SRM INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

AFMD 2024

International Conference on
Advanced Functional Materials and Devices (AFMD-2024)

February 26-29, 2024

PROCEEDINGS

Co-sponsored by

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Organized by

NRC Nanotechnology Research Centre SRMIST

Editors
Dr. M. Navaneethan
Dr. E. Senthil Kumar

International Conference on

Advanced Functional Materials and Devices (AFMD-2024)

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Organized by

Nanotechnology Research Center
SRM Institute of Science and Technology
Kattankulathur, Chennai, Tamilnadu, India.

Edited By

Dr. M. Navaneethan
Dr. E. Senthilkumar

Co-Sponsored by

In Association with

Shizuoka University Japan

University of Paris France

Alexandru Ioan Cuza University Iasi (UAIC), Romania

University of Montpellier, France

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The Ceramic Society of Japan

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SPD Laboratory Inc., Japan

IPGI Instruments, India

JEOL, India

Biologic, India

Dr. P. Sathyanarayanan
Pro Chancellor (Academics)

22 Feb 2024

MESSAGE

I am very happy to note that the International Conference on Advanced Functional Materials and Devices (AFMD-2024), is being organized by the Nanotechnology Research Centre at SRM Institute of Science and Technology, in collaboration with many national and international institutions, on 26th - 29th February 2024. The convergence of over 1000 participants and nearly 160 esteemed delegates at AFMD 2024 is truly a great international event.

The AFMD conference reinforces our commitment to foster an environment for exchanging ideas and technological advancements. The conference comprises the researchers around the world from Asian countries (Japan, Taiwan, Malaysia...), European countries (France, Poland…), the Middle east (Turkey), and so on. I am sure the conference will address current scientific issues on advanced materials technology and will also feature a highly interactive atmosphere among interdisciplinary materials science researchers.

I am confident that this conference is an excellent opportunity for young researchers to exchange their ideas and will pave the way for establishing great scientific connections for their collaborative research.

I extend my warmest greetings and congratulations to the organizing committee and all participants, and I offer my best wishes for the success of the AFMD-2024 conference.

Pro Chancellor (Academics)

Prof. C. Muthamizhchelvan, Ph.D
Vice Chancellor

SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

MESSAGE

I am extremely happy to know that the first edition of the International Conference on Advanced Functional Materials and Devices (AFMD-2024) is organized by the Nanotechnology Research Centre, SRM Institute of Science and Technology in association with some of the leading National and International Research Institutes and Laboratories from February 26-29, 2024 at SRM Institute of Science and Technology, Kattankulathur campus.

Material science and nanotechnology offer boundless potential to transform industries and improve daily life. The possibilities are endless, from advanced electronics to medical breakthroughs and sustainable energy solutions. By exploring the capabilities of material science and nanotechnology, we can tackle urgent global challenges and propel innovation toward a more promising future. I am sure this conference will serve as a pivotal forum for deliberating on interdisciplinary cooperation and facilitating the interchange of ideas and skills essential for pushing the frontiers of material science and nanotechnology globally. AFMD -2024 draws in speakers and participants from a diverse spectrum of countries, including India, Japan, Australia, Malaysia, the United Kingdom, and many other countries. This eventually promises a vibrant exchange of knowledge, fosters new collaborations, and engages in state-of-the-art research endeavors.

I wish AFMD-2024 a grand success.

20/2/24

Prof. C. Muthamizhchelvan
VICE CHANCELLOR
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603203
Chengalpattu Dist. Tamilnadu, India.

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Dr. S. Ponnusamy, Ph.D.
Registrar

Greetings from SRM Institute of Science and Technology!!!

I am elated that the International Conference on Advanced Materials and Devices (AFMD 2024) during February 26-29, 2024 is being organized by the Nanotechnology Research Center, SRM Institute of Science and Technology in association with Shizuoka University, Japan; NAIST, Japan; University of Paris Cité, France; University of Gustave Eiffel, France; University of Montpellier, France; Riga Technical University, Latvia; Polish Academy of Sciences, Poland; The Ceramic Society of Japan, SPD Laboratory. inc, Japan; Fuji Electronic Industrial Co., Ltd, Japan; Japan Society of Applied Physics, National Cheng Kung University, Taiwan; Universiti Tun Hussein Onn Malaysia, Malaysia; Daegu Gyeongbuk Institute of Science & Technology, South Korea; University of Malaya, Malaysia, University of Indonesia, Indonesia; JEOL India, Biologic India, IPGI Instruments, and also by various private industries.

The Nanotechnology Research Center enthralled us with the effort to gather research scientists and professionals across the globe into one platform.

The AFMD'24 conference explores 14 captivating symposia, each a springboard for groundbreaking discoveries. From the intricate nanostructures to the power-packed potential of energy materials, delve into diverse themes tailored to ignite your scientific spirit. This conference is believed to facilitate spirited discussion among participants, researchers and subject experts from India and the rest of the world on the latest trend in Functional Materials, their modern applications, and their usefulness to society.

I wish the AFMD-2024 conference a grand success.

Registrar

Registrar
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603 203
Chengalpattu Dist, Tamilnadu,India.

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Email: registrar@srmist.edu.in, Website: www.srmist.edu.in

Prof. T. V. Gopal
Dean
College of Engineering and Technology
SRMIST

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MESSAGE

I am happy that the Nanotechnology Research Centre, SRM Institute of Science and Technology, in association with global partners, is organizing an International Conference on Advanced Functional Materials and Devices (AFMD-2024) during February 26-29, 2024. Learning about the impressive 1000+ attendees and 160 speakers across 33 countries at the AFMD-2024 conference fills me with excitement and anticipation.

This conference will cover various interdisciplinary and current research topics related to functional materials in the various fields such as Optoelectronic devices, Sensors and Wearable Devices, Energy Conversion and devices, Functional Nanomaterials, Biomaterials, Nano catalytic, Sustainable energy materials, Environmental Nanotechnology, Magnetic materials, and Computational Informatics.

As we all know that the functional materials play a pivotal role in technological advancement and daily life improvement. I am sure that this Conference will provide valuable opportunities for budding researchers in expanding their knowledge and network with professionals from diverse backgrounds.

I wish the AFMD-2024 conference a great success.

Prof. T. V. Gopal

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R E C T O R'S O F F I C E

Iaşi, February, 2024

To: Organizers of the International Conference on Advanced Functional Materials and Devices
Nanotechnology Research Centre, SRM Institute of Science and Technology (SRMIST)
https://afmdsrmist2024.in/
Kattankulathur- 603203, Chennai, Tamil Nadu, India

On behalf of the academic community of *Alexandru Ioan Cuza* University of Iași, Romania, allow me to extend to you my most cordial greetings and sincere congratulations for the organisation of the first edition of the International Conference on Advanced Functional Materials and Devices, AFDM 2024. It is our hope that the AFMD 2024 event will become a regular opportunity to bring together researchers and students with common interests in each of the multiple symposia proposed by the organisers.

We are genuinely happy to be part of this community, together with universities and organizations from many countries: Shizuoka University, Japan, Université Paris Cité, France, Nara Institute of Science and Technology, Japan, University of Gustave Eiffel, France, Daegu Gyeongbuk Institute of Science & Technology, South Korea, University of Malaya, Malaysia, Tun Hussein Onn University of Malaysia, National Cheng Kung University, Taiwan.

I avail myself of this opportunity to convey my best wishes on behalf of *Alexandru Ioan Cuza* University – as a partner institution of AFMD, to both the organizers and participants in this conference. It is our hope that our university's participation and contribution to the conference can develop and strengthen the research connections with the host SRM Institute of Science and Technology and the other many partner institutions supporting this event.

In light of all the above, I wish you every success in your future endeavours, and I extend warm thanks to the entire team who contributed to the organization of the forthcoming event.

Yours sincerely,

Rector,
Prof.dr. Tudorel TOADER

Shizuoka University

Message for the 1st International Conference on Advanced Functional Materials and Devices (AFMD-2024)

I am delighted to deliver a welcome speech for the 1st International Conference on Advanced Functional Materials and Devices (AFMD-2024) which is organized at the SRM Institute of Science and Technology (SRMIST), India. It is an honor for Shizuoka University to join the hands with SRMIST in the academic and research activities.

Shizuoka University has currently seven Faculties such as Humanities and Social Science, Education, Informatics, Science, Engineering, Agriculture, Global Interdisciplinary Science and Innovation, and School of Regional Development. There are five Graduate Schools for master and doctoral course. In addition to that, we have Research Institute of Electronics and Research Institute of Green Science and Technology to promote the research activity. Shizuoka University's staff and students uphold the philosophy of "freedom and enlightenment" as a mainstay of education, research and collaboration with society, industry and overseas.

Collaboration between Shizuoka University and SRMIST started in 2009 before the Memorandum of Understanding was signed in 2014. Since then, the colleagues in both Universities have been fostering the relationship steadily, which have led to the promotion of Double Degree Program (DDP) in the doctoral course and exchange program of students. This collaboration is now one of the most active frameworks among the collaborations between the other foreign Universities and Shizuoka University. Shizuoka University has organized Inter Academia Asia Conference since 2014. In 2016, the 3rd conference was held in India and the community of Asian higher education Institutions from Japan, India, Bangladesh, Sri Lanka, Hong Kong, Malaysia, Thailand, Vietnam, Indonesia gathered together and discussed the global education and research at SRMIST.

Shizuoka University is grateful to SRMIST for their tremendous support as host of many joint conferences including AFMD and ICONN which is another conference hosted jointly by Shizuoka University and SRMIST. I hope that all the speakers and researchers will enjoy the scientific discussions and strengthen the collaboration.

Finally, I would like to express my sincere thanks to all members of conference committee, and participants.

Kazuyuki Hizume

Prof. Kazuyuki Hizume

President of Shizuoka University

RIGA TECHNICAL
UNIVERSITY

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Rīgā

15.02.2024. No. 04000-2.2.1-e/5

International Conference on Advanced Functional Materials and Devices-2024 (AFMD-2024)

Address on the occasion of the opening of the conference "International Conference on Advanced Functional Materials and Devices-2024 (AFMD-2024)" in Nanotechnology Research Centre of SRM Institute of Science and Technology, Chennai, India

Dear Colleagues,

It is with great pleasure and excitement that I address you on behalf of Riga Technical University (RTU). As we gather here to exchange ideas, share insights, and foster collaborations in the field of advanced materials and devices, RTU is honoured to be a part of this esteemed gathering.

AFMD-2024 serves as a platform for collaboration and partnership building, and RTU is eager to engage with fellow researchers, industry leaders, and policymakers to explore new avenues for cooperation. By fostering international collaborations and knowledge exchange, we can accelerate the pace of innovation and address global challenges more effectively.

As we navigate the complexities of the 21st century, the role of advanced functional materials and devices in driving progress and shaping our future cannot be overstated. Whether it is developing next-generation materials for renewable energy systems, designing smart sensors for healthcare monitoring, or creating innovative solutions for environmental remediation, the potential impact of our collective efforts is immense.

We are committed to leveraging our expertise and resources to contribute meaningfully to the discussions and initiatives emerging from this conference. Together, let us harness the power of advanced functional materials and devices to create a more sustainable and equitable world for future generations.

Sincerely,

Prof. Dr. ing.sc.
Acting Vice-Rector for Research

G. Bažbauers

Sedova, anna.sedova@rtu.lv

It is a great honor for me to participate this Year to the International Conference on Advanced Functional Materials and Devices 2024 organized by the Nanotechnology Research Center, SRM Institute of Science and Technology of Chennai. I am extremely grateful to the organizers for their very kind invitation to contribute to this extremely rich scientific program that encompasses a wide spectrum of material-related applications in chemistry, biology and electronics among others to tackle the most topical challenges society faces today in terms of energy, environment and health. The diverse symposia assembled talks from worldwide experts in these respective field completed by poster sessions that are expected to stimulate fruitful exchanges with early-stage researchers as well as students. I envision this conference as an ideal platform for the young generation to communicate their achievements in a pleasant environment and actively participate to the general discussions with advanced researchers. This is also an optimum platform to discover opportunities for future doctorate or postdoctoral positions in world leading laboratories. The recent agreement between SRM and University Montpellier my research group is affiliated with, offers a great chance to build a bridge for students motivated to spend visiting periods in France. I wish all you an excellent conference in the very beautiful and pleasant city of Chennai.

Guillaume Maurin, Professor Université Montpellier/Institut Universitaire de France
ICGM UMR 5253 CNRS UM ENSCM
Bâtiment Pôle Chimie Balard, Campus CNRS, 1919 route de Mende, 34293 Montpellier, France
☎ +3348792105 – 🖂 guillaume.maurin1@umontpellier.fr

UNIVERSITI MALAYA

Greeting Message

We are honored to extend its steadfast support to the International Conference on Advanced Functional Materials and Devices-2024 (AFMD-2024) as a prestigious gathering of global scholars and researchers. Through our unwavering commitment to academic excellence, we uphold the values of collaboration, discovery, and the advancement of knowledge. We invite all participants to join us in forging new frontiers in the dynamic field of advanced materials and devices. Together, let us illuminate the path towards a future enriched by groundbreaking research and scholarly exchange.

Your sincerely

.....

Prof. Ir. Dr. Sulaiman Wadi Harun
Head of Department of Electrical Engineering
Faculty of Engineering
Universiti Malaya

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Greetings from the Dean Faculty of Engineering, Universitas Indonesia

First and foremost, I would like to express my greetings to our esteemed colleagues, distinguished guests and participants. It is an honor opportunity for us to participate in the International Conference on Advanced Functional Materials and Devices (AFMD-2024) from 26-29 February 2024 is being organized by the Nanotechnology Research Center, SRM Institute of Science and Technology.

We are sure that this event will be a good opportunity for researchers from all over the world to share ideas and exchange advanced knowledge in the crucial role of material and its advancement, covered in fifteen symposia, such as quantum materials, functional nanomaterials, and more including their development techniques and applications. This field has been becoming a central concern to reach cutting-edge research and development in future technologies that are beneficial to humankind and the environment.

The Faculty of Engineering Universitas Indonesia has seriously committed and focused on preserving the environment and creating a green, sustainable, and comfortable campus for our students and academics. We also give special attention to the amount of renewable energy production on campus by installing solar panels in several locations, using fuel cells as hydrogen fuel (clean biomass) and creating waste management programs.

Our profound appreciation goes to all those who have contributed to making AFMD 2024 a reality to share, discuss, and establish networks in the field of Advanced Functional Materials and Devices. I hope everyone enjoys and takes from their experiences on the field, discussions, and talks from speakers and experts. May more cooperation be built and continued during this conference into more joint research and various collaborations.

Dean Faculty of Engineering Universitas Indonesia

Prof. Dr. Ir. Heri Hermansyah, S.T., M.Eng., IPU.

Organizers

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INTERNATIONAL CONFERENCE ON
ADVANCED FUNCTIONAL MATERIAL AND DEVICES (AFMD - 2024)
February 26-29, 2024

AFMD-2024 PROGRAM SCHEDULE (Day - 1)

26.02.2024 (MONDAY)

Time (IST)								
07.30-09.45	**Registration @ Dr. T. P. Ganesan Auditorium (TPGA)**							
10.00 - 11.10	**Inaugural Program @ Dr. T. P. Ganesan Auditorium (TPGA) - Main Hall**							
11.10 - 11.30	**High Tea**							
ROOM	**TPGA Mini Hall -1**	**TPGA Mini Hall - 2**	**SBE 101**	**SBE 102**	**SBE 103**	**SBE 104**	**SBE 201**	**SBE 202**
	Symposium A	**Symposium B**	**Symposia C & M**	**Symposium D**	**Symposia E,J & I**	**Symposium F**	**Symposium G**	**Symposia H & K**
	Paraell Session 1							
11.35 - 12.10	**Chair:** *Prof. Mohamed Chehimi, CNRS, France* **Co-chair:** *Dr. Trilochan Sahoo, Physics, SRMIST, KTR*	**Chair:** *Prof. Mei-Jywan Syu, National Cheng Kung University, Taiwan* **Co-chair:** *Dr. Anbumozhi Angayarkanni, Physics, SRMIST, KTR*	**Chair:** *Dr. Daniel Moraru, Shizuoka University, Japan* **Co-chair:** *Dr. P. Malar, Physics, SRMIST, KTR*	**Chair:** *Prof. Nji Raden Poespawati, Universitas Indonesia, Indonesia* **Co-chair:** *Dr. Payel Bandyopadhyay, Physics, SRMIST, KTR*	**Chair:** *Prof. Yueh-Heng Li, National Cheng Kung Uni, Taiwan* **Co-chair:** *Dr. C. Preferencial Kala, Physics, SRMIST, KTR*	**Chair:** *Prof. Ryo Teranishi, Kyushu University, Japan* **Co-chair:** *Dr. Debabrata Sarkar, Physics, SRMIST, KTR*	**Chair:** *Prof. Chien-Hsiang Chang, National Cheng Kung University, Taiwan* **Co-chair:** *Dr. Tusharabhai H Rana, Physics, SRMIST, KTR*	**Chair:** *Dr. Katarzyna Krukiewicz, Silesian University of Technology, Poland* **Co-chair:** *Dr. M. Kovendhan, Physics, SRMIST, KTR*
	KN 01: **Prof. Naoki Wakiya** Shizuoka University, Japan ***Title:*** *Computer simulation of spontaneous superlattice formation in S-Ti-O thin film by dynamic aurora PLD*	**KN 02:** **Dr. T.N. Narayanan** Tata Institute of Fundamental Research, Hyderabad ***Title:*** *Engineering electrode-electrolyte interfaces in heterogeneous catalysis*	**KN 03:** **Prof. Ajay Agarwal** Indian Institute of Technology Jodhpur ***Title:*** *Do Nano-sensors need AI?*	**KN 04:** **Prof. Mohd Khairul Bin Ahmad** Universiti Tun Hussein Onn Malaysia, Malaysia ***Title:*** *Unlocking the potential of rutile TiO2: innovations and applications*	**KN 05:** **Prof. Ramesh Chandra Mallik** Indian Institute of Science, Bangalore ***Title:*** *Tetrahedrite and Skutterudite: Two important crystal structures in thermoelectric research*	**KN 06:** **Prof. T. Serkan Kasirga** Bilkent University, Turkey **Title:** Substrate effects and ionic phase transitions at two-dimensions	**KN 07:** **Prof. Muhammet S. Toprak** KTH Royal Institute of Technology, Stockholm, Sweden ***Title:*** *Development of inorganic nanoparticles for biomedical imaging*	**KN 08:** **Prof. C. Clark Kendrick** Ateneo de Manila University, Philippines **Title:** Topological data analysis:Fundamentals and use-cases
12.10 - 12.40	**IT 01:** **Dr. Pavels Onufrijevs** Riga Technical University, Latvia *Title: Laser-assisted tailoring of semiconductors properties for advanced microelectronics: unleashing the possibilities for GeSn epitaxial layers*	**IT 02:** **Dr. Soorathep Kheawhom** Chulalongkorn University, Thailand *Title: Innovative integration of MOF-derived NiFeO nanocrystals and Ti_3C_2Tx MXene nanosheets in oxygen electrocatalysis for rechargeable zinc-air*	**IT 03:** **Dr. Aman Mahajan** Guru Nanak Dev University, Amritsar ***Title:*** *Self-powered monitoring of biomarkers and environment pollutants by integrating MXene based sensors with nanogenerators*	**IT 04:** **Dr. Ursic Hana** Jožef Stefan Institute, Slovenia ***Title:*** *Aerosol deposition of functional thick films on metal and polymer substrates*	**IT 05**: **Dr. Maizatul Azrina Yaakob** Universiti Tun Hussein Onn Malaysia, Malaysia ***Title:*** *Dual role of microalgae in wastewater treatment for bioproduct (fish feeds alternative)*	**IT 06:** **Prof. Chao-Wei Huang** National Cheng Kung University, Taiwan *Title: Metal-organic frameworks composites for dye degradation via adsorption, heterogeneous photo-fenton and photocatalysis*	**IT 07:** **Dr. Ionut Topala** Alexandru Ioan Cuza University of Iasi, Romania ***Title:*** *Atmospheric pressure plasma deposition of interstellar dust analogues based on amorphous hydrogenated carbon and evolution after proton irradiation*	**IT 08:** **Dr. Chi-cheng Chiu** National Cheng Kung University, Taiwan ***Title:*** *Molecular design of ion pair amphiphiles for biomimetic catanionic bilayers with designated phase and morphological properties*
12.40 - 14.00	**Lunch Break**							
	Parallel Session 2							
14.00 - 14.35	**Chair:** *Dr. Paul Joseph Daniel, National Institute of Technology, Warangal* **Co-chair:** *Dr. Ajay Rakesh, Physics, SRMIST, KTR*	**Chair:** *Prof. Bhagwati Prasad, IISc, Bangalore* **Co-chair:** *Dr. Rohit dir, Physics, SRMIST, KTR*	**Chair:** *Prof. Suman De Sarkar, IISER, Kolkata* **Co-chair:** *Dr. Chandra Mohan, Physics, SRMIST, KTR*	**Chair:** *Dr. Rabindra Nath Mahato, Jawaharlal Nehru University, New Delhi* **Co-chair:** *Dr. M. Bhaskar Chandra Behara, Physics, SRMIST, KTR*	**Chair:** *Dr. Vanchiappan Aravindan, IISER, Tirupati* **Co-chair:** *Dr. P. Malar, Physics, SRMIST, KTR*	**Chair:** *Dr. Sujit Das, Indian Institute of Science, Bangalore* **Co-chair:** *Dr. Meenal S. Deo, Physics, SRMIST, KTR*	**Chair:** *Dr. Taketomo Sato, Hokkaido University, Sapporo, Japan* **Co-chair:** *Dr. C. Preferencial Kala, Physics, SRMIST, KTR*	**Chair:** *Dr. Ravichandar Babarao, RMIT University, Australia* **Co-chair:** *Dr. K. Shadak Alee, Physics, SRMIST, KTR*
	KN 09: **Prof. Kazuhiko Hara** Shizuoka University, Japan ***Title:*** *Issues on substrates for the thin film growth of hexagonal boron nitride by low-pressure chemical vapor deposition*	**KN 10:** **Prof. Suman De Sarkar** IISER, Kolkata ***Title:*** *Regulating chemoselectivity of organic transformations through electrolysis*	**KN 11:** **Dr. Pratima Agarwal** Indian Institute of Technology Guwahati, Guwahati ***Title:*** *Dopant free c-Si heterojunction solar cells: Prospective and challenges*	**KN 12:** **Dr. Suvankar Chakraverty** Institute of Nano Science and Technology, Mohali ***Title:*** *Anomalous Shubnikov-De Haas oscillations and room temperature spin polarizations at oxide interfaces*	**KN 13:** **Prof. Tomoaki Watanabe** Meiji University, Japan ***Title:*** *Recent advance in photocatalyst for new hydrogen energy source*	**KN 14:** **Prof. Hiroki Kondo** Kyushu University, Japan ***Title:*** *Novel plasma-assisted syntheses of functional carbon nanomaterials, their mechanism, and applications*	**KN 15:** **Dr. Mrinmoy De** Indian Institute of Science, Bangalore ***Title:*** *Functionalization of different phases of 2D-MoS2 and related applications*	**KN 16:** **Prof. Neha Gandhi** Manipal Institute of Technology, Manipal ***Title:*** *Nanoparticle translocation across the lung surfactant film: Unravelling its mechanism at the molecular scale*
14.35 - 15.05	**IT 09:** **Prof. P. Rajamalli** Indian Institute of Science, Bangalore ***Title:*** *Systematic investigation to enable the high-efficiency thermally activated delayed fluorescence emitter for OLEDs*	**IT 10:** **Dr. Mohammad Abul Hasnat** Shahjalal University of Science and Technology, Bangladesh ***Title:*** *Electro-oxidation of ethanol on IrOx-Pt and oxidation of hydrogen peroxide on GCE/Nafion/Ni electrode surface in alkaline medium*	**IT 11:** **Dr. Nurul Asyikeen Ab Mutalib** Universiti Malaya, Malaysia ***Title:*** *Redox cycling amplification in microgap-based bipolar electrodes using an ion-selective membrane*	**IT 12:** **Prof. Hiroshi Masumoto** Tohoku University, Japan ***Title:*** *Novel multi-functional properties by magnetic metal-ceramics nano-granular films*	**IT 13:** **Dr. V. Kameswara Rao** University of Delhi, New Delhi ***Title:*** *Nano gold in immunosensing applications*	**IT 14:** **Dr. Bruce (Jun-Yu) Ou** University of Southampton, UK ***Title:*** *Nanomechanical metamaterials*	**IT 15:** **Dr. Marlia Binti Morsin** Universiti Tun Hussein Onn Malaysia (UTHM), Malaysia ***Title:*** *Potential of gold nanobipyramids as an antifungal agent in biomedical and agricultural*	**IT 16:** **Dr. T.J. Dhilip Kumar** Indian Institute of Technology, Ropar ***Title:*** *Ab initio insights of 2D carbon lattices and doped analogues as alkali ion batteries materials*
15.05 - 15.35	**IT 17:** **Dr. Catur Apriono** Universitas Indonesia, Indonesia ***Title*** *: Design of LO phase shifter based on quadrature hybrid branchline coupler for IQ mixer in synthetic aperture radar applications*	**IT 18:** **Prof. A. J. Saleh Ahammed** Jagannath University, Bangladesh ***Title:*** *Fabrication of electrode materials for sustainable energy applications*	**IT 19:** **Prof. N. Gopalakrishnan** National Institute of Technology, Tiruchirappalli ***Title:*** *Sn and Cr doped β-[(Ga]_2 O_3 Inter Digitated Electrode (IDE) gas sensors*	**IT 20:** **Dr. J. Judith Vijaya** Loyola College, Chennai ***Title:*** *Multifunctional pristine magnetic copper ferrite (CuFe2O4) and CuFe2O4/rGO binary nanocomposites: Electrochemical performance and heavy metals adsorption*	**IT 21:** **Dr. Easwaramoorthi Ramasamy** ARCI, Hyderabad ***Title:*** *Materials and device concepts of large-area perovskite solar cells*	**IT 22:** **Dr. Noor Kamalia Binti Abd Hamed** Universiti Tun Hussein Onn Malaysia, Malaysia ***Title:*** *Synergistic coupling {101}-{111} facet of N-doped TiO2 film enhance spatial charge separation for methylene blue photodegradation*	**IT 23:** **Er. Puan Faezahana Binti Mohkhter** Universiti Tun Hussein Onn Malaysia, Malaysia ***Title:*** *The challenge in study of topography properties using Atomic Force Microscope (AFM)*	**IT 24:** **Mr. Katsuhiko Nobeta** Fuji Electronics, Japan ***Title:*** *SPS latest technology/application, production system and new model*
15.35 - 16.15	**Oral Presentation (OP 01 - OP 04)**	**Oral Presentation (OP 05 - OP 08)**	**Oral Presentation (OP 09 - OP 12)**	**Oral Presentation (OP 13 - OP 16)**	**Oral Presentation (OP 17 - OP 20)**	**Oral Presentation (OP 21 - OP 24)**	**Oral Presentation (OP 25 - OP 28)**	**Oral Presentation (29 - 32)**
16.15-16.30	**Tea Break**							
16.30 - 17.30	**Poster Presentation (Venue: Dr. T. P. Ganesan Auditorium) (PP 01 - PP 150)**							
17.30-18.30	**Cultural Program (Venue: Dr. T. P. Ganesan Auditorium)**							
18.30-20.30	**Dinner**							

Note : PL - Plenary Talk; KN - Keynote; IT: Invited Talk; TT-Technical Talk **TPGA - Dr. T. P. Ganesan Auditorium Mini Hall; SBE - School of Bio-Engineering Buliding**

INTERNATIONAL CONFERENCE ON
ADVANCED FUNCTIONAL MATERIAL AND DEVICES (AFMD - 2024)
February 26-29, 2024

AFMD-2024 PROGRAM SCHEDULE (Day-2)

27.02.2024 (TUESDAY)

Time (IST)								
ROOM	**TPGA Main Hall**		**TPGA Mini Hall - 1**		**TPGA Mini Hall - 2**		**SBE Prof. G. N. Ramachandran Hall**	
	Paraell Session 3							
09.00-09.40	**Chair:** *Prof. T. Serkan Kasirga, Bilkent University, Turkey* **Co - chair:** *Dr. S. Shanmugam, Chemistry, SRMIST , KTR*		**Chair:** *Dr. Pavels Onufrijevs, Riga Technical University, Latvia* **Co - chair:** *Dr. C. Preferencial Kala, Physics, SRMIST, KTR*		**Chair:** *Prof. Nobuyasu Adachi Nagoya Institute of Technology, Japan* **Co-chair:** *Dr. Rohit Dir, Physics, SRMIST, KTR*		**Chair:** *Prof. Guillaume Maurin University of Montpellier, France* **Co - chair:** *Dr. M. Alagiri, Physics, SRMIST, KTR*	
	PL 01: **Dr. Judy Lee** University of Surrey, UK ***Title:*** *The unique chemical and physical effect of ultrasound cavitation for material synthesis*		**PL 02: Prof. A. Ajayaghosh** SRM Institute of Technology, KTR Campus, Chennai ***Title:*** *Molecular self-assembly and superhydrophobic soatings for energy saving application*		**PL 03: Dr. Rohini Kitture** Deputy Editor, Wiley, Pune ***Title:*** *Effective research publishing: Insider tips and techniques*		**PL 04: Dr. Hyung Chul Ham** Inha University, Republic of Korea ***Title:*** *Computational design of single/double atom catalysts for efficient electrochemical NH_3 production*	
ROOM	**TPGA Mini Hall 1**	**TPGA Mini Hall 2**	**SBE 101**	**SBE 102**	**SBE 103**	**SBE 104**	**SBE 201**	**SBE 202**
	Symposium A	**Symposium B**	**Symposium C & M**	**Symposium D**	**Symposium E, J & I**	**Symposium F**	**Symposium G**	**Symposium H & K**
	Paraell Session 4							
09.45 - 10.20	**Chair:** *Prof. Sebastian Lourdudoss, KTH Royal Institute of Technology, Sweden* **Co-chair:** *Dr. T. Vijayakumar, Physics, SRMIST, KTR*	**Chair:** *Prof. Tomoya Ohno, Kitami Institute of Technology, Japan* **Co - chair:** *Dr. T. Kalaivani, Physics, SRMIST, KTR*	**Chair:** *Prof. N. Gopalakrishnan, National Institute of Technology, Tiruchirappalli* **Co - chair:** *Dr. R. M. Hariharan, Physics, SRMIST, KTR*	**Chair:** *Dr. Ursic Hana, Jožef Stefan Institute, Slovenia* **Co - chair:** *Dr. Angeline Little Flower, Physics, SRMIST, KTR*	**Chair:** *Prof. Tomoaki Watanabe, Meiji University, Japan* **Co - chair:** *Dr. K. Mani Rahulan, Physics, SRMIST, KTR*	**Chair:** *Prof. Ramesh Chandra Mallik, Indian Institute of Science, Bengaluru* **Co - chair:** *Dr. P. Malar, Physics, SRMIST, KTR*	**Chair:** *Dr. Mrinmoy De, Indian Institute of Science, Bangalore* **Co - chair:** *Dr. Sandeep Lakhera, Physics, SRMIST, KTR*	**Chair:** *Prof. Neha Gandhi, Manipal Institute of Technology, Manipal* **Co - chair:** *Dr. V. Ramesh, Physics, SRMIST, KTR*
	KN 17: Prof. Tomoaki Yamada Nagoya University, Japan ***Title:*** *Electro-optic effect of ferroelectric thin films: strain engineering and exploration of emerging materials*	**KN 18: Dr. M. Sathish** Central Electrochemical Research Institute, Karaikudi ***Title:*** *Fabrication of high energy supercapacitors using porous activated carbon: a journey from lab scale to prototype device*	**KN 19: Prof. Mohamed Chehimi** CNRS, France ***Title:*** *Agrowaste conversion to reactive and functional biochar for biomedical, environmental and energy applications*	**KN 20: Dr. N. Kamaraju** IISER, Kolkata ***Title:*** *Antiferromagnetic topological insulator, MnBi2Te4 investigated using time domain THz spectroscopy and Pump-Probe Spectroscopy*	**KN 21: Dr. C. N. Tharamani** Indian Institute of Technology, Ropar ***Title:*** *Designing a greener energy conversion system for a sustainable future*	**KN 22: Prof. Ryo Teranishi** Kyushu University, Japan ***Title:*** *Miniaturization of BaHfO3 flux pinning centers in YBa2Cu3Oy superconducting thin film using solution-based metal organic deposition process*	**KN 23: Prof. Chien-Hsiang Chang** National Cheng Kung University, Taiwan ***Title:*** *Fabrication of microalgae oil drug delivery carriers*	**KN 24: Dr. Ravichandar Babarao** RMIT University, Australia ***Title:*** *Accelerating the Discovery of Novel Materials for a Sustainable Society: Integrating High Throughput Screening and Machine Learning*
10.20 - 10.50	**IT 25: Prof. Paul Joseph** National Institute of Technology, Warangal ***Title:*** *Nano-dimensional films for novel devices – elucidating the role of hierarchy, architecture and doping strategies*	**IT 26: Prof. Prasit Pattananuwat** Chulalongkorn University, Thailand ***Title:*** *Development of bismuth-based materials for light-driven-assisted -charging supercapacitor*	**IT 27: Prof. Dr. Govind Gupta** National Physical Laboratory, New Delhi ***Title:*** *Fabrication of gas sensors utilizing semiconductor heterostructures*	**IT 28: Prof. Bhagwati Prasad** Indian Institute of Science, Bangalore ***Title:*** *Electric field control of magnetism: energy-efficient spintronics for AI and IOT applications*	**IT 29: Dr. Mohd Faiz Bin Mohd Salleh** Universiti Malaya, Malaysia ***Title:*** *Thermoelectric energy harvester for floating system application*	**IT 30: Dr. T. S. Shyju** Sathyabama Institute of Science and Technology, Chennai ***Title:*** *Earth abundant nitride thin films for energy applications*	**IT 31: Dr. Sujit Das** Indian Institute of Science, Bangalore ***Title:*** *Manipulation of polar topology*	**IT 32: Prof. Sangaraju Shanmugam** DGIST, South Korea ***Title:*** *Electrocatalysts for sustainable carbon-free E-fuels*
10.50 - 11.05	**Tea Break**							
	Paraell Session 5							
11.05 - 11.35	**Chair:** *Prof. Sudakar Chandran, Indian Institute of Technology, Madras* **Co - chair:** *Dr. Elangovan Elamurugu, Physics, SRMIST, KTR*	**Chair:** *Prof. A. J. Saleh Ahammed, Jagannath University, Bangladesh* **Co - chair:** *Dr. Balaji, Mechanical, SRMIST, KTR*	**Chair:** *Dr. Hiroki Kase, Shizuoka University, Japan* **Co - chair:** *Dr. B. Hariharan, Cintel, SRMIST, KTR*	**Chair:** *Prof. Hiroshi Masumoto, Tohoku University, Japan* **Co - chair:** *Dr. G.T. Senthil Andavan, Chemistry, SRMIST, KTR*	**Chair:** *Prof. Kenji Murakami, Shizuoka University, Japan* **Co - chair:** *Dr. Mathimalar, Physics, SRMIST, KTR*	**Chair:** *Dr. P. Malar, SRMIST, Chennai* **Co - chair:** *Dr. P.C. Karthika, Physics, SRMIST, KTR*	**Chair:** *Dr. Yuta Kubota Tokyo Institute of Technology, Japan* **Co - chair:** *Dr. A. Tamilselvan, Physics, SRMIST, KTR*	**Chair:** *Dr. Chi-cheng Chiu, National Cheng Kung University, Taiwan* **Co - chair:** *Dr.Subhojyoti Sinha, Physics, SRMIST, KTR*
	IT 33: Prof. Hiroaki Satoh Shizuoka University, Japan ***Title:*** *Silicon-on-insulator photodiode with SP antenna and its applications to advanced light detection*	**IT 34: Dr. Suttipong Wannapaiboon** Synchrotron Light Research Institute, Thailand ***Title:*** *Synchrotron-based characterizations of electrocatalytic metal-organic frameworks and covalent organic framework-based solid electrolyte interphase for stabilizing anode of rechargeable batteries*	**IT 35: Dr. Suhana Binti Mohamed Sultan** Universiti Teknologi Malaysia, Malaysia ***Title:*** *Hydrothermal optimization of one-dimensional zinc oxide nanostructure arrays for resistive based biosensors*	**IT 36: Dr. Rabindra Nath Mahato** Jawaharlal Nehru University, New Delhi ***Title:*** *Structural, magneto-caloric and unusual magnetic behavior in the nanocrystalline manganites*	**IT 37: Dr. Vasundhara Mutta (Virtual)** CSIR-Indian Institute of Chemical Technology, Hyderabad ***Title:*** *Synthesis mechanisms of chalcogenide nanostructures via aqueous based reflux method for enhanced room temperature thermoelectric performance*	**IT 38: Prof. Atsushi Nakamura** Shizuoka University, Japan ***Title:*** *Visible light-driven Z-scheme photocatalyst of SnS2/g-C3N4 for dye decomposition*	**IT 39: Dr. Ranita Basu** Bhabha Atomic Research Centre, Mumbai ***Title:*** *Development of high performance thermoelectric material in mid-and high temperature regime for viable power generators*	**IT 40: Dr. Sakura N. Takeda** NARA Institute of Science and Technology, Japan ***Title:*** *Search of band bending potential curve consistent with the observed electronic states*
11.35 - 12.05	**Oral Presentation (OP 33 - OP 35)**	**Oral Presentation (OP 36 - OP 38)**	**Oral Presentation (OP 39 - OP 41)**	**Oral Presentation (OP 42 - OP 44)**	**Oral Presentation (OP 45 - OP 47)**	**Oral Presentation (OP 48 - OP 50)**	**Oral Presentation (OP 51 - OP 53)**	**Oral Presentation (OP 54 - OP 56)**
12.05 - 13.00	**Poster Presentation (PP 151 - PP 300)**							
13.00-14.00	**Lunch Break**							
	Paraell Session 6							
14.00 - 14.35	**Chair:** *Dr. Arief Udhiarto, Universitas Indonesia, Indonesia* **Co - chair:** *Dr. P. Malar, Physics, SRMIST, KTR*	**Chair:** Dr. Maizatul Azrina Yaakob, UTHM, Malaysia **Co - chair:** *Dr. S. Chandramohan, Physics, SRMIST, KTR*	**Chair:** *Dr. Riyaz Ahmad Mohamed Ali, UTHM, Malaysia* **Co - chair:** *Dr. C. Prefrencial Kala, Physics, SRMIST, KTR*	**Chair:** *Dr. K. Mohan Kant, VNIT, Nagpur* **Co - chair:** *Dr. R. Annie Sujatha, Physics, SRMIST, KTR*	**Chair:** *Prof. S. Anandan, NIT, Tiruchirappalli* **Co - chair:** *Dr. K. Shanthi, Physics, SRMIST, KTR*	**Chair** Dr. *Mohd Faiz Bin Mohd Salleh Universiti Malaya, Malaysia* **Co - chair:** *Dr. Tusharbhai H Rana, Physics, SRMIST, KTR*	**Chair:** *Dr. Elangovan Elamurugu, SRMIST, KTR* **Co - chair:** *Dr. R. Ajay Rakkesh, Physics, SRMIST, KTR*	**Chair:** *Dr. Jaivardhan Sinha, SRMIST, KTR* **Co - chair:** *Dr. G. Bakiyaraj, Physics, SRMIST, KTR*
	KN 25: Prof. Shikha Varma (Virtual) Institute of Physics, Bhubaneswar ***Title:*** *Designing Graphene Quantum dots and their Photo-response*	**KN 26: Prof. Senthilarasu Sundaram** Teesside University, United Kingdom ***Title:*** *Nanocellulose from waste for energy applications*	**KN 27: Dr. Najla Fourati** SATIE Laboratory, UMR CNRS, France ***Title:*** *Electrochemical sensors for sustainable agriculture: trends and challenges*	**KN 28: Dr. Shintaro Yasui** Tokyo Institute of Technology, Japan ***Title:*** *κ-Al2O3-type ferroelectrics*	**KN 29: Prof. Venkata Krishnan (Virtual)** Indian Institute of Technology Mandi ***Title:*** *Green chemistry and heterogeneous catalysis for energy and environmental applications*	**KN 30: Dr. Virgil Andrei (Virtual)** University of Cambridge, United Kingdom ***Title:*** *Integrated light harvesting systems for scalable artificial photosynthesis*	**KN 31: Prof. Muthupandian Ashokkumar (Virtual)** University of Melbourne, Australia *Title: Ultrasonic synthesis of functional materials*	**KN 32: Prof. Majdi Hochlaf (Virtual)** Université Gustave Eiffel, France ***Title:*** *First principles methodologies for Probing interfacial interactions and applications*
14.35 - 16.15	**Oral Presentation (OP 57- OP 66)**	**Oral Presentation (OP 67- OP 76)**	**Oral Presentation (OP 77- OP 86)**	**Oral Presentation (OP 87- OP 96)**	**Oral Presentation (OP 97- OP 106)**	**Oral Presentation (OP 107 - OP 116)**	**Oral Presentation (OP 117 - OP 126)**	**Oral Presentation (OP 127 - OP 136)**
16.15-16.30	**Coffee Break**							
16.30 - 17.30	**Poster Presentation (PP 301 - PP 450)**							
17.30-18.30	**Cultural Program**							
18.30-20.30	**Dinner**							

Note : PL - Plenary Talk; KN - Keynote; IT: Invited Talk; TT-Technical Talk **TPGA - Dr. T. P. Ganesan Auditorium Mini Hall; SBE - School of Bio-Engineering Buliding**

INTERNATIONAL CONFERENCE ON ADVANCED FUNCTIONAL MATERIAL AND DEVICES (AFMD - 2024)

February 26-29, 2024

AFMD-2024 PROGRAM SCHEDULE (Day - 3)

28.02.2024 (WEDNESDAY)

Time (IST)								
ROOM	**TPGA Main Hall**		**TPGA Mini Hall - 1**		**TPGA Mini Hall - 2**		**SBE Prof. G. N. Ramachandran Hall**	
	Paraell Session 7							
09.00-09.40	**Chair:** *Prof. Mohamed Chehimi, CNRS, France* **Co-chair:** *Dr.Jaivardhan Sinha, Physics, SRMIST, KTR*		**Chair:** *Prof. Naoki Wakiya, Shizuoka University, Japan,* **Co-chair:** *Dr. G. Maduraiveeran,Chemistry,SRMIST, KTR*		**Chair:** *Dr. Takafumi Ishibe* *Osaka University, Japan,* ***Co-chair:*** *Dr. Elangovan Elamurugu, Physics, SRMIST, KTR*		**Chair:** *Prof. C. Clark Kendrick,* *Ateneo de Manila University, Philippines* **Co-chair:** *Dr.V. Kumaran, Chemistry, SRMIST, KTR*	
	PL 05: Dr. D. K. Aswal Bhabha Atomic Research Centre, Mumbai ***Title:*** *Utilization of uranium mill tailings for construction materials: A pathway for sustainable uranium mining and milling*		**PL 06: Prof. Benoit Piro** CNRS, France, ***Title:*** *Printed electronics in sensors and medical devices*		**PL 07: Prof. Dr.-Ing. Olfa Kanoun** Technische Universität Chemnitz, Germany ***Title:*** *Potential of electrode surface modification by nanomaterials for sensors with high performance*		**PL 08: Prof. Guillaume Maurin** University of Montpellier, France ***Title:*** *Computational-aided development of MOF-based membranes for molecular separation*	
ROOM	**TPGA Mini Hall - 1**	**TPGA Mini Hall - 2**	**SBE 101**	**SBE 102**	**SBE 103**	**SBE 104**	**SBE 201**	**SBE 202**
	Symposium A	**Symposium B**	**Symposium C & M**	**Symposium D**	**Symposium E, J & I**	**Symposium F**	**Symposium G**	**Symposium H & K**
	Paraell Session 8							
09.45 - 10.20	**Chair:** *Dr. Catur Apriono, Universitas Indonesia, Indonesia* **Co-chair:** *Dr. C. Prefrencial Kala, Physics, SRMIST, KTR*	**Chair:** *Prof. Kunio Hayakawa, Shizuoka University, Japan* **Co-chair:** *Dr. R. Maheswaran, Physics,SRMIST, KTR*	**Chair:** *Dr. Najla Fourati, SATIE Laboratory, UMR CNRS, France* ***Co-chair:*** *Dr. G. T. Senthil Andavan, Physics,SRMIST, KTR*	**Chair:** *Prof. P.N. Santhosh, IIT Madras, Chennai* **Co-chair:** *Dr. T. Maiyalagan, Chemistry,SRMIST, KTR*	**Chair:** *Dr. Hiromu Hamasaki Osaka University, Japan* **Co-chair:** *Dr. AVM Manikandan, ECE, SRMIST, KTR*	**Chair:** *Dr. Bruce (Jun-Yu) Ou, University of Southampton, UK* **Co-chair:** *Dr.Piyush Sharma, Mechanical,SRMIST, KTR*	**Chair:** *Dr. Ionut Topala, Alexandru Ioan Cuza University of Iasi, Romania* **Co-chair:** *Dr. J. Chandra dass, Automobile, SRMIST, KTR*	**Chair:** *Dr. T.J. Dhilip Kumar Indian Institute of Technology, Ropar,* **Co-chair:** *Dr. M. Prakash, Chemistry,SRMIST, KTR*
	KN 33: Prof. Sebastian Lourdudoss KTH Royal Institute of Technology, Sweden ***Title:*** *Light emitting diodes and semiconductor lasers*	**KN 34: Prof. C Retna Raj** Indian Institute of Technology, Kharagpur ***Title:*** *Aqueous rechargeable Zn batteries: anode and cathode engineering*	**KN 35: Prof. Madhu Bhaskaran** RMIT University, Australia ***Title:*** *Wearables sensors for health care and aged care*	**KN 36: Prof. Palani Iyamperumal Anand** Indian Institute of Technology, Indore ***Title:*** *A novel thin film based micro-3D printer for printing microscale structures for MEMS applications*	**KN 37: Dr. Ajay Singh** Bhabha Atomic Research Centre, Mumbai ***Title:*** *Defect and interface engineering to realize high performance thermoelectric materials and power generators*	**KN 38: Dr. Takafumi Ishibe** Osaka University, Japan ***Title:*** *Simultaneous control of carrier and phonon transports in nanostructured thermoelectric films with the controlled interfaces*	**KN 39: Prof. S. Sindhu** Birla Institute of Technology and Science, Pilani ***Title:*** *Advancing green technology exploring polymer based electrochromic windows to sustainable energy efficiency*	**KN 40: Prof. Katarzyna Krukiewicz** Silesian University of Technology, Poland ***Title:*** *Modulating cell-surface interactions through electroactive materials*
10.20 - 10.50	**IT 41: Dr. Tomy Abuzairi** Universitas Indonesia, Indonesia ***Title:*** *Flash joules heating methods with high voltage capacitor for lab-scale graphene*	**IT 42: Dr. Vanchiappan Aravindan** IISER, Tirupati ***Title:*** *Li-ion capacitors and recycling Li-ion batteries*	**IT 43: Dr. Yuta Kubota** Tokyo Institute of Technology, Japan ***Title:*** *Fabrication of CeO2 and Cu2O films for humidity and bending sensors by using solution processes based on thermochemical calculations*	**IT 44: Dr. Tetsuo Oikawa** JEOL, Japan ***Title :*** *Electron Microscopy*	**IT 45: Prof. Nji Raden Poespawati** Universitas Indonesia, Indonesia ***Title:*** *Effect of carbon electrode annealing temperature on perovskite solar cells*	**IT 46: Dr.-Ing. Vincent** Linseis Messgeräte GmbH ***Title:*** *Thermoelectric Metrology: A Comprehensive Review from a Manufacturer's Perspective*	**IT 47: Dr. D. Durgalakshmi** Anna University, Chennai ***Title:*** *Functional nanomaterials for theranostic applications*	**IT 48: Dr. Mahesh Kumar Ravva** SRM University-AP, Amaravati ***Title:*** *Computational insights into metal corrole complexes as single atoms catalysts for electrochemical hydrogen evolution reactions*
10.50 - 11.05	**Tea Break**							
	Paraell Session 9							
11.05 - 11.35	**Chair:** *Prof. P. Rajamalli Indian Institute of Science, Bangalore* **Co-chair:** *Dr. A. Geetha, Physics,SRMIST, KTR*	**Chair:** *Dr. Soorathep Kheawhom Chulalongkorn University, Thailand* **Co-chair:** *Dr. K. Shadak Alee, Physics, SRMIST, KTR*	**Chair:** *Prof. Madhu Bhaskaran RMIT University, Australia* **Co-chair:** *Dr. Meenal S Deo,Physics, SRMIST, KTR*	**Chair:** *Dr. Baskar Bhera, SRMIST, Chennai* **Co-chair:** *Dr. T. Viyayakumar, Physics, SRMIST, KTR*	**Chair:** *Dr. Assayidatul Laila Binti Nor Hairin,International Islamic University, Malaysia* **Co-chair:** *Dr. R. Annie Sujatha, Physics, SRMIST, KTR*	**Chair:** *Dr. Atsushi Nakamura, Shizuoka University, Japan* **Co-chair:** *Dr. J. Chandra dass,Automobile, SRMIST, KTR*	**Chair:** *Dr. Ranita Basu, Bhabha Atomic Research Centre, Mumbai* ***Co-chair:*** *Dr.M. Kovendhan, Pysics,SRMIST, KTR*	**Chair:** *Dr. Sakura N. Takeda NAIST, Japan* ***Co-chair:*** *Dr. Sandeep K lahera, SRMIST, KTR*
	IT 49: Dr. Arief Udhiarto Universitas Indonesia, Indonesia ***Title:*** *Analysis of performance degradation in single-layer OLEDs fabricated using vacuum-free lamination methods*	**IT 50: Prof. R. Kothandaraman** Indian Institute of Technology Madras, Chennai ***Title:*** *Mechanistic Investigation on the Capacity Loss in Phosphonated Anthraquinone Based Redox Flow Battery*	**IT 51: Prof. Mei-Jywan Syu** National Cheng Kung University, Taiwan ***Title:*** *Fabrication of magnetic nanoclusters modified gold electrode for the impedimetric detection of serum albumin*	**IT 52: Dr. Ir. Retno Wigajatri Purnamaningsih** Universitas Indonesia, Indonesia ***Title :*** *A visible light wide angle optical divider based on III/nitride for under water application*	**IT 53: Dr. Vibha Saxena** Bhabha Atomic Research Centre, Mumbai ***Title:*** *Langmuir-Blodgett technique: a versatile method to prepare high quality and ordered ultra-thin films for various applications*	**IT 54: Dr. N. Krishna Chandar** Vellore Institute of Technology, Vellore ***Title:*** *Nanostructured manganese oxide based two dimensional nanocomposites for the removal of organic pollutants*	**IT 55: Prof. M. Arivanandhan** Anna University, Chennai ***Title:*** *Growth of Si1−xGex (0 < x < 1) alloy semiconductor under rapid cooling*	**IT 56: Prof. Sulaiman Wadi Harun** Universiti Malaya, Malaysia ***Title:*** *Nanomaterial applications in ultrafast photonics*
11.35 - 11.55	**Oral Presentation (OP 137 - OP 138)**	**Oral Presentation (OP 139 - OP 140)**	**Oral Presentation (OP 141 - OP 142)**	**Oral Presentation (OP 143 - OP 144)**	**Prof. Shoji Kaneko SPD Laboratory, Japan**	**Oral Presentation (OP 145 - OP 146)**	**Oral Presentation (OP 147 - OP 148)**	**Oral Presentation (OP 149 - OP 150)**
11.55-13.00	**Lunch Break**							
13.00-19.30	**Sight Seeing (Trip to Mahabalipuram)**							
19.30 -21.00	**Conference Banquet Dinner @ Downtown Building, Mahindra World City near Singaperumal Kovil**							

Note : PL - Plenary Talk; KN - Keynote; IT: Invited Talk; TT-Technical Talk **TPGA - Dr. T. P. Ganesan Auditorium Mini Hall; SBE - School of Bio-Engineering Buliding**

INTERNATIONAL CONFERENCE ON
ADVANCED FUNCTIONAL MATERIAL AND DEVICES (AFMD - 2024)
February 26-29, 2024

SRM INSTITUTE OF SCIENCE & TECHNOLOGY (Deemed to be University u/s 3 of UGC Act, 1956)

Nanotechnology Research Centre

AFMD 2024

AFMD-2024 PROGRAM SCHEDULE (Day - 4)

29.02.2024 (THURSDAY)

Time (IST)								
ROOM	**TPGA Main Hall**		**TPGA Mini Hall - 1**		**TPGA Mini Hall - 2**		**SBE Prof. G. N. Ramachandran Hall**	
	Parallel Session 10							
09.00-09.40	**Chair:** *Prof. Benoit Piro, CNRS, France* **Co-chair:** Dr. M. Alagiri , Physics, SRMIST, Chennai		***Chair:*** *Prof. Toru Aoki, Shizuoka University, Japan* ***Co-chair:*** *Dr. G. Bakyaraj, Physics, SRMIST, Chennai*		**Chair:** *Prof. Hiroya Ikeda, Shizuoka University, Japan* ***Co-chair:*** *Dr. R. Maheswaran, Physics, SRMIST, Chennai*		**Chair:** *Prof. Mohd Khairul Bin Ahmad,UTHM, Malaysia* **Co-chair:** Dr. G. T. Senthil Andavan, Chemistry, SRMIST, Chennai	
	PL 09: Prof. Aziz Amine Hassan II University of Casablanca, Morocco ***Title:*** *Recent advances in carbon nanomaterials-based electrochemical sensors and biosensors*		**PL 10: Prof. Kim Daasbjerg** Aarhus Univesrsity, Denmark ***Title:*** *Use of manganese bipyridine complexes and single-atom catalysts in the electroreduction of carbon dioxide*		**PL 11: Prof. Mohamed Jouini** CNRS, France ***Title:*** *CO2 reduction on dye sensitized NiO photocathodes decorated with palladium nanoparticles*		**PL 12: Prof. Shahzada Ahmad** University of Basque Country Science Park, Spain ***Title:*** *Engineering the emerging semiconductors for thin-film photovoltaics*	
ROOM	**TPGA Mini Hall - 1**	**TPGA Mini Hall - 2**	**SBE 101**	**SBE 102**	**SBE 103**	**SBE 104**	**SBE 201**	**SBE 202**
	Symposium A	**Symposium B**	**Symposium C & M**	**Symposium D**	**Symposium E, J & I**	**Symposium F**	**Symposium G**	**Symposium H & K**
	Parallel Session 11							
09.45 - 10.20	**Chair:** *Prof. Yasuhiro Hayakawa, Shizuoka University, Japan* **Co-chair:** *Dr. Maduraiveeran, Chemistry, SRMIST, KTR*	**Chair:** *Prof. R. Kothandaraman, IIT Madras, Chennai* **Co-chair:** *Dr. C. Siva, Physics, SRMIST, KTR*	**Chair:** *Dr. Chao-Wei Huang, National Cheng Kung University, Taiwan* **Co-chair:** *Dr. P.C. Karthika, Physics, SRMIST, KTR*	**Chair:** *Dr. Vibha Saxena, BARC, Mumbai* **Co-chair:** *Dr.R. Annie Sujatha , Physics, SRMIST, KTR*	**Chair:** *Dr. Naonori Sakamoto, Shizuoka University, Japan* **Co-chair:** *Dr. V. Kathirvel, Physics, SRMIST, KTR*	**Chair:** *Dr. T. S. Shyju, Sathyabama Institute of Science and Technology, Chennai* **Co-chair:** *Dr. Trilochan Sahoo, Physics, SRMIST, KTR*	**Chair:** *Prof. Muhammet S. Toprak KTH Royal Institute of Technology, Stockholm, Sweden* **Co-chair:** *Dr. Gopirajan, Physics, SRMIST, KTR*	**Chair:** *Dr. Nurul Asyikeen Ab Mutalib Universiti Malaya, Malaysia* **Co-chair:** *Dr. Venkatesh kumara mangalam, Chemistry, SRMIST, KTR*
	KN 41: Prof. Sudakar Chandran Indian Institute of Technology, Madras ***Title:*** *Sublattice distortion controlled electronic and optical properties of Cs2B'B''X6 (B' = Ag, Na; B'' = Bi, In; X = Cl, Br) double perovskites*	**KN 42: Prof. Tomoya Ohno** Kitami Institute of Technology, Japan ***Title:*** *Control of the coating structure on a cathode particle for Li-ion battery*	**KN 43: Prof. Toru Aoki** Shizuoka University, Japan ***Title:*** *Single crystal diamond photon-counting X-ray imaging device*	**KN 44: Prof. Nobuyasu Adachi** Nagoya Institute of Technology, Japan ***Title:*** *Ferromagnetic properties of zinc and magnesium ferrite prepared by MOD technique*	**KN 45: Dr. Ch. Subrahmanyam** Indian Institute of Technology, Hyderabad ***Title:*** *Nonthermal plasma assisted CO2 conversion to value-added chemicals*	**KN 46: Prof. Taketomo Sato** Hokkaido University, Sapporo, Japan ***Title:*** *Photoelectrochemical etching of III-nitride semiconductors for nanostructure fabrication*	**KN 47: Prof. S. Balakumar** University of Madras, Chennai ***Title:*** *Productizing nanostructured functional bioactive materials for advanced healthcare hemostats and tissue regenerative aids*	**KN 48: Prof. Kazushi Ikeda** NAIST, Japan ***Title:*** *Machine learning approaches to materials*
10.20 - 10.50	**IT 57: Dr.P. Koteswara Rao Peta** University of Delhi, New Delhi ***Title:*** *Growth and defects challenges of wide bandgap electronic materials: Applications*	**IT 58: Prof. Kenji Murakami** Shizuoka University, Japan ***Title:*** *Research on the Energy Conversion Devices: Focusing on Solar Cells and Mechanoluminescence*	**IT 59: Dr. Hiroki Kase** Shizuoka University, Japan ***Title:*** *Spatial representation of multi-energy 3D X-ray CT using mixed reality for nondestructive testing*	**IT 60: Dr. Assayidatul Laila Binti Nor Hairin** International Islamic University, Malaysia ***Title:*** *Upgraded recycling of cast-iron scrap chips towards Fe-based thermoelectric materials for waste-heat energy harvesting*	**IT 61: Dr. Srinivasan Anandan** ARCI, Hyderabad ***Title:*** *Indigenous materials for energy storage applications: From lab innovations to semi-pilot scale production*	**IT 62: Dr. Maneesh Chandran** National Institute of Technology Calicut ***Title:*** *Template assisted sol-gel synthesis of BiFeO3 hollow tubes*	**IT 63: Dr. E.V.A. Premalal** University of Sri Lanka ***Title:*** *Development of Chemical Vapor Deposition Technology for the Synthesis of Carbon Nanotube and Nanofiber Forest*	**IT 64: Dr. Shamima Hussain** UGC-DAE CSR, Kalpakkam
10.50 - 11.05	**Tea Break**							
	Parallel Session 12							
11.05 - 11.35	**Chair:** *Dr.P. Koteswara Rao, University of Delhi, New Delhi* ***Co-Chair:*** *Dr. Sandepan Roy, Mechanical, SRMIST, KTR*	**Chair:** *Dr. M. Sathish, Central Electrochemical Research Institute, Karaikudi* ***Co-Chair:*** *Dr. Meenal S. Deo, Physics, SRMIST, KTR*	**Chair:** *Dr. Suhana Binti Mohamed Sultan, Universiti Teknologi Malaysia, Malaysia* ***Co-chair:*** *Dr. Anbumozhi Angayarkanni, Physics, SRMIST, KTR*	**Chair:** *Prof. Kazushi Ikeda, NAIST, Japan* ***Co-chair:*** *Dr. A. Tamil selvan, Physics, SRMIST,KTR*	**Chair:** *Dr. Ch. Subrahmanyam, Indian Institute of Technology, Hyderabad* ***Co-chair:*** *Dr. Angeline Little Flower, Physics, SRMIST, KTR*	**Chair:** *Dr. Taketomo Sato, Hokkaido University, Sapporo, Japan* ***Co-chair:*** *Dr. Shobana, Maths, SRMIST, KTR*	**Chair:** *Dr. E.V.A. Premalal University of Sri Jayewardenepura, Sri Lanka* ***Co-chair:*** *Dr. Chandradoss, Automobiles, SRMIST, KTR*	***Chair:*** *Dr. Maheswaran, Physics, SRMIST, KTR*
	IT-65: Dr. Darius Gailevicius Vilnius University, Lithuanian ***Title:*** *3D printed phase retarders*	**IT 66: Dr. R. Ramesh** Periyar University, Salem ***Title:*** *Metal-organic framework derived 3D hierarchical metal oxides for high energy density supercapacitor application*	**IT 67: Prof. Hiroya Ikeda** Shizuoka University, Japan ***Title:*** *Wearable thermoelectric power generator for self-powered physiological sensor*	**IT 68: Dr. Shailesh Narain Sharma** National Physical Laboratory, New Delhi ***Title:*** *Nanotechnology advancements for sustainable energy: Addressing critical materials challenges*	**IT 69: Dr. Manjusha Battabyal** ARCI, Chennai ***Title:*** *Nanostructured antimonides for waste heat harvesting*	**IT 70: Dr. Ranu Bhat** Bhabha Atomic Research Centre, Mumbai ***Title:*** *Designing high efficiency Bi-Te thermoelectric power generators: challenges and approaches*	**IT 71: Dr. P. Prathap** National Physical Laboratory, New Delhi ***Title:*** *Atomic layer deposition of oxide layers for efficient passivation of silicon solar cell surface*	**IT 72:Dr. Biplab Sanyal** Uppsala University, Sweden ***Title:*** *Understanding of magnetism in 2D materials by first principles theory*
11.35 - 11.55	**Oral Presentation (OP 151 - OP 152)**	**Oral Presentation (OP 153 - OP 154)**	**Oral Presentation (OP 155 - OP 156)**	**Oral Presentation (OP 157 - OP 158)**	**Oral Presentation (OP 159 - OP 160)**	**Oral Presentation (OP 161 - OP 162)**	**Oral Presentation (OP 163 - OP 164)**	**Oral Presentation (OP 165 - OP 166)**
11.55 - 12.55	**Poster Presentation (PP 451 -PP 600)**							
12.55-14.00	**Lunch Break**							
	Parallel Session 13							
14.00 - 14.35	**Chair:** *Dr. Darius Gailevicius, Vilnius University, Lithuanian* **Co-chair:** *Dr. R.M. Hariharan, Physics, SRMIST, KTR*	**Chair:** *Dr. R. Ramesh, Periyar University, Salem* **Co-chair:** *Dr. S. Mathimalar, Physics, SRMIST, KTR*	**Chair:** *Prof. Aziz Amine, Hassan II University of Casablanca, Morocco* **Co-chair:** *Dr. Shubojyothi Sinha, Physics, SRMIST, KTR*	**Chair:** *Dr. Mohd Faiz Bin Mohd Salleh, Universiti Malaya, Malaysia* **Co-chair:** Dr.M. KovendHan, Physics, SRMIST, KTR	**Chair:** *Prof. Kim Daasbjerg Aarhus Univesrsity, Denmark* **Co-chair:** *Dr. Karthika, Physics, SRMIST, KTR*	**Chair:** *Prof. Shahzada Ahmad University of Basque Country Science Park, Spain* **Co-chair:** *Dr.K. Santhi, Physics, SRMIST, KTR*	**Chair:** *Prof. S. Balakumar University of Madras, Chennai* **Co-chair:** *Dr. Maduraiveeran, Chemistry, SRMIST, KTR*	**Chair:** *Prof. Sulaiman Wadi Harun Universiti Malaya, Malaysia* **Co-chair:** *Dr. Jaivardhan Sinha, Physics, SRMIST, KTR*
	KN 49: Prof. Daniel Moraru Shizuoka University, Japan ***Title:*** *Quantum Tunneling Functionalities based on Silicon Nanomaterials and Nanodevices*	**KN 50: Prof. Kunio Hayakawa** Shizuoka University, Japan ***Title:*** *Electro-thermo-mechanical finite element analysis on SPS sintering process of zirconia part*	**KN 51: Prof. Jun Kondoh** Shizuoka University, Japan ***Title:*** *Finite element analysis of surface acoustic wave on 36YX-LiTaO3/36Y90X-qaurtz structure for sensor application*	**KN 52: Prof. P.N. Santhosh** Indian Institute of Technology, Madras, Title: Competing magnetic interactions and exchange bias behaviour in complex oxides materials	**KN 53: Prof. Yueh-Heng Li** National Cheng Kung University, Taiwan ***Title:*** *Iron particles: Applications in aerospace and energy industries*	**KN 54: Dr. Hiromu Hamasaki** Osaka University, Japan ***Title:*** *Electrical conductivity and Seebeck coefficient of a single contact between carbon nanotubes*	**KN 55: Dr. Naonori Sakamoto** Shizuoka University, Japan ***Title:*** *Control of encapsulated chemical species into cage-structured crystal 12CaO·7Al2O3*	**KN 56: Prof. Yuichi Sakumura** NARA Institute of Science and Technology, Japan ***Title:*** *Derivation of nonlinear dynamics of silicon structure under indium adsorption*
14.35 - 15.05	**IT 73: Prof. Yasuhiro Hayakawa** Shizuoka University, Japan ***Title:*** *Effect of gravity on the growth of InGaSb alloy semiconductor crystals*	**IT 74: Technical Talk**	**IT 75: Dr. Riyaz Ahmad Mohamed Ali** Universiti Tun Hussein Onn Malaysia, Malaysia ***Title:*** *Nanoplasmonic micro- structured chip for single cell sensing application*	**IT 76: Technical talk**	**IT 77: Prof. S. Anandan** National Institute of Technology, Tiruchirappalli ***Title:*** *Current scenario of dye-sensitized solar cells - modifications and large-scale production*	**IT 78: Prof. Te-Wei Chiu** National Taipei University of Technology, Taiwan ***Title:*** *Synthesis and versatile applications of Cu-based delafossite compounds*	**IT 79: Technical talk**	**IT 80: Dr. Nasrul Anuar Bin Abd Razak** Universiti Malaya, Malaysia ***Title:*** *Recycling of polyethylene terephthalate wastes for prosthetic applications*
15.05-16.00	**Closing Ceremony**							
16.00-16.20	**High Tea**							

Note : PL - Plenary Talk; KN - Keynote; IT: Invited Talk; TT-Technical Talk **TPGA - Dr. T. P. Ganesan Auditorium Mini Hall; SBE - School of Bio-Engineering Buliding**

Invited Speakers abstract

Contributed Lecturers Abstract

Symposia A: Electronic, Optical, Optoelectronic, Quantum Materials and Devices

Symposia B: Electrochemical Energy Conversion, storage & Devices

Symposia C: Sensors and Wearable Devices

Symposia D: Ferroelectric, Magnetic & Multiferroic Materials for Spintronics and Memory applications

Symposia E: Energy Harvesting for sustainable Future

Symposia F: Functional Nanomaterials and Applications

Symposia G: Structural Materials, Composites, Coatings and Additive Manufacturing

Symposia H: Soft Materials, Biomaterials and Healthcare Materials

Symposia I: Materials for Environment & Sustainable Development Goals

Symposia J: Waste-to-Wealth

Symposia K: Computational Materials Science and Materials Informatics

Symposia M: Women Scientific Symposia on Advanced Functional Materials

List of Sponsors

ABSTRACTS

PL 01

The Unique chemical and physical effect of ultrasound cavitation for material synthesis

Dr. Judy Lee

University of Surrey, UK

ABSTRACT

Acoustic cavitation has found itself in a diverse range of applications, from cancer treatment to possible sonofusion. More well-known are the use of low frequency ultrasonic baths and horns for physical processes such as cleaning, mixing, dispersion and emulsification. In addition, high frequency ultrasound has been used to generate chemically reactive radicals and conditions to facilitate degradation of pollutants and synthesis of polymers, as well as nanomaterials such as metal colloids, metal nano-composites and hollow shelled micro/nano-spheres. These ultrasonic effects stem from the creation of acoustically driven cavitation bubbles as the sound waves propagate through a liquid medium. Liken to "a star in a jar", these cavitation bubbles can emit light (sonoluminescence) and undergo violent collapses to generate extreme temperatures (> 5000 k), pressures (> 1000 atm) and jet velocities (up to 120 m/s has been reported). It is these remarkable conditions which create the unusual physical and chemical effects that we observe. However, to capitalise on these effects, one needs to understand the fundamental mechanisms behind the physical and chemical conditions created and the importance of solution and sonication conditions used.

PL 02

Molecular Self-assembly and Superhydrophobic Coatings for Energy Saving Application

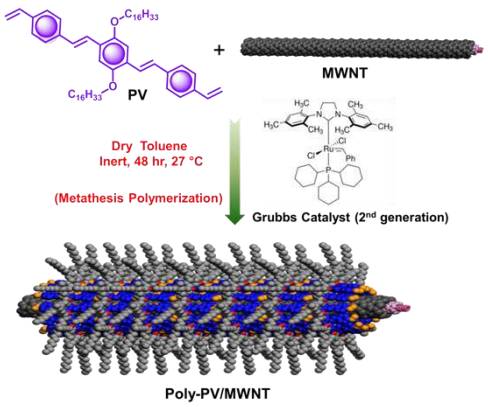
Ayyappanpillai Ajayaghosh

CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram, Kerala

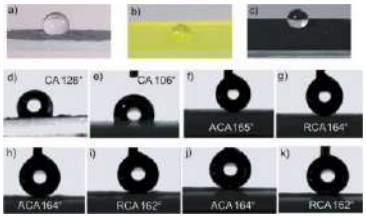
SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu

ABSTRACT

Nature exploits the bottom-up self-assembly approach for the construction of functional materials. Many of such natural creations are superhydrophobic which facilitate their self-cleaning ability. The science and engineering behind these creations are inspiration for scientists to design artificial self-cleaning materials, which mimick the lotus leaf and rose petal like superhydrophobicity [1]. We have been exploring the possibility of the bottom-up molecular self-assembly approach [2-4] to create superhydrophobic organic-inorganic nanocomposites and gels [5,6]. We have chosen π-conjugated molecules such as OPVs and carbon nanotubes to prepare hybrid materials. The strong π-interaction of OPVs with CNTs allows dispersion of the latter in organic solvents. This well-dispersed nanocomposite can be coated on surfaces of glass, metals and mica, resulting in water repellent self-cleaning surfaces.



Detailed TEM and AFM studies revealed that coatings of the OPV self-assembly on CNTs form a rough surface with nano and microsized topography which is responsible for the self-cleaning property. Further, we attempted polymerization of the self-assembled molecules on the surface of the CNT using Grubb's metathesis approach, which resulted stable superhydrophobic coating for aquatic vessels to improve the fuel efficiency [7]. These coatings have binary surface topography with large amount of trapped air and very small contact angle hysteresis, which facilitate frictionless motion. The proposed lecture will be focused on the details of our results in this topic.



References:

1. Ajayaghosh, V. K. Praveen, *Acc. Chem. Res.* **2007,** *40*, 644.
2. Ajayaghosh, V. K. Praveen, S. Srinivasan, R. Varghese, *Adv. Mater*. **2007**, *19*, 411.
3. S. S. Babu, V. K. Praveen, A. Ajayaghosh, *Chem. Rev*. **2014,** *114*, 1973.
4. S. Srinivasan, S. S. Babu, V. K. Praveen, A. Ajayaghosh, *Angew. Chem. Int. Ed*. **2008,** *47,* 5746.
5. S. Srinivasan, V. K. Praveen, R. Philip, A. Ajayaghosh, *Angew. Chem. Int. Ed*. **2008,** *47,* 5750.

PL 03

Effective Research Publishing: Insider Tips and Techniques

Dr. Rohini Kitture

Deputy Editor, Small AND Physical Science Portfolio, Wiley.

ABSTRACT

Despite an increase in submissions from India, the acceptance rate has not proportionally risen. Through this talk, I aim to guide budding researchers in making their publications effective, thereby bridging the gap and improving their chances of acceptance. This talk on 'Effective Research Publishing: Insider Tips and Techniques' will provide attendees with invaluable insights into navigating the research publishing process. Beginning with an overview of the Wiley portfolio journals, researchers will discover options for submitting their findings. Further, meticulous evaluation process undertaken by editors, including pre-checks and peer review protocols will be discussed. By understanding these intricacies, attendees will learn to identify common pitfalls and minimize the risk of editorial desk rejection, empowering them to enhance the quality and success of their manuscript submissions. This talk offers actionable strategies to improve publication outcomes and elevate research impact.

PL 04

Computational Design of Single/Double Atom Catalysts for Efficient Electrochemical NH_3 production

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ABSTRACT

Green ammonia production via electrochemical nitrogen reduction is one of the most attractive and emerging chemical processes in hydrogen storage applications. In particular, the development of highly efficient catalysts is essential for the electrochemical ammonia synthesis process. However, such development is still a challenging issue owing to the difficulty of direct characterization of electro-catalyst property. Quantum mechanics-based first-principles density functional theory (DFT) calculation is one of flexible and powerful means which can provide the quantitative information on the electro-catalysis and in turn help to design the novel electro-catalyst composition. In this talk, we present the effect of ligand and support on the ammonia productivity of single and double atom catalyst by using DFT calculation [1,2]. Here, the ligand effect is related to the catalytic activity modification of a single atom catalyst by the addition of hetero atom into a single atom, while the support effect is the activity change of catalyst by the strong interaction between a single atom and support. Our study provides the key insight on how such ligand and support affect the NH_3 production catalysis on the single atom level catalyst.

References

1. S.-H. Kim, H. C. Song, J. Han, K.-Y. Lee and H. C. Ham, “Impact of Dopant-induced Ensemble Structure of Hetero Double Atom Catalysts in Electrochemical NH_3 Production”, Journal of Materials Chemistry A, 10, 6216-6230 (2022)
2. H. C. Song, and H. C. Ham On the role of metal cation in MXene in boosting the catalytic activity of single/double atom toward electrochemical NH3 production, Chemical Engineering Journal, 470, 144243 (2023)

PL 05

Utilization of uranium mill tailings for construction materials: A pathway for sustainable uranium mining and milling

D. K. Aswal* and S.K. Jha

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ABSTRACT

Uranium mining and ore processing is the most visible sector of nuclear industry due to its processing of large volume of low specific active and low-grade uranium ore and generation of equivalent quantity of solid waste, called tailings. Uranium mill tailings contain uranium series radionuclides along with a small fraction of residual parent uranium and process chemicals. In India, currently eight uranium mines are operating in two states (i.e. Jharkhand and Andhra Pradesh) and proposed to expand the existing operations (Narwapahar and Tummalapalle) and establishment of new operations at Rohili, Rajasthan in near future. Long term storage in engineering impoundment systems and management of the bulk volume of tailings for centuries with a modified chemical form of radionuclides and other chemical contaminants are the major technical challenge for all the stakeholders' i.e. mining agencies, the department, regulator and the union government. There is a general recognition that at some level, society is now expecting practices that put less pressure on natural resources and entail the recycling and reuse of materials. The background for this position is that our society is consuming natural resources way beyond any sustainable level. As per international/AERB norms, uranium mill tailings are required to be confined in order to exercise proper source term control. The concern arises, since very large amounts of U tailings need recycling or proper disposal. The coal ash is the one of the other largest stream of NORM waste. Million tonnes of fly ashes are arising globally each year, which carry U-238 along with all its non-gaseous decay products, as well as Th-232 and its progeny.

PL 06

Printed Electronics in Sensors and Medical Devices

Prof. Benoît PIRO

Distinguished Professor in Chemistry at Université Paris Cité , France

Laboratory ITODYS, CNRS, France

ABSTRACT

In the history of mankind, every era is marked by innovations that transform society. Since 1947, when the transistor was discovered, the constant progress of electronics has transformed the world in a digital revolution. In this hyper-connected world, another type of electronics, printed, organic and flexible electronics, is preparing a new revolution in the medical device industry with the discovery of new materials. Printed electronics technology for the manufacture of components consists of materials deposited on substrates using various printing processes. Materials account for around half or even two-thirds of the total cost of manufacturing a device. This demonstrates the strategic importance of materials. Expertise and mastery of production processes are also very important for entering the printed electronics market, an industry that is developing at an impressive rate. Printable materials are needed to make electrical contacts (in this case, the most common are metallic inks, e.g. silver, gold or platinum), but also to make the functional parts of chemical sensors, e.g. conducting polymers, nanostructured oxides, organic or inorganic semiconductors, graphene or carbon nanotube derivatives... Printing (inkjet printing, screen printing, aerosol printing, to name the most common techniques) allows these materials to be deposited as thin films in a very reproducible way and is one of the most reliable methods for producing sensors in laboratories, but also on an industrial scale for use in medical devices. Another issue that needs to be addressed is the environmental impact of printed chemical sensors. Reducing the amount of active material deposited on a sensor is the primary objective, and digital printing technologies such as on-demand inkjet printing, where each droplet has a volume of only a few pL, are perfect for this.

PL 07

Potential of electrode surface modification by nanomaterials for sensors with high-performance

Olfa Kanoun,

Chemnitz University of Technology

ABSTRACT

Nowadays, sensors are one of the most important enablers for various current developments in highly societal-sensitive areas such as health and environmental monitoring. Sensor developments have to meet several requirements, not only for improved accuracy and cost reduction but also for higher performance through increased flexibility, specificity, reliability, and multifunctionality. In electrochemical sensors, electrode modification is crucial as it mediates the charge transfer and can reduce the oxidation potential of the analyte at the formal potential of the carbon modification and increase the current density. Carbon-based nanomaterials, e. g. carbon nanotubes (CNTs), graphene or graphene oxide (GO), in Laser-Induced Graphen (LIG) electrodes and surface modification lead to a high electron transfer performance and large specific surface area compared to other nanomaterials. They bring excellent properties to electrochemical sensors and biosensors, such as a high surface area/volume ratio. CNTs and GO have a high surface area, which leads to high catalytic activity. Further chemical attachments to the ends of carbon nanomaterials and dedicated surface functional groups create chemical bonds that can be used to tailor the interaction with other entities, such as a polymer, and improve the electron transfer rate.

This plenary talk focuses on the contribution of carbon-based nanomaterials in LIG electrodes and their modification towards electrochemical and biosensors with outstanding properties.

PL 08

Computational-aided development of MOF-based Membranes for molecular separation

Guillaume Maurin

ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France.

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ABSTRACT

Mixed matrix membranes (MMMs) incorporating Metal-organic frameworks (MOF) into polymeric matrices show promising properties for several industrial applications, such as gas separation, water desalination and pervaporation among others. Especially in the field of gas separation and in particular for CO_2 capture, MMMs have attracted a great attention owing to their potential for merging the processability of polymers and the excellent selectivity of MOF materials. One of the key challenges in the field is the fabrication of continuous and mechanically stable membranes, with high MOF loading and homogeneous dispersion of MOF nanoparticles into the polymer matrices that call for a good interfacial adhesion of the two components. A systematic computational exploration of the interface structures for a series of MOF/polymer composites has been achieved by our group via deploying an innovative modeling approach integrating quantum calculations and force-field equilibrium Molecular Dynamics simulations. This enabled us to unravel key features of both MOFs and polymers that control their adhesion (1). Further concentration-gradient driven molecular dynamics (CGD-MD) calculations revealed that the MOF/polymer interface plays also a key role in the overall molecular transport in the MMM. We demonstrated recently that the interfacial structuring can be finely controlled to achieve a selective enhancement of the CO_2 transport which is of great interest for improving the productivity of the corresponding MMM (2). This lecture will deliver an illustration of our latest modelling achievements in the field that paved the way towards a rational design of MMMs with outstanding performance for the separation of industrially relevant gas mixtures (3).

Reference:

1. Carja, I.-D. et al., ACS Appl. Mater. Interfaces 13, 29041, 2021.
2. Fan, D. et al., Journal of Membrane Science Letters 2, 100029, 2022.
3. Jit Datta, S. et al., Science!"#$%!"&’(’!")’))*"

PL 09

Recent advances in carbon nanomaterials-based electrochemical sensors and biosensors

Aziz Amine[1]

[1]*Hassan II University of Casablanca, Faculty of Sciences and Techniques, Mohammedia, Morocco.*

*Corresponding author e-mail: aziz.amine@fstm.ac.ma

ABSTRACT

In this presentation, we will focus on the electrochemical behavior and electroanalytical applications of laser-scribed graphene electrodes, as well as screen-printed electrodes modified through microwave-assisted functionalization of carbon nanofibers and various types of carbon blacks. Noteworthy advancements, such as the non-enzymatic oxidation of glucose, nanomolar detection of dopamine, and a negative shift in the oxidation peak of electroactive molecules, characterize these electrodes, setting them apart from conventional methodologies. The structural and morphological characterization of sensors based on various carbon nanomaterials, employing techniques such as Raman spectroscopy, transmission electron microscopy (TEM), and scanning electron microscopy (SEM), will be elucidated. The increasing prominence of these carbon nanomaterials can be attributed to their superior performance, including a decrease in applied potential or peak-to-peak separation, improved peak intensity, and reduced resistance in electron transfer. Key features contributing to their success include nanostructure, low electron transfer resistance, a high number of defect sites, stability, tunable properties, and cost-effectiveness. This presentation will also provide a brief overview of our latest work on the design, preparation, and electrochemical sensing applications of these carbon nanomaterials. Furthermore, challenges and future perspectives in this field will be outlined and discussed.

PL 10

Use of Manganese Bipyridine Complexes and Single-Atom Catalysts in the Electroreduction of Carbon Dioxide

Kim Daasbjerg*

Novo Nordisk Foundation (NNF) CO2 Research Center, Aarhus Univesrsity, Gustav Wieds Vej 10, 8000 Aarhus C, Denmark

*Corresponding author e-mail: kdaa@chem.au.dk

ABSTRACT

Electrocatalysis presents a promising avenue for utilizing CO_2 as a feedstock in the chemical industry. However, effectively controlling the selectivity for different CO_2 reduction products remains a significant challenge. We report a series of manganese complexes featuring bipyridine ligands that can reduce CO_2 to either HCOOH, if the ligand structure incorporates strategically positioned tertiary amines, or CO if the amine groups are absent in the ligand or positioned far from the metal center.1-6 The amine-modified complexes are benchmarked to be among the most active catalysts for reducing CO_2 to HCOOH, demonstrating remarkable activity even at overpotentials as low as 300 mV. Mechanistically, the formation of a Mn−hydride species aided by in situ protonated amine groups is identified as a key intermediate using cyclic voltammetry, infrared spectroelectrochemistry, and DFT calculations. Another highly effective type of catalyst in CO_2 reduction is the single-atom catalyst (SAC). We present findings on the nitrogen-stabilized SACs containing low-valence zinc or indium atoms in a carbonaceous network (M-NC; M = Zn or In).7,8 These catalysts comprise saturated four-coordinate (M-N4) and unsaturated three-coordinate (M-N3) sites, where the latter results in the metal center adopting a low-valence state. Both metal-based materials exhibit a remarkable catalytic in the electrochemical reduction of CO_2 to CO with near-unity selectivity in water at an impressively low overpotential of 310 mV. Utilizing the SACs in a flow cell allows for the attainment of a current density of up to 1 A cm−2 with a high CO selectivity of >95 %. Computational analyses suggest that the unsaturated M-N3 sites play a critical role in reducing the energy barrier by stabilizing the COOH* intermediate. This work not only sheds light on the intricate relationship among coordination number, valence state, and catalytic performance but also demonstrates the potential for achieving high current densities relevant to industrial applications.

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PL 11

CO_2 Reduction on Dye Sensitized NiO Photocathode Decorated with Palladium Nanoparticles

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ABSTRACT

The thin-layer-stacked dye-sensitized NiO photocathodes decorated with palladium nanoparticles (nPd) can be used for the visible-light-driven selective reduction of CO_2, mostly to CO, at potentials starting as low as 0 V vs. RHE (compared to 0.6 V in the dark for electrocatalysis). The photosensitization of NiO by the organic dye P1, with a surface coverage of 1.5 $.10^{-8}$ mol cm^{-2}, allows the hybrid material to absorb light in the 400–650 nm range. In addition, it improves the stability and the catalytic activity of the final material decorated with palladium nanoparticles (nPd) through the electron-transfer-cascade mechanism. The photosensitizer P1 plays a central role as it generates excited-state electrons and transfers them to nPd. The formation of CO as the main reaction product is postulated, though the formation of traces of other small organic molecules (e.g. methanol) cannot be excluded.

PL 12

Engineering the Emerging Semiconductors for Thin-film Photovoltaics

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ABSTRACT

Our societal quest for clean energy generation and to reduce emissions has pushed the scientific community to discover sustainable energy sources. Photovoltaics is an effective and cost-competitive source to harvest solar energy. In the last decade, perovskite solar cells (PSC) have emerged as a potentially attractive thin-film PV technology in the laboratory, and power conversion efficiency as high as 26.2%, has been measured in the lab. Though the performance improvement is remarkable, their long-term stability, and reproducibility, have plagued its rapid commercialization endeavor. In our efforts to develop effective light harvesters, current efforts are being made to the employment of formamidinium lead triiodide ($FAPbI_3$) due to its favorable optical band gap (1.47 eV), high tolerance factor, and phase stability. In this talk, I will discuss our laboratory efforts in inducing reliability, through interface optimization, compositional engineering, developing rational charge selective layers in perovskites, and uncovering the underlying mechanisms, along with kesterites-based photovoltaics.

KN 01

Computer Simulation of Spontaneous Superlattice Formation in S-Ti-O This Film by Dynamic Aurora PLD

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ABSTRACT

We have reported spontaneous superlattice formation in epitaxial Sr-Ti-O thin film deposited on SrTiO3(001) having A-site excess composition (Sr/Ti=1.4) by PLD under magnetic field of 2,000 G (dynamic aurora PLD).(Fig. 1)[1] This spontaneous superlattice formation is not observed without applying magnetic field during deposition. The purpose of this work is to reproduce spontaneous superlattice formation in Sr-excess SrTiO3 thin film using phase-field method without limiting the direction of propagation of the composition wave. For this calculation, the open source-code for AB binary alloy [2] was modified. In this simulation, phase separation from uniform solid solution to SrTiO3 and SrO. To consider the temporal evolution of a composition field, the Cahn-Hilliard diffusion equation Figure 2 shows the results of simulating the time evolution of the composition under the following conditions: Sr/Ti = 1.4, temperature 700 °C, activation energy of diffusion 1.81 eV, and external magnetic field 2000 G. Here, calculation area is set to 100 nm square. This result shows that the superlattice structure is formed. This means that the spontaneous formation of the superlattice by spinodal decomposition can be reproduced by computer simulation without limiting the direction of propagation of composition wave.

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KN 02

Engineering Electrode-Electrolyte Interfaces in Heterogeneous Catalysis

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ABSTRACT

Electrolyte effects on the kinetics of electrochemical reactions is an emerging phenomenon in electrocatalysis. Recently we have shown that engineering aqueous electrolytes with high/low amounts of additives to achieve tunable products can be a facile strategy in different electrocatalytic processes. For example, a large amount of salt in water changes the structure of the hydration sphere around the ions and this can affect the water splitting process kinetically or thermodynamically. Water-in-Salt electrolytes based catalysis is found to be playing different roles in different metals and hence enhancing or decreasing the water splitting process. Such electrolyte engineering processes can be useful in different electrocatalytic processes such as hydrogen generation, nitrogen reduction, CO_2 reduction reaction etc. The talk will be focussing on such aspects of electrochemical reaction control in aqueous electrolytes and also will be on the importance of electrolyte structure probing near the electrode surface. Such engineering approaches are also important in energy storage devices such as metal-air batteries and phenomena such as photoluminescence.

KN 03

Do Nano-sensors need AI?

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ABSTRACT

Numerous nanomaterials are being developed to create extremely sensitive systems. Nanosensors are enabling portable devices/ systems that can quickly detect various bio/ chemical analytes or disease biomarkers at point-of-use. The major challenge of nanosensors is the extraction of meaningful data which is also described as the selectivity of the sensor. These nanosensors target to detect analytes in extremely low concentrations, many time in nano-molar or even lower at trace-levels; but these analytes are not alone in the sample. The other bio/ chemical molecules in such samples create a huge noise in the sensor output.

Conventional data analytics limit the progress of nanosensor systems research. This talk will elaborate the importance of Artificial Intelligence (AI) or Machine learning (ML) algorithms in advancing nano-sensing strategies toward diagnosis or any bio/ chemical identification. Various nanosensor device platforms, their applications and some use-cases with AI interventions will be discussed.

KN 04

Dual Role of Microalgae in Wastewater Treatment for Bioproduct (Fish Feeds Alternative)

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ABSTRACT

Wastewater is heavily polluted water which rich in organic and inorganic matters depend on the source of the wastewater itself. The direct discharge of wastewater into water body is associated with eutrophication and spreading of the disease's phenomenon, despite exceed the standard limit for Sewage Characteristics and Effluent Discharge. Thus, treatment of wastewater before disposal shall be implemented and microalgae have potential to this treat wastewater by uptake of organic matters to produce biomass via phycoremediation process. Phycoremediation might be an alternative technology, because it is cheaper and more effective for removing nutrients compared to other physicochemical process. Microalgae biomass have high nutritional values in term of lipids, protein and carbohydrates as an alternative for fish feeds. Microalgae can adapt to harsh condition in wastewater to produce quality biomass depend on the light exposure, aeration, pH, temperature and also nutrient content such as nitrogen, carbon and phosphate in the wastewater. Microalgae biomass from treated wastewater may be an alternative to replaced traditional fish feeds production in aquaculture industry that expensive. This microalgae biomass from treated wastewater have potential to support fish growth, fish development, fish feeding efficiency, fish resistance to diseases, fish stress response and low cost compared to wild catch fish feeds from juvenile fish. Hence, this study aims to highlight the dual roles potential of microalgae to treat wastewater and produce biomass as an alternative to traditional fish feeds. The phycoremediation techniques for wastewater treatment and microalgae biomass as fish feed were reviewed.

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KN 05

Tetrahedrite and Skutterudite: Two important crystal structures in thermoelectric research

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ABSTRACT

Thermoelectricity could be one of the solutions for the rapidly increasing energy demand. It can be used to recover waste heat into valuable electricity. There are several approaches to improving the efficiency of thermoelectric devices by enhancing the figure of merit. One of the approaches is to tune the crystal structure. In this talk, I will discuss two crucial crystal structures, Skutterudite and Tetrahedrite, which played important roles in optimising thermoelectric figures of merit. Skutterudite has a highly symmetric body-centred cubic (bcc) structure and space group of Im. The unit cell of Co_4Sb_{12} consists of 8 formula units, 32 atoms, and two voids can be filled with electropositive rattler to minimize the lattice part of thermal conductivity. Choosing InSb and GaSb as nanocomposites because the different Fermi level positions of the matrix phase and the inclusion phase will generate a potential barrier at the interfaces, blocking the low energy charge carriers. Therefore, the Seebeck coefficient is enhanced because the increase in the average effective mass of charge carriers improved the TE figure of merit. Another crystal structure is tetrahedrite ($Cu_{12}Sb_4S_{13}$), which has a complex crystal structure with many atoms (58 atoms) per unit cell; they are helpful for low thermal conductivity and have a high symmetric crystal structure (cubic). Substituting multi-oxidation states of element (Sn) at the Cu site enhanced the Seebeck coefficient and the power factor to realize a high thermoelectric figure of merit.

KN 06

Substrate Effects and Ionic Phase Transitions at Two-Dimensions

Prof. T. Serkan Kasirga

ABSTRACT

In this talk, I would like to present my research efforts over the past five years, starting with a one-of-a-kind chemical vapor deposition (CVD) chamber that allowed us to monitor the crystal formation optically. This unique ability enabled us to synthesize materials in novel morphologies, mostly as two-dimensional single crystals. I will talk about the products of this furnace, in particular, how intrinsically alkali-intercalated van der Waals (vdW) materials can be used as neuromorphic devices thanks to the reversible phase transitions, which can be controlled electrically and optically. Then, I will talk about materials where ionic motion can be controlled to change electrical and optical properties thanks to vacancy ordering. Finally, I will depart from the synthesis and ionics of atomically thin materials to introduce how functional devices of vdW materials can be created by modifying the substrate supporting the vdW crystals. I will show two exemplary cases by using semiconducting transition metal dichalcogenides: one with thermoelectric and the other with photoluminescence properties.

KN 07

Development of Inorganic Nanoparticles for Biomedical Imaging

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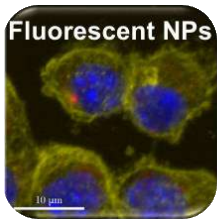
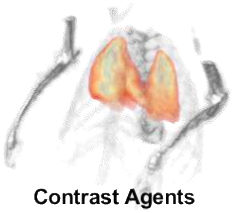
ABSTRACT

Nanoparticles (NPs) have found use in many areas from hybrid materials, to sensors, antiviral/antibacterial coatings and various biomedical applications. Each application area has its own set of NP attributes that has to be complied in order to assure their successful implementation. We have been designing different families of ceramic nanoparticles for a diverse set of biomedical applications, using specifically bottom-up solution chemical techniques. Whenever needed the individual NPs were assembled into larger micron-scale architectures by the use coupling mechanisms using their surface functionality. In this respect, it is of utmost importance to have the right surface chemistry to minimize the number of process steps, in order to reach the desired material attributes. In this talk, I will briefly present the special X-ray fluorescence (XRF) imaging set-up developed for preclinical imaging at KTH. Furthermore, recent activities and materials dedicatedly designed for XRF, starting from the first-generation nanoparticles, to the development of composite and core-shell particles and various surface functionalization schemes will be presented, along with recent results achieved using the developed NPs for in-vitro and in-vivo studies.





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KN 08

Topological Data Analysis: Fundamentals and Use-cases

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ABSTRACT

The past decade has seen rapid changes in the way we collect and analyse data. Concurrently, machine learning and mathematical modelling methods have evolved to handle the complexity and intricacies of high-dimensional data. In this talk, we introduce an increasingly popular approach to study the 'shape' of data and the information this 'shape' contains – topological data analysis (TDA). TDA, whose foundations rest on the mathematical field of topology, refers to a set of tools designed to help summarise and visualise complex data sets[1]. In this talk, we introduce fundamental concepts and intuitions surrounding topological data analysis (TDA). In particular, the talk will begin with key concepts of homology and the Mapper algorithm. Furthermore, we explore some groundbreaking examples on how TDA has been applied in various fields: identifying subtypes of breast cancer[2], roles of players in a basketball game[3], politics in the United States[4]. Finally, we close the talk by giving some results and open questions regarding the use of TDA in the field of materials science[5].

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KN 09

Issues on Substrates for the Thin Film Growth of Hexagonal Boron Nitride by Low-Pressure Chemical Vapor Deposition

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ABSTRACT

There has been increasing interest in hexagonal boron nitride (h-BN), which is a wide bandgap (~ 6 eV) material crystalized in a layered structure consisting of sp2-hybridized atomic sheets of boron and nitrogen, because of its potential use for novel electronics such as Van der Waals heterostructures based electronic devices,[1] deep ultraviolet devices,[2] neutron detectors,[3] single photon emitters[4] and so on. Very thin BN layers grown on sapphire substrates have also proven to be useful as exfoliation layers for GaN-based devices.[5] Thin film growth techniques on large scale substrates for h-BN are essential to further promote the development of such devices. We have grown h-BN films on c-plane sapphire substrates by chemical vapor deposition (CVD) with BCl_3 and NH_3 as sources and characterized their properties.[6-8] The probability of carbon incorporation in the film is expected to be much lower for this carbon-free boron source than for organic boron compounds. So far, we have succeeded in the epitaxial growth of h-BN films, which exhibits pronounced intrinsic excitonic luminescence at room temperature. On the other hand, the type of substrate and their surface condition significantly affect growth behavior and film quality. For example, a notable difference we have found for the growth on a-plane sapphire compared to c-plane sapphire is that the substrate surface is easily nitrided during growth, resulting in the degradation of film quality. However, at growth temperatures, T_g, lower than 1200 °C, the properties of the films on a-plane sapphire were comparable to or even better than those on c-plane sapphire, suggesting that a-plane sapphire is suitable for growing high-quality h-BN films at relatively low T_g. The influences of other factors including surface pretreatment will also be discussed. A part of this work was carried out under the Cooperative Research Project Program of RIEC, Tohoku University.

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KN 10

Regulating Chemoselectivity of Organic Transformations through Electrolysis

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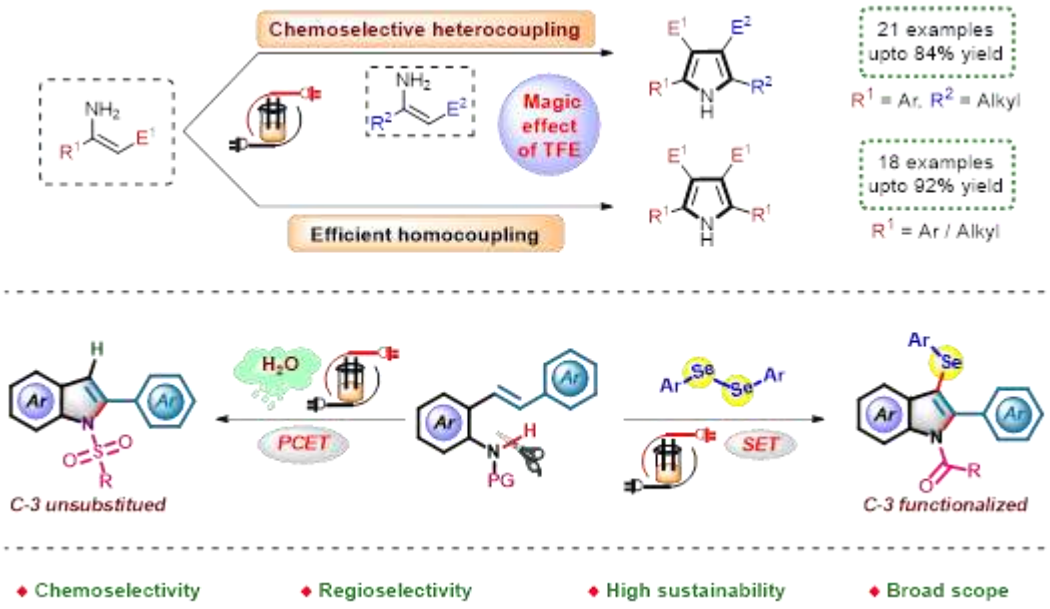
ABSTRACT

Chemoselectivity is a critical concept in organic synthesis, where precise control over the reactions occurring at different functional groups is essential.[1] In the first part of the talk, an electrochemical strategy will be presented for the efficient heterocoupling of aryl- and alkyl-substituted enamines to synthesize tetrasubstituted NH-pyrroles by controlling the reactivity of in situ generated radicals.[2] In the second part, a regio-divergent synthetic approach to access highly substituted indole scaffolds will be illustrated. The developed tuneable electrochemical strategy exploits two analogous styrylaniline precursors and permits nice control on the chemoselectivity over the C-3 substitution pattern, governed by the acidity of the amide proton.[3]



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KN 11

Dopant free c-Si heterojunction solar cells: Prospective and Challenges

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ABSTRACT

In order to achieve the optimal performance to cost ratio, photovoltaic technology requires advances in both production cost effectiveness and device efficiency. The combination of low sheet resistance transparent conducting oxide and doped nano-crystalline silicon layer as carrier selective contacts made it possible for silicon heterojunction (SHJ) solar cells to attain an efficiency of 26.81%, the highest in the world1. Nevertheless, the need for toxic dopants and costly manufacturing processes for device fabrication are creating challenges to the commercial viability of this technology. The aforementioned challenges have prompted researchers to look for dopant-free carrier selective connections (DF-CSC) that require cheaper fabrication processes, as a replacement for doped carrier selective contacts. Transition metal oxides (TMO) with large band gap and variable work function can function as DF hole and electron selective contacts (HSC and ESC)2. Non-stoichiometric MoO3 and V2O5 are being explored as hole selective contacts for c-Si (n) heterojunction solar cells, whereas TiO2 and ZnO are proposed as electron selective contacts. The carrier transport across CSC/c-Si junction is either caused by band to band tunneling or trap assisted tunneling, depending on the work function of CSC and/or the presence of oxygen vacancies, which affect the I-V characteristics and solar cell performance. The talk will focus on the effects of oxygen deficiency and work function on performance of CSC and c-Si heterojunction solar cells. We shall also discuss how the work function of these carrier selective layers can be controlled by choosing appropriate deposition conditions and post-deposition treatments, such as oxygen plasma treatment. Furthermore, the modifications done to improve our MoO_x/c-Si(n) solar cells efficiency from 4.44% to 11.88% will also be covered in this talk.

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KN 12

Anomalous Shubnikov-De Haas oscillations and Room temperature spin polarizations at Oxide interfaces

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ABSTRACT

In recent times, momentum dependent splitting of spin-bands in an electronic system, the "Rashba effect", has gained a lot of interest because of its applications in future generation spintronic devices.[1,2] The Rashba effect is important not only because it has tremendous potential for technical applications, but also because it is a hunting ground for emergent physical properties owing to the linear dispersion relation at the crossing point of the two spin bands.[3] In this work, we present the observation of emergent phenomena arising at the interface of two insulating perovskite oxides due to Rashba spin-band splitting. In our first work, we improvise a novel conducting interface by juxtaposing $KTaO_3$ (KTO) with another insulator, namely $LaVO_3$ (LVO).[4] This heterointerface exhibits strong spin-orbit coupling which is the highest among perovskite oxide heterostructures reported so far. The system is also found to show the signature of topological chiral anomaly via observation of planar Hall effect (PHE) and anomalous in-plane magnetoresistance (AMR) similar to that observed for topological systems. [5] In addition, surprising quantum oscillations have been observed in magneto-resistance. A nonlinear dependence of Landau index as a function of the inverse of applied magnetic field has been observed. In our next work, we show the realization of a spin polarized optically transparent interface. The quest for realizing highly spin-polarized conduction in materials at room temperature is one of the central themes of material physics. We report the realization of a conducting interface of two insulating perovskite oxides namely $LaFeO_3$ (LFO) and $SrTiO_3$ (STO) that demonstrates the signatures of spin-polarization, namely negative magnetoresistance, and anomalous Hall resistivity above 150 K and even up to the room temperature. However, the same system shows positive magnetoresistance and normal Hall effect at temperatures below 150 K. The origin of this could be understood phenomenologically as magnetic proximity and a topological effect of Berry's phase originating from the nonlinear spin arrangement in the system due to thermal fluctuations at high temperatures. In addition, this interface appears to be almost transparent in the entire range of visible light. Our observation is not only of interest to fundamental science but is also viewed as a step towards "room-temperature transparent oxide-spintronics."

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KN 13

Recent advance in photocatalyst for new hydrogen energy source

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ABSTRACT

In recent years, the growing significance of environmental and energy issues has become evident. Amidst this context, one promising candidate as a next-generation environmentally friendly energy source is green hydrogen. Green hydrogen is produced through the photocatalytic process of water splitting using, for example, solar energy. Although this principle is fundamentally based on the Honda-Fujishima effect discovered in Japan in 1972, practical implementation has long been considered challenging. However, recent prototype experiments conducted in outdoor large-scale test facilities[1] have brought a glimmer of hope for its practical application. This presentation focuses on summarizing recent research on photocatalysts, particularly nitride photocatalysts, shedding light on the advancements made towards the realization of green hydrogen production.

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KN 14

Novel plasma-assisted syntheses of functional carbon nanomaterials, their mechanism, and applications

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ABSTRACT

Plasma-assisted techniques are widely used in academic research and industry as a powerful method for thin film deposition and nanomaterial synthesis. However, plasma processes are generally complex processes that involve a variety of active species, making it difficult to elucidate the mechanism and control the process. Efforts have been made mainly in academic research to measure active species in process plasmas and elucidate their generation mechanisms.[1] On the other hand, in recent years, attempts have been made to control this complex plasma process using machine learning approaches. However, since learning models are black boxes, it is difficult to understand their mechanisms of plasma-excited reactions. In recent years, on plasma-enhanced chemical vapor deposition (PECVD) to deposit carbon hard masks for plasma etching, based on active species measurement using quadrupole mass spectrometry and a contribution analysis method based on game theory, we succeeded in quantitatively clarifying the interactions between active species.[2] On the other hand, we have developed a new high-speed synthesis method for functional nanographene materials using gas-liquid plasma with alcohols. Its synthesis mechanism has been clarified by analyzing active species in the gas phase and measuring products in the liquid phase. Furthermore, in the nanographene material synthesized using this method, pyridinic nitrogen is essentially involved in the expression of catalytic activity.[3] In this way, analysis based on active species measurement allows us to scientifically interpret complex plasma processes and lead to innovations in new processes and materials.

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KN 15

Functionalization of Different Phases of 2D-MoS_2 and Related Applications

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ABSTRACT

Two-dimensional MoS_2 nanosheets (2D-MoS_2) have been widely used in many biological applications due to their distinctive physicochemical properties. In the past, it was theorized that chemically exfoliated MoS_2 can be modified using thiol. In this regard, we provide the first experimental evidence for this process using a facile solution based method. We demonstrated the ability to tune the surface of the conjugates for selective enzyme targeting, inhibition and antibacterial activity. Moreover, 2D-MoS_2 generally exists in two different polymorphic structures, metallic (1T phase) and semiconducting (2H phase). The functionalization of 2H phase is even more difficult due to the inertness of the surface. We report a new method for the exfoliation and direct functionalization of 2H-MoS_2. We found that this can be extended to other TMDs. Apart from that, effect of possible ligand exchange on 2D-MoS_2 has never been explored, which can play an important role in diverse biological applications. Recently we have observed the ligand exchange phenomenon on 2D-MoS_2 in presence of different thiolated ligands. We have used that phenomenon for detection of several bio-thiols and drug delivery application. This strategy can be applied to the development of 2D-TMD based materials for various biological applications related to ligand exchange.

KN 16

Nanoparticle translocation across the lung surfactant film: Unravelling Its Mechanism at the Molecular Scale

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ABSTRACT

In the era of nanosciences, the widespread utilization of nanomaterials spans various scientific domains, including cosmetics, electronics, and medicine. The increased prevalence of nanoparticles (NPs) in the environment, particularly those with gold cores (AuNPs), poses a potential health risk due to their interaction with the lungs upon inhalation. While AuNPs have been employed for targeted drug delivery in cancer treatment, their environmental exposure remains a concern. Our work focused on the molecular-scale mechanism underlying the penetration of environmental and engineered AuNPs into the lung surfactant (LS), a crucial first barrier encountered by these particles upon contact with the alveolar surface. The LS monolayer, composed of lipids, four protein types, and other molecules, plays a pivotal role in regulating the entry of NPs into the circulatory system. Despite extensive experimental efforts, a comprehensive understanding of the translocation and permeation of AuNPs into the lung surfactant was lacking. To address this gap, we employed coarse-grained molecular dynamics simulations to investigate the interaction between a model pulmonary surfactant film and AuNPs of varying sizes, shapes, and concentrations. Additional simulations include the presence of cholesterol and proteins SP-B and SP-C to explore their impact on the interaction at the air-water interface. Simulations were performed at the surface tension 0 mN/m and 23 mN/m to mimic lung surfactant during inhalation and exhalation in the presence and absence of AuNP. Various properties of the surfactant monolayer such area per lipid, lateral diffusion coefficients, density profiles, lipid chain order parameter were analysed after the simulation. Analysis of molecular-scale structural and dynamical properties of the surfactant film in the absence and presence of nanoparticles showed how the nanoparticle affects the structure and packing of the lipids and also aggregation of nanoparticles. Our findings shed light on the inhalation toxicity of AuNPs and their potential role in pulmonary diseases, emphasizing the need for caution in designing inhaled nanoparticles to minimize adverse effects. These studies laid the groundwork for future research and design considerations in the development of inhaled nanoparticles with reduced side effects.

KN 17

Electro-optic effect of ferroelectric thin films: strain engineering and exploration of emerging materials

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ABSTRACT

In recent years, novel thin-film-based electro-optic (EO) modulators, which are compact, energy-saving, and high-speed, have attracted a great deal of attention. In such devices, the use of ferroelectric materials, which show large EO coefficients, is preferable compared to that of non-linear polymers from the viewpoint of long-term stability. However, it is widely observed that the EO coefficients of thin, ferroelectric films are often different from those of the bulks, and these origins have not been deeply understood, unlike the ferroelectric and piezoelectric effects. Therefore, the strategy to enhance the EO effect in ferroelectric thin films has not been established yet. In this presentation, we first theoretically and experimentally demonstrate the influence of strain on the EO effect in thin films of classical perovskite ferroelectric (Ba, Sr)TiO_3,[1,2] and discuss the extrinsic contribution, owing to the dynamic domain switching, to the total EO response in classical perovskite Pb(Zr, Ti)O_3 thin films.[3] Then, we explore the EO response in emerging ferroelectric thin films compatible with Si-based CMOS technology. Y-doped HfO_2 thin films showed the evident EO response based on their ferroelectricity,[4,5] and the EO coefficient of Mg-doped ZnO thin films was increased with increasing Mg content and reached 7.6 pm/V, which is over three times larger than the reported values for ZnO-based thin films and over twice larger than that of ZnO single crystals.[6]

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KN 18

Fabrication of High Energy Supercapacitors Using Porous Activated Carbon: A Journey from Lab Scale to Prototype Device

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ABSTRACT

Electrochemical capacitors or supercapacitors has high power density compared to other energy storage devices. It will also reduce the cost of the energy storage device by serving long and delivering high power. However, their poor energy density limits their potential applications in electric and hybrid electric vehicles. Porous carbon and carbon based nanomaterials have been extensively used for electrochemical supercapacitor applications owing to their high surface area. It is also interesting to develop carbon-based nanomaterials with different pore sizes and nanostructured architectures for improved performance in supercapacitors. Various attempts have been made to exploit the porous carbon-based electrode materials for supercapacitor applications and it has been proposed that a combination of mesopores and micropores is essential for high specific capacitance. Though several carbon materials prepared from different bio-waste/sources have been demonstrated for excellent performance in supercapacitors, lack of large-scale preparation with similar electrochemical properties, high production cost, seasonal deviations, and sustainability of the process makes them nonviable for commercial production. CSIR-CECRI has developed a cost-effective large-scale production of supercapacitor grade carbon electrode materials from commercial low-price carbon powders. The present process relates to the design, development, and manufacturing of carbon electrode materials using proprietary high-performance carbon materials. Supercapacitor-grade carbon owns high surface area with good electrical conductivity to perform as an efficient electrode material in supercapacitors. CSIR-CECRI also developed an electrode formulation, and supercapacitor fabrication expertise that can exhibit performance at par with commercial supercapacitor-grade carbon materials. In this presentation, fabrication of 2.7 V, 100 F proto-type supercapacitor devices using the in-house developed carbon material and challenges handled during the lab-scale to prototype fabrication will be discussed.

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KN 19

"A growaste conversion to reactive and functional biochar for biomedical, environmental and energy applications"

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ABSTRACT

Biochar is a porous carbon allotrope obtained by thermochemical conversion of biomass (agrowastes, manure, leather…) under inert or oxygen-deficient atmosphere, in the 300-1000 °C temperature range. Biochar has raised much hope recently and falls into the concept of « *Waste-to-Wealth* ». Indeed, high added value materials could be obtained from biochar, such as pollutant adsorbents, supports for nanocatalysts, porous materials for soil amendment , composite materials for fighting pathogenic micro-organisms, and for energy storage to name but a few. Biochar has been coined « new black gold. Interestingly, biochar particle composition, size and texture can be suitably be controlled with pyrolysis parameters, wet impregnation and loading of nanomaterials within the porous structures. The initial biomass composition has also dramatic effect on the final properties of biochar. In this lecture, we will summarize our research on biochar-based functional materials obtained from a large set of agrowastes such as olive stones, palm wastes, sugarcane bagasse, walnut and peanut shells, millet, marine algae, rose petals and brewer spent grains. We will discuss control over porosity via maceration, grinding, pre-hydrothermal treatment, and wet impregnation. We will then present some interesting applications of biochar as electrode material and adsorbent of perfluorinated compounds (« eternal pollutant »), biochar-based Fenton-like catalysts for water treatment, leishmania treatment using biochar@nanoAg, and CO_2 methanation over biochar@Ni composite catalysts.

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KN 20

Antiferromagnetic topological insulator, $MnBi_2Te_4$ investigated using time domain THz spectroscopy and Pump-Probe Spectroscopy

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ABSTRACT

$MnBi_2Te_4$, an intrinsic antiferromagnetic topological insulator, has garnered significant attention due to its involvement with exotic quantum phenomena such as anomalous quantum hall effect and axion insulator state. The Fermi level of $MnBi_2Te_4$ can be tuned across the bulk band gap via Sb-substitution, yielding phases with enhanced topological functionality and facilitating its implementation in device fabrication. In this study, THz time-domain spectroscopy was employed to investigate $MnBi_2Te_4$ and Sb-substituted $MnBi_2Te_4$ thin films, which were grown using the pulsed laser deposition technique. THz conductivity spectra (in the 0.4-2 THz range) at various temperatures (from 7K to room temperature) were obtained from our measurements. The THz studies indicate metallic behaviour for both samples, while the transport studies reveal a metallic nature for $MnBi_2Te_4$ and a semiconducting nature for $Mn_{1.7}Sb_{0.7}Te_4$. Ultrafast studies on these materials will also be discussed.

KN 21

Designing a greener energy conversion system for a sustainable future

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ABSTRACT

Highly efficient and cost-effective hydrogen production (H_2) promises to play a vital role in green energy production due to its high energy density, low-pollution, and renewable nature. The electrocatalytic decomposition of H_2O to H_2 and O_2 considered to be the most sustainable method for pure H_2 production, unfortunately, it stumbles due to potentially uphill and energy-consuming sluggish anodic oxygen evolution reaction (OER).[1] Contrary to H_2O isostructural hydrogen sulfide (H_2S) possesses lower bond dissociation energy. Therefore, anodic sulfide oxidation reaction (SOR) will be more energy-efficient than OER. Presently, the Claus process is the most popular industrial technology for removing H_2S, but energy wasted in the form of steam. Therefore, electrochemical conversion of environment pollutant H_2S into H_2 and S provide a way to remove pollutant H_2S and also emerges as new energy source.[2] However, the industrialization of such energy-efficient technology never meets the expectation in reality in the absence of cost-effective and robust electrocatalyst. Therefore, talk addresses the non-noble metal based catalyst that exhibited lower onset potential of 0.23 V vs. RHE towards SOR, which is 1.25 V lower than OER. Notably, only a 1.2 V commercial battery easily derives H_2S electrolysis, which is impossible for H_2O splitting demonstrating the tremendous future prospective of H_2S for cheaper hydrogen production for a sustainable economy.

Scheme 1. Schematic representation of H_2S electrolysis into cathodic H_2 and anodic S.

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KN 22

Miniaturization of $BaHfO_3$ flux pinning centers in $YBa_2Cu_3O_y$ superconducting thin film using solution-based metal organic deposition process

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ABSTRACT

$REBa_2Cu_3O_y$ (REBCO, RE = rare earth elements such as Y, Gd, Eu so on) coated conductors (CCs) have been considered as the prime materials for the electric power applications as extremely strong coil, due to its high current properties. Metal organic deposition (MOD) is the most low-cost process to fabricate REBCO-CCs because of its inexpensiveness, high material yield and facileness. The composition of starting solution of MOD can easily be controlled, so that to introduce artificial pinning centers (APCs) into REBCO thin films, for the enhancement of critical current density (Jc) in magnetic fields. In this work, YBCO films with $BaHfO_3$ (BHO) particles as APCs were fabricated by the MOD and the influences of heat-treatment profile on particle size of BHO were investigated. The starting solution was prepared by dissolving Y and Ba-trifluoroacetates, and Cu-octylate in the organic solvent with the Hf salts of 1 mol%. The solution was deposited on two $CeO_2/LaMnO_3/MgO/Gd_2Zr_2O_7$/Hastelloy substrates using a spin-coating method. The coated films were calcined at 703 K in a humid oxygen atmosphere to obtain the precursor films. After the cooling of precursor films, one sample was crystallized by a constant heating rate until 1053 K and keep the temperature for 150 min, the other one was done by additional heating process at 823 K in prior to the above constant heating rate process. As a result, particle size of BHO was miniaturized in the film prepared with additional heating process than the one prepared without additional process. Then, in-field Jc of the film was increased more than 50% at 77.3 K in 3 T, after the introduction of additional heating temperature. Acknowledgement This work was supported by JSPS KAKENHI grant numbers 22H0219, Japan.

KN 23

Materials Fabrication of Microalgae Oil Drug Delivery Carriers

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ABSTRACT

Microalgae oil is abundant in fatty acid components and is used in health products. It has been reported drug delivery carriers were possible to be fabricated from fatty acids. To develop drug delivery systems from microalgae oils will be able to expand high-value applications of microalgae biomass. By using microalgae oil as the raw material, a forced formation process was developed. The applicability of the vesicle formation process was then demonstrated by using microalgae oils with different fatty acid compositions. For microalgae oils, a stable vesicle dispersion with single size distribution and negative zeta potential could be fabricated by applying the vesicle formation process. The negative zeta potential of the vesicles was most likely caused by partial dissociation of the fatty acid components in the microalgae oils. Comparatively, the bilayer structure of microalgae oil vesicles was more fluidic or flexible than that of traditional phospholipid vesicles. This could be attributed to unsaturated structures of some fatty acid components in the microalgae oils. The existence of aqueous cores/regions in the microalgae oil vesicles was confirmed by encapsulation capability for a hydrophilic model material. By encapsulating a hydrophilic material, the size, zeta potential and bilayer fluidity of the vesicles were almost unchanged. This can be expected for encapsulation of a hydrophilic material by aqueous cores/regions of the vesicles. The capability of the microalgae oil vesicles to encapsulate hydrophobic materials was demonstrated by using lutein and curcumin as the model materials. The average diameter of the vesicles was apparently increased after encapsulating a hydrophobic material, and the bilayer structures became ordered or rigid after the encapsulation. However, the vesicles still possess high stability. In summary, microalgae oil can be used as a raw material to prepare vesicle structures with the potential of being applied as delivery carriers.

KN 24

Integrating High Throughput Screening and Machine Learning

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ABSTRACT

Porous materials especially, coordination polymers (CP) or metal-organic frameworks (MOFs) have emerged as a special class of hybrid nanoporous materials. The variation of metal oxides and the vast choice of controllable organic linkers allow the pore size, volume and functionality of MOFs to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new functional materials and are considered as versatile candidates for storage, separation, sensing, catalysis, drug delivery and other important applications. With ever-growing computational resources and advance in mathematical techniques, molecular simulations have become an indispensable tool for materials characterization, screening and design. At a molecular level, simulations can provide microscopic insights from the bottom-up and establish structure-function relationships. This presentation will highlight on how molecular modelling combining with machine learning approach can a powerful tool in complementing experiments and thus aid in designing of new smart porous materials for storage, sensing, catalysis and separation applications. 1-5.

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KN 25

Designing Graphene Quantum dots and their Photo-response

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ABSTRACT

We discuss the tuning of the photo-response and electronic behaviour of graphene quantum dots (GQDs). Prepared by the process of ion irradiation of monolayer graphene, the results display a method that can be useful in designing GQD based photodetectors without incorporation of any metal-nanoparticles. Ion energy is a crucial parameter that can be used for effectively modulating many characteristic properties of GQDs. These results can be significant in designing conjugated Visible and UV range photodetectors from graphene quantum dots.

KN 26

Nano Cellulose from Waste for Energy Applications

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ABSTRACT

Sustainable energy generation for the net zero applications are prime focus of the "Sustainable Energy Materials" group in the Teesside University. The focus of the research is to obtain net zero capacity in materials, devices, and systems development. The major focus of the group is to innovate materials, applying circular economy concepts for Energy-Food-Water-Healthcare nexus problems and extending its impact towards society. The use of sustainable materials as alternatives to fossil fuel derived materials is vital to tackle the current environmental challenges. Cellulose, as a naturally occurring polymer, is a good candidate for the above endeavour due to its excellent intrinsic properties. When considering the sources used for processing cellulose materials, it is wise to consider waste materials that are rich in cellulose content, rather than using high-grade resources like wood; integrating with the concept of circular economy to address environmental and economic challenges from the waste, as well as provide a sustainable solution of processing environmental-friendly materials. This work innovates the upscale of cow slurry collected from local dairy farm as a feedstock to process nanocellulose using a combined chemical and mechanical method. The resultant materials were characterised using various method to proof that such a circular economical method is a practical solution to provide abundant source for nanocellulose processing, as well as mitigate the environmental issues of farm animal waste.

KN 27

Electrochemical sensors for sustainable agriculture: trends and challenges

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ABSTRACT

The field of electrochemical sensors in sustainable agriculture is experiencing significant innovation growth driven by the need for more efficient and environmentally friendly farming practices [1]. Research is focused on making these sensors more affordable and scalable for widespread use, especially in developing countries where sustainable agriculture is crucial for food security. The ultimate goal is to take advantage of the sensitivity, selectivity, and portability of these devices to enable: i) climate monitoring by tracking parameters such as temperature and humidity, which give crucial information for planning the best times for planting and harvesting; ii) early detection of plant health issues before they become visible to the naked eye, iii) precision agriculture where inputs like water, fertilizer, and pesticides are applied in exact quantities needed by crops, and iv) detection of contaminants such as heavy metals and pesticides to maintaining soil quality and promote sustainable agricultural practices [2-3]. Trends in electrochemical sensors for sustainable agriculture concern: i) the use of nanomaterials, like graphene, carbon nanotubes, and metallic nanoparticles, to enhance the sensitivity of these devices and reduce their limit of detection [4], ii) the integration of electrochemical sensors with wireless networks which can continuously monitor various parameters like pH, moisture levels, and nutrient content, and transmit real-time data for analysis [5]. The large amounts of data generated by electrochemical sensors can be analyzed by artificial intelligence to predict models for crop management and early warning systems for potential issues like nutrient deficiencies or pest infestations, iii) and the use of wearable sensors able to on-site quantification of harmful substances concentrations, and to determine in a rapid way if regulatory thresholds are exceeded [6]. Beyond monitoring, electrochemical sensors play a vital role in advancing environment-friendly farming practices, reducing the use of chemical fertilizers and pesticides, and promoting organic farming methods.

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KN 28

κ-Al_2O_3-type ferroelectrics

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ABSTRACT

Perovskite type structured ferroelectric materials such as $BaTiO_3$ and $Pb(Zr,Ti)O_3$ and related compounds have been used for memory, sensor, and various applications since they are found around 70 years ago. Since Perovskite-type ferroelectrics are found, they have been used until now because of their superior ferroelectric and piezoelectric properties. To evolve forward from this situation, we would like to suggest novel ferroelectric/ferrimagnetic ferroelectric which has κ-Al_2O_3-type crystal structure classified as polar $Pna2_1$ space group. This structure consists of the corundum-type and spinel-type staking layers along c-axis. The corundum and spinel layers consist of only oxygen-octahedra, and mixture of oxygen-octahedra and oxygen-tetrahedra, respectively. The spontaneous polarization direction is c-axis. It is note that coordination recombination from octahedra to tetrahedra (6 to 4) and tetrahedra to octahedra (4 to 6) in spinel layer is occurred during polarization switching. At the same time, corundum layer moves right and left alternately along in-plane a-axis which is like shear motion. This polarization switching system is optimized by the first principal calculation. However, almost all of the materials with κ-Al_2O_3-type crystal structures are metastable phases, which makes it difficult to prepare conventional techniques in chemical equilibrium. Here, we succeeded in preparing this structure's materials through the physical vapor deposition technique.[1-9] We would like to introduce ferroelectricity of this material's family.

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KN 29

Green Chemistry and Heterogeneous Catalysis for Energy and Environmental Applications

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ABSTRACT

Energy crisis and environmental deterioration has emerged as major problems around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of solar energy to produce chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. Our research group has recently developed several two-dimensional materials supported nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles, which can utilize the full solar spectrum from ultraviolet to infrared regions for energy generation and environmental remediation applications. In addition to photocatalytic hydrogen generation, nitrogen fixation and pollutants degradation, our group has also utilized these materials for biomass valorization, carbon dioxide conversion and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research works of our group will be presented.

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KN 30

Integrated light harvesting systems for scalable artificial photosynthesis

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ABSTRACT

Photoelectrochemical (PEC) artificial leaves can lower the costs of sustainable solar fuel production by integrating light harvesting and catalysis within a compact panel.[1] However, most prototypes can only perform water splitting over a few hours on a cm^2 scale, whereas conventional light absorbers limit solar-to-fuel efficiencies and product rates.[2,3] Here, we explore alternative routes to expand the performance and functionality of PEC devices, by designing integrated systems which benefit from unconventional materials and complementary energy harvesting. To this end, we first demonstrate the fabrication of lightweight artificial leaves by employing thin, flexible substrates and carbonaceous protection layers,[4,5] which are compatible with modern fabrication techniques.[6] These materials allow 100 cm^2 perovskite-$BiVO_4$ artificial leaves to float along River Cam (UK), showcasing the potential of floating solar fuel farms.[5] The same carbonaceous protection layers can be employed to increase the moisture stability of an underexplored BiOI photocathode from minutes to >500 h, whereas a pixelated design provides the additional photovoltage required for unassisted water and CO_2 splitting.[7] Product rates can be significantly boosted by integrating PEC devices onto thermoelectric (TE) generators, which harvest waste heat from thermalisation and IR photons.[8,9] Accordingly, a Pt-TE-$BiVO_4$ device can already yield unassisted water splitting under 2 sun irradiation, while the photocurrent of a Pt-perovskite-TE-Fe_2O_3 device is boosted 30-fold under 5 sun irradiation.[9] Further up-scaling of PEC systems towards m^2 areas can be performed by taking advantage of the modularity of artificial leaves,[10] however, manual fabrication must be replaced by high-throughput techniques for large scale applications.[6]

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KN 31

Ultrasonic synthesis of functional materials

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ABSTRACT

The interaction between sound waves and microbubbles in solutions generates acoustic cavitation, the growth and collapse of bubbles, under certain experimental conditions. The near adiabatic collapse of microbubbles during acoustic cavitation generates local temperatures as high as 5000 °C, and local pressures of the order of 500 atmospheres. Under such extreme conditions, light emission (sonoluminescence) and chemical reactions (sonochemistry) occur. Sonochemistry is an evolving area in science and has the potential for many applications (Figure 1). Sonochemically generated radicals, such as OH and H can be used for a variety of redox reactions. Syntheses of metal, semiconductor and polymer nanoparticles are some of the potential applications of sonochemistry.

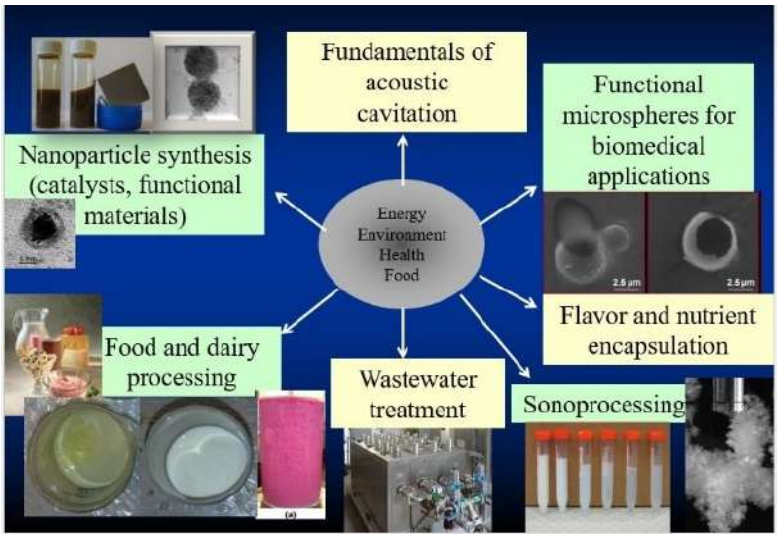

Figure 1: Applications of ultrasonics and sonochemistry

For example, the reducing radicals generated during acoustic cavitation have been used to synthesise metal and other inorganic nanoparticles and the oxidising radicals have been used to generate oligomeric structures from simple organic molecules that ultimately form nanoparticles with fluorescence properties. The fundamental aspects of ultrasonics and sonochemistry and their application in nano and functional materials synthesis will be discussed.

KN 32

First principles methodologies for Probing interfacial interactions and applications

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ABSTRACT

We use first principles methodologies to characterize and to probe the interfacial interactions occurring at solid – liquid and gas – solid and gas – liquid interfaces. We thus determine the equilibrium structures of the interacting entities and their binding energies or adsorption energies. Diverse analyses are performed to probe the intermolecular van der Waals interactions, the charge transfers and the induced spectroscopic shifts (both vibrational and electronic). We show that these effects, either of weak magnitudes, are crucial to activate molecules and to transform them in value-added products. For illustration, we will present several examples covering the fields of CO2 activation, gas sequestration by porous materials, proton transfer induced catalysis.

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KN 33

Applications of III-V semi-insulating materials for discrete and integrated photonic devices

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ABSTRACT

Realization of silicon integrated circuits was feasible mainly due to the native oxide of silicon, silicon dioxide, which is extremely insulating and thereby imparts electrical isolation between the adjacent components. There exists no such resistive native oxide of III-V semiconductors to facilitate similar integration feasibility. To overcome this, semi-insulating III-V semiconductors come to help. These are the III-V semiconductors doped with deep acceptors or deep donors that can quench the residual acceptors or holes, respectively. These are highly resistive materials and hence can be used for integration of III-V devices. When employed in buried heterostructures (BH) as current blocking layers, these also enhance heat dissipation and at the same time reduce the capacitance of the whole chip leading to high-speed modulation. We have employed Fe as the deep acceptor in InP, GaAs, $Ga_{0.51}$ $In_{0.49}P$ (lattice matched to GaAs) and GaN to impart insulating properties [1-3]. $Ga_{0.51}In_{0.49}P$ has been used as the current blocking layer in GaAs based BH in-plane (λ = 808 nm) and vertical cavity surface emitting (λ = 850 nm) lasers [4-5]. Similarly, InP:Fe has been used to fabricate BH telecom lasers emitting at 1.55 µm for high speed modulation [6] as well as BH quantum cascade lasers (BH-QCL) in the mid-IR range for high power [7-8] and free space communication applications [9]. Several types of BH-QCL designs to improve thermal dissipation have been proved to be successful. The usefulness of InP:Fe has also been demonstrated for photonic integration in a vertical integration of an InGaAsP/InP HBT and a 1.55 µm strained MQW p-substrate laser [10], in an Optical Code Division Multiplex Access (OCDMA) system [11] and in an Optical Arbitrary Waveform Generation (OAWG) system [12].

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KN 34

Aqueous Rechargeable Zn Batteries: Anode and Cathode Engineering

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ABSTRACT

The aqueous zinc-based energy devices are emerging as an ideal candidate to store the renewable energy resources and to power portable electronics, electric vehicle, etc.[1] The rechargeable zinc-ion batteries (ZIBs) are very promising as Zn has high theoretical capacity (820 $mAhg^{-1}$) and low reduction potential (-0.76 V vs SHE). The dendritic growth at anode and structural instability of cathode are some the concerns that limits the charge storage performance. Rationale engineering of anode as well as cathode is desired to improve the capacitive performance and cycling stability. We demonstrate the anode engineering of ZIB by artificial solid-electrolyte interface based on hybrid polymeric materials and the development of stable cathode by defect engineering.[2] The defect engineered ternary spinels $ZnMn_2O_4$ and ZnV_2O_4 deliver high specific capacity and has outstanding cycling stability. The fabricated $ZnMn_2O_4$||Zn full cell delivers a specific capacity of 265 $mAhg^{-1}$ (at 100 mAg^{-1}) and has long cycling stability without any capacity loss. On the other hand, specific capacity as high as 599.6 $mAhg^{-1}$ (at 100 mAg^{-1}) is achieved with ZnV_2O_4||Zn. The mechanism of charge storage is established with operando and density functional theory calculations. The recent progress on the engineering of cathode and anode will be discussed.

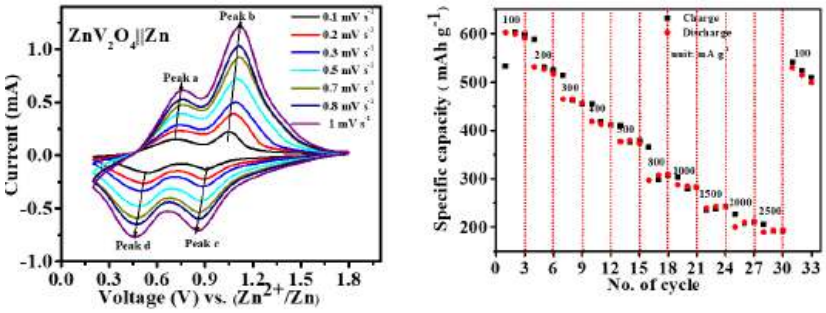

Figure 1. Cyclic voltammetric profile and plot illustrating the rate capability of ZnV2O4||Zn.

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KN 35

Wearable sensors for health care and aged care

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ABSTRACT

Imagine wearable sensors which you place on your skin – this band-aid like patch could measure your body parameters offering you a window to your health. Imagine nearable sensors embedded into a mattress cover which can non-invasively track a person's presence, position, and posture in bed overnight in residential aged care facilities. These nearable and wearable sensors are conformal, un-feelable and unbreakable. I will present the fundamental research and breakthroughs which has led to these technologies and the research challenges overcome. Following this, our collaborative efforts to translate and commercialise with industry, manufacturing and design partners will be highlighted .

KN 36

A Novel Thin film based μ-3D Printer for Printing Micro Scale Structures for MEMS Applications

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ABSTRACT

The majority of the microelectromechanical (MEMS) devices are fabricated using either a lithography process or some microfabrication system which goes through the phase change process during the fabrication process. The phase change during processing leads to the change in the chemical as well as the functionality of the fabricated devices hence it is essential to develop a process which retains the chemical and functionality of the structure before and after the fabrication process. The research work focuses on the development of a laser decal transfer-based micro 3D printing process by using a thin film as feed material for the printing of MEMS devices. In laser decal transfer, the thin film material is deposited on the sacrificial layer coated transparent substrate and the laser beam irradiates from the top of the transparent donor substrate. The laser energy gets absorbed in the sacrificial layer and vaporizes to form high-pressure gas. The high pressure tries to expand and apply a pressure force on the donor thin film that leads to the ejection of the thin film from the donor substrate and collected on another substrate. Since the laser spot size and the donor thin film are in the order of a few microns, the feature size will be the same. To fabricate micro-scale three-dimensional structures, the laser decal transfer process will be continuing to build pixel-by-pixel and layer-by-layer fashion for the fabrication of the microscale MEMS devices. The process involved a high energy density laser heat source as the driving force for the printing process hence a numerical simulation is performed to investigate the effect of laser interaction with material and estimate the temperature rise during the fabrication process. Moreover, the process involved the absorption of laser energy and leads to the formation of a plume beneath of thin film. The numerical simulation predicts the shape and size of the plume before the material ejection 2 from the donor substrate and the same is monitored using a high-speed camera using time resolve imaging technique. At last, Laser micro3D printing is deployed for the fabrication of the different microelectronics devices which can be used for different electronics circuits such as a microheater, antenna, etc. To shows the capabilities of micro 3D printing, multiple-layer NiTi-based stain gauge are printed on flexible PET sheets and performance were investigated at different loading conditions. For three-dimensional strain measurement, a rosette strain gauge is also printed, and its performance is measured at different strain conditions using the universal testing machine. To check the feasibility of the process towards device fabrication, the ZnO nanostructure was transferred on the PET sheet and its performance was investigated before and after the printing process for opto mechatronics applications. The process involved micro features printing on a substrate which can induce the roughness of the substrate, hence the micro 3D printing is performed to print the ZnO seed layer in a line pattern followed by the hydrothermal growth for the triboelectric nanogenerator for energy harvesting applications.

KN 37

Defect and interface engineering to realize high performance thermoelectric materials and power generators

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ABSTRACT

Thermoelectric generators (TEGs) are devices that convert temperature differences into electrical energy through a phenomenon known as Seebeck effect. TEG provides one of cleanest energy conversion method, which is noise-free, virtually maintenance free and can continuously produces power for several years. In recent years, energy generation through thermoelectric harvesting has witnessed an increased interest for various applications, including tapping waste heat from the exhaust of vehicles, from industries, radioisotopes etc. The development of an efficient TEG requires the fulfillment of several factors, which includes availability of n- and p-type thermoelectric materials with high figure-of-merit (ZT), preparation of Ohmic contacts between thermo-elements and metallic interconnects and management of maximum heat transfer though the device. From materials perspective the key parameter for obtaining high conversion efficiency is figure-of-merit i.e. $ZT = (S^2\sigma/k)T$, where S, σ, k, and T are respectively, Seebeck coefficient, electrical conductivity, thermal conductivity and temperature. For a given thermoelectric material S, σ and k are interdependent and therefore their ZT is limited to ≤ 1. One of the challenges to maximize ZT of a material is to lower down its κ without reducing the power factor ($S^2\sigma$), which can be achieved by designing a material that allows facile transport of charge carriers but blocks phonon flow. In this talk an overview on the various aspects of TEG development and deployment will be discussed, which includes synthesis of high ZT thermoelectric materials, creating electrical contacts with low specific contact resistivity and essential interfacial electronics required for the deployment of TEG for the field applications.

KN 38

Simultaneous control of carrier and phonon transports in nanostructured thermoelectric films with the controlled interfaces

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ABSTRACT

Thermoelectric films are drawing much attention as a stand-alone and small power source. The thermoelectric conversion efficiency monotonically increases with a dimensionless figure-of-merit ZT; $ZT=S^2\sigma T\kappa^{-1}$, where S is Seebeck coefficient, σ is electrical conductivity, κ is thermal conductivity, and T is absolute temperature. Simultaneous realization of high $S^2\sigma$ and low κ has been difficult because of trade-off relationship among the three parameters. Previous studies have mainly utilized heavy element-based materials with intrinsically-low κ. However, these elements are not suitable to industrial application because of toxicity and expensiveness [1, 2]. On the other hand, light element-based materials, which are non-toxic and low-cost, have low ZT because of high κ. In 2000s, nanostructuring approaches were spotlighted because the nanostructured interfaces intensified phonon scatterings, reducing κ. These outstanding approaches allowed us to reduce κ even in light element-based materials [1]. However, carriers are also scattered at the nanostructured interfaces, resulting in κ reduction. For simultaneous realization of high $S^2\sigma$ and low κ, the interfaces enabling the phonon scattering and the carrier transmission are required. We have developed nanostructured thermoelectric films with the controlled interfaces [3-5]. For example, by engineering nanostructure domains of SnO_2 films on the basis of the symmetry of crystal structure, high σ and low κ were simultaneously realized [4]. This domain engineering was also applied to GeTe film [5], indicating that domain engineering is universally applicable approach. This talk will discuss the interface control based on the film growth technique and its influence on thermoelectric properties.

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KN 39

Advancing Green Technology: -Exploring Polymer-Based Electrochromic Windows for Sustainable Energy Efficiency

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ABSTRACT

Over the last decades we have observed a substantial increase in energy demand. This calls for an increased use of renewable energy and energy-efficient technologies. Electrochromic devices will find a wide range of applications in smart windows for energy-efficient buildings, low-power displays, self-dimming rear mirrors for automobiles, electrochromic e-skins, and so on. Electrochromic devices generally consist of multilayer structures with transparent conductors, electrochromic films, ion conductors, and ion storage films. Synthetic strategies and new materials for electrochromic films and transparent conductors, comprehensive electrochemical kinetic analysis, and novel device design are areas of active study worldwide. These are believed to be the key factors that will help to significantly improve the electrochromic performance and extend their application areas. The building sector is responsible for 10% of the total energy consumed. Smart windows, electrochromic devices offer great potential for the fabrication of cheap, smart, switchable, and energy-efficient architectural fenestration. A highly transparent low cost stable electrochromic devices were explored by using a high contrast electrochromic polymer (ECP).

KN 40

Modulating cell-surface interactions through electroactive materials

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ABSTRACT

The development of electroactive organic materials has been an unquestionable breakthrough for organic electronics, allowing for the design of polymer-based electrochromic and optoelectronic devices. Electroactive materials have been also considered as promising in the wide-field biomedical engineering, particularly considering their similarity with a living tissue in terms of elemental composition, surface morphology and mechanical properties. The aim of this talk is to present recent achievements of the Bioelectrochemistry Group to develop biocompatible, antibacterial and electrically conducting biomaterials based on conducting polymers and diazonium-derived electroactive monolayers. With the use of electrochemical techniques, we have fabricated a library of electroactive materials with various physicochemical characteristics, differing in the way how they interact with a living matter. Unique combination of biological activity of developed materials with their electroactivity allows for further enhancement of their *modus operandi*, through the possibility of applying electrical stimulation to facilitate treatment.

KN 41

Sublattice distortion controlled electronic and optical properties of $Cs_2B'B''X_6$ (B' = Ag, Na; B'' = Bi, In; X = Cl, Br) double perovskites

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ABSTRACT

Halide perovskites have attracted the materials research community for their intriguing optical and electronic properties. However, due to the material instability and toxicity issues, it is highly desirable to explore functional analogs which are stable and non-toxic, while retaining the structural attributes. Lead-free halide double perovskites have been considered as promising alternative to lead-halide single perovskites for photovoltaics and optoelectronics. However, due to larger bandgaps, their applicability is limited. We demonstrate that in lead-free $Cs_2Ag_{1-x}Na_xBiCl_6$ (x = 0 to 1) alloys the difference in the ionic radii between Ag^+ and Bi^{3+} lead to octahedral mismatch and induces sub-lattice distortions in the lattice which imparts bandgap bowing effect in HDP. The bandgap is shown to vary from 3.01 eV to 2.64 eV as Na^+ at B' site gets replaced with Ag^+ cation. A strong correlation among the bandgap variation, Raman mode frequency shift due to sublattice distortion, Raman peak width and the ratio of intensities of Raman modes show the role of sublattice distortions on the bandgap behaviour as a function of Na substitution concentration (x). Further, sublattice distortion also influences self-trapped excitons (STE) photoluminescence emission. The end members show negligible photoluminescence, whereas double perovskite alloys exhibit broad photoluminescence. Change in sublattice distortions are shown to play significant role in the formation and recombination of STEs. The STE emission intensity and quantum yield greatly depend on x, with highest intensity observed for x = 0.75, consistent with a large change in sublattice distortion observed at this x. Variation in photoluminescence properties with composition follows a similar trend as that of bandgap and phonon vibrational changes observed due to sublattice distortion. Temperature dependent phonon vibrations and photoluminescence studies reveal a giant electron-phonon coupling. A strong synergy between STE emissions, electron-phonon coupling, bandgap, and phonon vibrations in double-perovskites with sublattice distortions is revealed through this work. Finally, we also shown how to infer the presence of sublattice distortion by monitoring the asymmetric stretching vibration modes (Eg) in Raman spectra of wide range of double perovskites.

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KN 42

Control of the Coating Structure on a Cathode Particle for Li-ion battery

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ABSTRACT

Coating of Li ion conductors on cathode particles is indispensable not only for all-solid-state Li-ion batteries but also for those employing liquid electrolytes [1]. However, there are various reports discussing the optimal structure of the coating layer for these demands. In this presentation, we introducea nanocoating process for Li-ion conductors on cathode particles using chemical reactions and deposition phenomena. In our previous study, our research group demonstrated that the coating structure can be controlled by manipulating key process parameters, including electrostatic interactions [2]. Consequently,this presentation serves an example for material development in the realm of Li-ion batteries based on thistechnology. As an example, Figure 1 elucidates TEM+EDS results, portraying the uniform oxide-based Li-ion conductor coating on the cathode particle's surface. Furthermore, this presentation delves into the impacts on cell properties when employing nano-coated cathode particles, showcasing an array of structures prepared using this technique, all within the context of a Li-ion battery system.

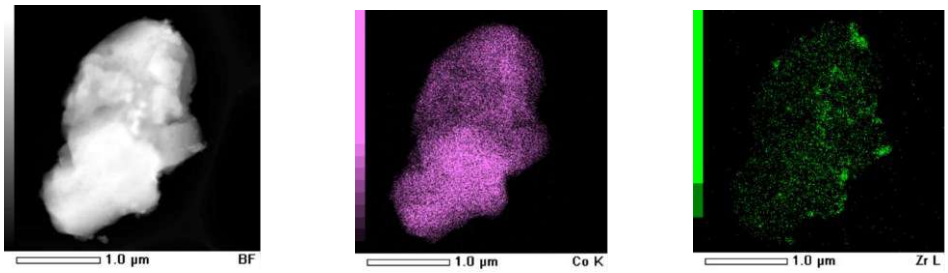

Fig.1 TEM+EDS analysis for $Li_7La_3(Zr_{1.75}Ta_{0.25})O_{12}$ coated $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ particle. Co: core part,Zr: Shell part

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KN 43

Single Crystal Diamond Photon-Counting X-ray Imaging device

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ABSTRACT

In an exploration of diamond's utility in high-dose radiation measurements due to its radiation tolerance, researchers have developed a pixelated diamond detector for X-ray detection. Taking advantage of diamond's close atomic number to human tissue, which ensures similar radiation absorption rates, this study exploits the material's ability to convert X-ray photons into electron-hole pairs, ensuring high spatial resolution. The detector uses single-crystal diamond grown by chemical vapour deposition (CVD), specifically heteroepitaxial diamond grown on sapphire substrates. The detector architecture includes a 3mm x 3mm x 0.5mm crystal with indium film electrodes and a photon and charge counting application specific integrated circuit (ASIC) that digitises the charge of X-ray photons across a matrix of electrodes covering the same area as the crystal. Operating at a bias of -500 V and a frame rate of 200 Hz, the imaging capabilities of the system were tested with an X-ray tube set at 100 kV and placed 20 cm from the detector, supplemented by lead plate shielding. The empirical results indicate that the diamond crystal is solely responsible for detection, and although improvements in image quality are required, the initial results are promising. The study concludes with a positive outlook on the applicability of the pixelated diamond detector in X-ray imaging, supported by the satisfactory performance of the current technology.

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KN 44

Ferromagnetic Properties of Zinc and Magnesium Ferrite Prepared by MOD Technique

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ABSTRACT

Zinc ferrite (ZnFe2O4 : ZFO) is known for antiferromagnetic materials and Magnesium ferrite (MgFe2O4 : MFO) is known for ferromagnetic materials at room temperature1), however, the sputtering technique or PLD technique have reported the possible preparation of ferromagnetic ZFO at room temperuture2,3). The ferromagnetic ZFO or MFO are an attractive material for new magneto-optical devices because they show transparency in short wavelength region of the visible light. This property compensates the poor transparency of magnetic garnet materials in the short wavelength region. In this report, we have investigated the preparation of ferromagnetic ZFO, MFO and their mixed crystal with the metal organic decomposition (MOD) technique and have compared the detail magnetic properties depending on crystalizing conditions. The thicknesses of the prepared the films were approximately 250 nm and the spinel single phase was confirmed by the XRD analysis. The saturation magnetizations Ms of the ZFO films were depend on both the annealing temperatures and the annealing time, whereas the coercive force Hc indicated approximately 700 Oe for the all ZFO specimens. The valence of the Fe ions in ZFO was confirmed only 3+ by the Mossbauer spectroscopy. The Curie temperature was estimated to be of approximately 190 K. The hysteresis magnetic curves showed that the MFO films were ferromagnetic at room temperature. Both Ms and Hc of the films depend on the annealing temperatures and time and they have trade-off relation. The Hc of the film annealed at 510 degreeC was approximately 2 kOe and the film annealed at 900 degreeC was approximately 60 emu/g.

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KN 45

Nonthermal plasma assisted CO_2 conversion to value-added chemicals

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ABSTRACT

CO_2 conversion to value added chemicals was carried out in a catalytic DBD plasma reactor. The integration of heterogeneous catalyst in plasma improves the value-added products selectivity. Typical results indicated that the modified Al_2O_3 catalyst (Metal loading of around 5.0% - 20%) combined with plasma provided the best performance. The physiochemical properties of the prepared catalysts as well as the spent catalysts was done by PXRD, spectroscopy (Emission, XPS), BET, TGA, SEM and TEM. Conventional methods of CO_2 conversion methods such as thermal decomposition, require higher temperature (3000K-3500K). As CO_2 is a highly stable and inert molecule, the process of CO_2 activation requires a significant amount of energy to overcome the kinetic inertia and thermodynamic barrier. Recently, non-conventional methods such as non-thermal plasma (NTP) have gained much attention for CO_2 conversion. NTP technology provides a promising alternative solution for converting CO_2 into value-added fuels and chemicals at ambient conditions. In NTP, the electron temperature is higher than the gas temperature. Reactor outlet gaseous molecules are analyzed by gas chromatography. Initially, reaction performs with a DBD reactor without catalyst and same reaction performs with Ni/Al_2O_3 catalyst. The role catalyst improves the reaction performance, due to the synergistic effect between the plasma and catalyst. We performed a reaction with 70 mL/min CO_2 and CH_4 are 1:1 ratio. At maximum applied power ~ 2.1 W, the conversion of CO_2 and CH_4 are 7.5% and ~10% with no packing and 21% and 24% respectively with 15 wt% Ni/Al_2O_3 packing respectively. The syngas ratio ~1.0 and ~ 1.6 with no packing and Ni/Al_2O_3 packing respectively.

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KN 46

Photoelectrochemical Etching of III-Nitride Semiconductors for Nanostructure Fabrication

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ABSTRACT

Gallium nitride (GaN) has wide direct bandgap, high breakdown electric field and high saturation electron velocity. Based on these excellent material properties, significant progress has been made in devices based on GaN and III nitrides, such as laser diodes, light-emitting diodes, and high-power and high-frequency transistors. Furthermore, GaN and its alloys have attracted attention as building block materials for electrochemical (EC) energy conversion systems because of their excellent chemical stability and the ability to widely tune the band gap through alloying. Plasma-assisted dry etching have been commonly used to fabricate nitride semiconductor devices. However, various types of damage and defects induced by the plasma cause serious problems in the operational stability of GaN-devices. Photoelectrochemical (PEC) etching can solve these problems; PEC etching is a low-damage process that can be performed at room temperature and has significant advantages, including the ability to electrically control etching depth. In this talk, I will present our recent work on nanometer-order precisely controlled PEC etching of III nitride semiconductors by changing PEC etching properties such as smooth and porous etching. The porous structures formed by this method have attractive features such as high specific surface area and low reflectivity due to the densely arranged pores [1]. In addition, they are more productive than other nanostructure fabrication techniques because they do not require complex processes such as lithography. On the other hand, under smooth etching conditions, a flat etching surface with an rms roughness of less than 1.0 nm was obtained [2]. I would like to present an example of application of this etching technique to GaN-based transistor fabrication.

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KN 47

Productizing Nanostructured Functional Bioactive Materials for Advanced Healthcare Hemostats and Tissue Regenerative aids

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ABSTRACT

Considering their numerous applications in the form of scaffolds, foams, hydrogels, thin films, and other materials, as well as their health benefits, Bioactive materials are extremely admired in the medical field. Many patients are partially or completely recovering from implantations as well as from the routine replacement of fracture plates, screws, sutures, and other components due to the growing progress in bioactive material production methodologies and technologies. Biomaterials whose ability to regenerate bone via the formation of hydroxyapatite primarily depends on processing conditions. Our 70% of the bone weight comprises hydroxyapatite said to be a natural bone mineral. If a technology can be efficient in developing bio-materials with higher compatibility that could mimic natural bone, then it is worth it to mean that biomaterials are leading mankind to heaven. The biological function of biomaterials especially hydroxyapatite and bioactive glass are highly phase dependent. While synthesizing the bioactive materials, not only size matters. Various types of morphology, phase formation, facet setting, pH, room temperature, precursors, etc., everything matters. This greatly influences the biological and mechanical properties of the products which some researchers ignore to focus. Combeite ($Na_2Ca_2Si_3O_9$) is one of the high-temperature commonly occurring phases in the bioactive glass. This is considered to be one of the stable phases of bioactive glass where extraction as a single phase is highly troublesome via the sol-gel route. The behavioral nature of this common phase is studied and the importance of phosphate species on the crystal system is also investigated. Similarly, in hydroxyapatite synthesis, Monetite is an additional phase that occurs with hydroxyapatite phase. The ratio of phase and evolution of morphology is highly pH-dependent. Various benefits of the Monetite phase came to light through this study. Also, the nature of Equimolar Ca:P phase bioactive materials subjected to various sintering temperatures was studied and its improved bioactivity was reported. Parallelly, whether monovalent modifier cation is necessary or not in the network of bioactive glass is thoroughly inspected and their pros and cons are testified. Also, scaffolds and fibers made from these bioactive materials blended with polymers were prepared using various strategies and their dependency on the phase and structure of the bioactive materials will be presented.

KN 48

Machine Learning Approaches to Materials

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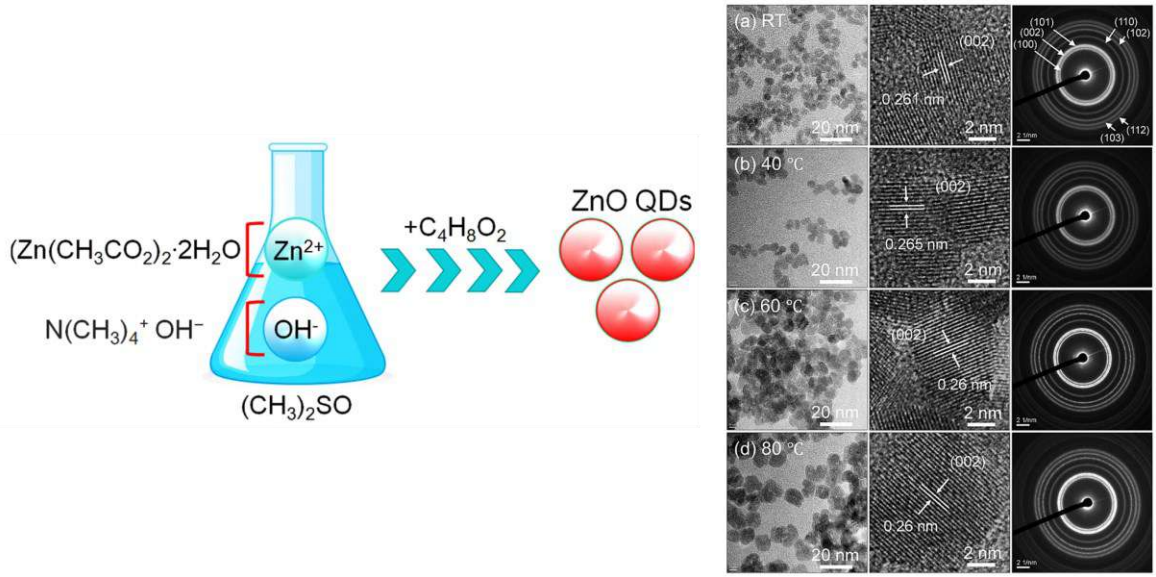
ABSTRACT

Materials Informatics has attracted much attention recently with the drastic development of artificial intelligence or machine learning in the big-data era. However, the wall between physicists/chemists and information scientists is too high to promote collaborative work in materials informatics. In this talk, we introduce general approaches to science/engineering in view of applied mathematicians/data scientists and show how we broke this wall, promoted materials informatics studies, and developed new mathematical/machine learning tools for materials informatics.



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KN 49

Quantum Tunneling Functionalities based on Silicon Nanomaterials and Nanodevices

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ABSTRACT

Silicon nanodevices form the building blocks of present-day nanoelectronics, either as pn diodes or as metal-oxide-semiconductor field-effect transistors (MOSFETs). As technology advances, quantum tunnelling becomes more and more dominant in developing new functionalities because of the lowdimensionality of the potential barriers, presence of quantum dots due to impurities (dopants) or high doping concentrations leading to ultra-narrow depletion layers in tunnel diodes. In our lab, we investigate quantum-tunneling functionalities emerging in both transistors and diodes, all fabricated in silicon-on-insulator (SOI) substrates using our cleanroom fabrication technology. In nanoscale SOI transistors, we rely on doping to increase the conductivity in the leads and also to create the quantum dots (QDs) in the low-dimensional channels. Following our reports on single-electron tunnelling (SET) via individual P-donors [1-3], when doping concentration is relatively low, we can demonstrate an ultimate level of electronics dealing with elementary charges and dopant-atom-induced QDs. When concentration is increased, clusters of P-donors act as QDs and they may have higher barriers under certain conditions [4]. With such structures, we demonstrated for the first time room-temperature SET operation by combining very high doping concentrations with very low dimensionality [5]. Furthermore, when counter-doping is done (with B-acceptors), SET functionalities emerge with higher yield [6], albeit only at lower temperatures still. In nanoscale diodes, we aim for high concentrations for both P-donors and B-acceptors forming the n-type and p-type regions in the SOI layer, so that tunnel (Esaki) diodes can be formed. Under such conditions, band-to-band tunnelling (BTBT) emerges as a key mechanism for transport, with applications also in tunnel FETs (TFETs). We reported BTBT mediated by dopant states [7], as well as dopant-induced QDs [8] in the nanoscale depletion layer of our SOI pn diodes, which suggests the possibilities for current enhancement by suitable arrangement of dopant states. Currently, we fabricate nanowire highly-doped pn diodes with the aim of demonstrating atomistic functionalities based on BTBT transport.

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KN 50

Electro-Thermo-Mechanical Finite Element Analysis on SPS Sintering Process of Zirconia Part

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ABSTRACT

Spark Plasma Sintering (SPS) process is pressure sintering with help of resistance heating by DC pulse current, which is more efficient process than other conventional sintering processes such as hot pressing sintering process. Parts can be sintered in shorter time by the combination of resistance heating and pressure. For the SPS process, fabrication of complex geometry part such as cup-shape is challenging, since simple compression of powder with different reduction in height cause non-uniform density distribution of the sintered part, which induce distributed hardness and strength. For the sintering of cup-shaped part, the specific tooling system has been developed by the present authors, which can fabricate cylindrical can of titanium and zirconia powder. Moreover, the precise prediction on the distribution of current density and temperature during process is also inevitable for the successful sintering. Numerical analysis such as FEM will help the development of proper sintering process design of the net shaped dense part with complex geometry. In the present paper, the tooling system of sintering of cylindrical can with uniform density, and the non-steady electro-thermo-mechanical finite element analysis of the SPS process of cylindrical can made of titanium and zirconia with the tooling system will be presented. Powder materials were modeled as a compressible elastic-plastic continuum material with large deformation by use of the plastic constitutive equation proposed by Shima and Oyane. The flow stress of was furnished by temperature-dependent Norton-Hoff model. Young's moduli were given as a function of relative density. The electric and thermal properties on the graphite and materials were assumed to be temperature dependence. The boundary conditions on the pressure and the voltage to the dies and tools during the sintering process were given as same as the experimental ones conducted by the present authors. The results of calculation were found in accordance with the experimental ones with sufficient accuracy. From the calculation of the sintering process of cylindrical cans, it was found that the enough compression pressure, heat generation by current, heating of the graphite dies that contacts with materials, and heat transmission from the die to materials was essential for the successful results. In case of zirconia cylindrical can, the lower density region at the inside of the can and large positive circumferential stress component during cooling were predicted, which corresponded to the region where the convex shape inside can and fracture, respectively in the experiments

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Finite Element Analysis of Surface Acoustic Wave on 36YX-LiTaO$_3$/36Y90X-Qaurtz Structure for Sensor Application

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ABSTRACT

Since the success of I. H. P. surface acoustic wave (SAW) device by Takai et.al[1], the development of SAW devices with a structure consisting of multiple crystals instead of piezoelectric single crystals has been active. For example, it is used for SAW devices with multiple crystals, such as piezoelectric crystal on insulator and piezoelectric crystal on piezoelectric crystal[2]. A sensor is realized using a SAW device. Its sensitivity depends on the piezoelectric crystal used. For example, a SAW on the 36Y90X-quartz is highly sensitive to mechanical perturbations but less sensitive to electrical perturbations. On the other hand, a SAW on 36YX-LiTaO$_3$ is the opposite: sensitive to electrical perturbations but insensitive to mechanical perturbations. If 36YX-LiTaO$_3$ and 36Y90X-quartz are bonded, we considered that a sensor that compensates for the shortcomings of both is realized. In this paper, the SAW sensor fabricated on a bonded structure of 36YX-LiTaO$_3$/36Y90X-Qaurtz is analyzed using the finite element method (FEM). Figure 1 shows the comparison results of mass sensitivity, one of the mechanical perturbations. The sensitivity for mechanical perturbation of 36YX-LiTaO$_3$/36Y90X-Qaurtz is the same as that of 36Y90X-quartz and higher than that of 36YX-LiTaO$_3$. The sensitivity for electrical perturbation was also simulated and found that the sensitivity of 36YX-LiTaO$_3$/36Y90X-Qaurtz is the highest. Therefore, we concluded that the bonded structure of 36YX-LiTaO$_3$/36Y90X-Qaurtz has a high potential as a high-sensitivity sensor.

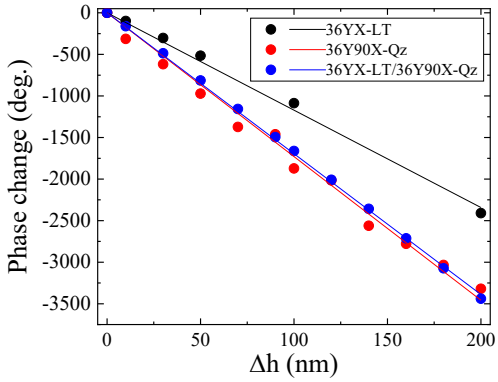

Fig. 1 Comparison of mass sensitivity. Phase change as a function of gold thickness.

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KN 52

Competing magnetic interactions and exchange bias behaviour in complex oxides materials

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ABSTRACT

Complex Oxides are of great importance in the field of strongly correlated materials. Amongst these Ruddlesden-popper phases as well as 6H perovskites are two structural class of materials that have found importance in the search for novel quantum materials. In this study we have investigated the magnetic properties of few compositions in both these structural families. Neutron-diffraction measurement rules out long-range magnetic ordering and together with dc magnetic measurements suggests formation of short-range magnetic domains. AC magnetic susceptibility, magnetic memory effect, and magnetic training effect confirm the systems to be cluster spin glasses. We have investigated the effect of competing magnetic interactions that can trigger exchange bias effects in these materials.

KN 53

Iron Particles: Applications in Aerospace and Energy Industries

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ABSTRACT

This presentation introduces two ongoing research projects conducted at ZAPlab. The first project involves incorporating iron particles into the PMMA propellant for a pulsed plasma thruster (PPT), with preliminary results indicating improved overall performance compared to traditional PMMA propellants. PPTs are crucial thrust units for microsatellites, enabling effective station-keeping and altitude adjustments. The second project explores the substitution of coal particles with iron particles in a coal-firing furnace for power plants. This innovative approach to energy generation using iron holds the promise of heat and power output without carbon emissions. I will delve into the details and provide insights into these groundbreaking applications of iron in the aerospace and energy sectors.

Electrical conductivity and Seebeck coefficient of a single contact between carbon nanotubes

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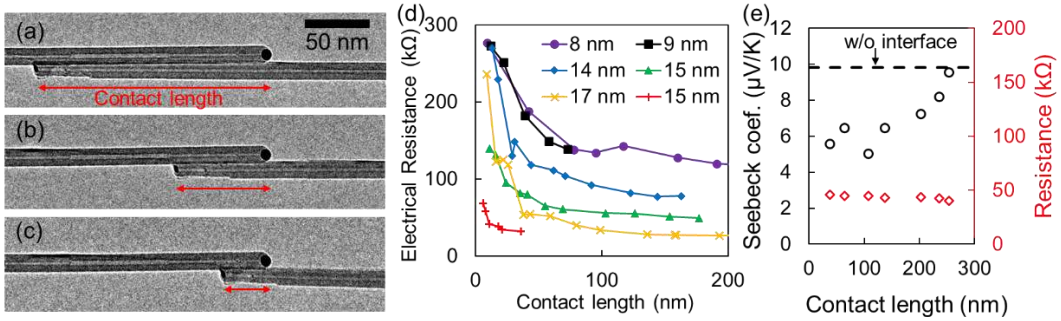
ABSTRACT

The interface plays a critical role in the transport properties of nanomaterial-based assemblies. However, understanding of interfacial transport remains limited because of the complexity of the interface morphologies and the difficulty of experimental approaches. Here, we report the in-situ measurements of the electrical resistance and Seebeck coefficient of multiwalled carbon nanotubes (MWCNTs) connected with a single parallel interface in a transmission electron microscope (TEM). Two protruding MWCNTs were prepared by cutting a bridged MWCNT by Joule heating. They were brought in contact with each other, and the length of contact was varied by controlling the manipulator under TEM observation. Figures 1(a), (b), and (c) present TEM images of parallel contact between the individual MWCNTs according to the contact length. Fig. 1(d) presents the measured electrical resistances for six pairs of MWCNT as a function of the contact length (outer diameters are indicated in the figure legends) [1]. The measured resistances were inversely proportional to the contact length below ~100 nm. The experimentally determined electrical conductivities of parallel contact were 10^2–10^3 S/m, which varied according to the specimen. MWCNTs connected with a single parallel interface exhibited a smaller thermoelectric power than that of a single nanotube [Fig. 1(e)]. The comparison of the contact-length-dependence between the electrical resistance and Seebeck coefficient suggested higher interfacial resistance in thermal transport than in electrical transport.



Figures 1. (a–c) TEM images of a parallel contact between MWCNTs. (d) Electrical resistance and (e) Seebeck coefficient as a function of the contact length. The legends in (d) denote the outer diameter.

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KN 55

Control of encapsulated chemical species into cage-structured crystal $12CaO{\cdot}7Al_2O_3$

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ABSTRACT

$12CaO{\cdot}7Al_2O_3$ (C12A7) has been known as a constituent of alumina cement for a long time. The crystal structure of C12A7 is cubic with lattice constant 11.99 Å, and consists of a framework (represented as $[Ca_{24}Al_{28}O_{64}]^{4+}$) which has 12 cages three-dimensionally connected and two oxygen ions, O^{2-}, clathrated in the cage. H. Hosono et al. reported remarkable findings on C12A7 series; the material can clathrate anion species e.g. anionic oxygen species (O^{2-}, O_2^- and O^-), hydride ion (H^-), electron (e^-) as well as hydroxyl ion (OH^-) and halogen anions (X^-) by treating them in appropriate atmospheres and/or temperatures[1, 2]. T. Dong et al., reported a direct oxidation of benzene yields phenol using the oxygen radicals[3]. There have been several reports about the substitution of the Al^{3+} site with other species with larger valence number in order to increase the amount and encapsulated species. In a case of tetravalent Si^{4+} substitution, the charge of the cage and the number of the encapsulated anion species increased [4]. On the other hand, there have been no report about substitution of the cations composed of C12A7 with smaller valence number cations, such as substitution of Ca^{2+} site by alkali metals. The substitution of the smaller valence cations is expected to result in the decrease of the charge of the cage and eventually the cage charge becomes negative. If the negative charge of the cage is achieved, it is expected that a new type of ion conductive material with cage structure which exhibits high ionic conductivity by encapsulating Li^+, Na^+ and K^+ etc., In the present study, we investigated the possible substitution amount of the Ca^{2+} sites of C12A7 with alkali metals and the doping effects on the C12A7 crystal structure.

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IT 01

Laser-Assisted Tailoring of Semiconductors Properties for Advanced Microelectronics: Unleashing the Possibilities for GeSn Epitaxial Layers

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ABSTRACT

The interaction between laser radiation and the semiconductor materials becomes particularly challenging when the laser intensity falls below the ablation threshold but remains close to it. This interaction can lead to various atomic rearrangements, material recrystallisation, the formation of nanostructures or microstructures, and even to the generation or recombination of intrinsic or extrinsic point defects. This study provides a comprehensive overview of laser-based methods for altering material properties. In particular, we focus on semiconductor materials and apply laser methods to modify epitaxial GeSn layers. Binary GeSn solid solutions present significant potential for mid-infrared Si photonics, due to their ability to achieve a direct band gap at more than 8% Sn content in GeSn and the possibility of forming devices directly on the Si chip. However, growing fully strain-relaxed GeSn epilayers with high Sn content and excellent material quality poses significant challenges for several reasons. These challenges include the high segregation coefficient of Sn in Ge, a substantial lattice mismatch of 14.7% (19.5%) between α-Sn and Ge (Si), and the limited equilibrium solid solubility of Sn in Ge, which is less than 1%. To address these concerns, our study investigates the redistribution of Sn atoms and the strain relaxation of GeSn alloys after employing post-growth laser processing techniques using nano-, pico-, and femtosecond lasers. Using the reciprocal space mapping (RSM) method, we investigated the impact of laser processing on nature of the strain in GeSn epilayers. Our observations revealed that the laser radiation induced partial compressive strain relaxation, and the extent of relaxation depended on the intensity of the laser. By employing TEM-EDS and X-ray photoelectron spectroscopy (XPS) analysis, we found that nanosecond laser radiation led to an increase in the Sn atomic concentration at the surface layer, reaching up to 14% for initial samples with a 4% Sn content. This increase can be attributed to the thermogradient effect. In contrast, pico- and femtosecond laser radiation had minimal influence on the redistribution of Sn atoms within the GeSn layers.

Acknowledgement

The authors gratefully acknowledge the ERA-NET Cofund project CHIST-ERA supported by the Horizon Europe: "NOEMIA - Nano-Opto-Electro-Mechanical Integrated Oscillator Arrays for Energy-Efficient Physical Reservoir Computing" (Nr. ES RTD/2023/16).

IT 02

Innovative Integration of MOF-derived NiFeO Nanocrystals and $Ti_3C_2T_x$ MXene Nanosheets in Oxygen Electrocatalysis for Rechargeable Zinc-Air

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ABSTRACT

In this work, we unveil an innovative study that focuses on enhancing the electrocatalytic efficiency in rechargeable zinc-air batteries (ZABs) through the integration of metal-organic framework (MOF)-derived NiFeO nanocrystals with $Ti_3C_2T_x$ MXene nanosheets. Addressing the challenges in oxygen electrocatalysis critical for ZABs, our approach overcomes the limitations of traditional MOFs, such as poor electrical conductivity and stability. The hybrid structure formed by combining NiFeO nanocrystals with $Ti_3C_2T_x$ nanosheets leads to improved conductivity and active site accessibility, thereby enhancing both oxygen evolution and reduction reactions. Our findings demonstrate the NiFeO@$Ti_3C_2T_x$ hybrid's exceptional bifunctional activity, highlighted by its notable half-wave potential and reduced overpotential. Its durability and alcohol tolerance in alkaline electrolytes are significant, with sustained performance over extended periods. In practical application, a ZAB with a NiFeO@$Ti_3C_2T_x$ air-cathode exhibits impressive open-circuit voltage, peak power density, and maintains cycling stability for prolonged hours. This research not only offers a successful strategy for improving oxygen reactions in ZABs but also paves the way for future advancements in MOF@MXene catalysts for energy conversion applications. This breakthrough highlights the potential of combining MOF-derived materials with conductive nanosheets, marking a significant step forward in the field of energy storage and conversion technologies.

IT 03

Self-powered monitoring of biomarkers and environment pollutants by integrating MXene based sensors with nanogenerators

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ABSTRACT

Gas sensor technology has provided an indispensable tool for the detection of toxic gases and volatile organic compounds as well as suggesting early diagnosis of diseases by detecting biomarkers to reduce the potential of risk to human beings. The ability of the gas sensor to operate at room temperature is imperative to keep pace with advancement in wearable and wireless technology. Up to now, metal oxide semiconductors based chemiresistive sensors have been widely explored but lack of pathway toward unresolved issues such as low sensitivity, low selectivity, high operating temperature, and flexibility are roadblocks toward bringing more sensors from laboratory to smart digital world. MXene (Ti_3C_2), as a forefront member of two-dimensional transition metal carbides and nitrides family, has aroused a boom based on its exceptional combination of numerous merits of high metallic conductivity, large specific surface area, adjustable surface chemistry, excellent mechanical and flexibility features. More significantly, the high hydrophilicity and electronegativity of MXene derived from its terminal functional groups make it an encouraging candidate for room-temperature gas sensing properties. During the last few years, utilizing these intriguing features of MXene, the researchers have put forward the innovative approaches to synthesize MXene-based hybrid nanomaterials and their associated devices for self-powered gas sensors systems. In this regard, the field of triboelectric/piezoelectric nanogenerators has been promoted which can scavenge environment mechanical energy into useful electrical output and couple with gas sensors as a source of energy for the real-time monitoring of gases without any external supply. In this talk, a brief overview of the fundamentals, current developments and our research contributions [1-4] towards potential applications of self-operating gas sensing system will be presented. This could serve as a road map for leading researchers in the field of self-powered sensors.

IT 04

Aerosol deposition of functional thick films on metal and polymer substrates

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ABSTRACT

To miniaturize functional devices, electroceramic components must be reduced in size down to the micrometer range. The aerosol deposition (AD) process (Figure 1a) offers a cost-effective way to deposit dense, micrometer-thick films at room temperature, enabling the integration of ceramic components on substrates such as metals and polymers. In this context, relaxor-ferroelectric (1-x)Pb(Mg1/3Nb2/3)O3– xPbTiO3 (PMN–100xPT) materials exhibit excellent electromechanical properties as well as energy storage and conversion capabilities suitable for electrical generators, capacitors and electrocaloric refrigerators. In this work, PMN–PT thick films were deposited on low-cost stainless steel [1] and flexible polymer substrates (Figure 1b) [2]. The films exhibit a relaxor-like hysteresis loop of polarization versus electric field, which makes them promising for energy storage applications. PMN–10PT films on polymer substrates exhibit a recoverable energy density of ~10 J·cm^{-3} at ~1000 kV·cm^{-1}. The energy storage properties of these films remain stable after 10^5 bending cycles at 1.0 % bending strain (Figure 1b) [2]. In addition, PMN–10PT films [3] and PMN–10PT/La-Fe-Si based alloy composites (Figure 1c) on polymer substrates show promising caloric properties, which are presented in this contribution. An analysis of the energy storage and piezoelectric properties of AD-processed PMN–35PT [4, 5] and lead-free BaTiO3-based thick films is also discussed.

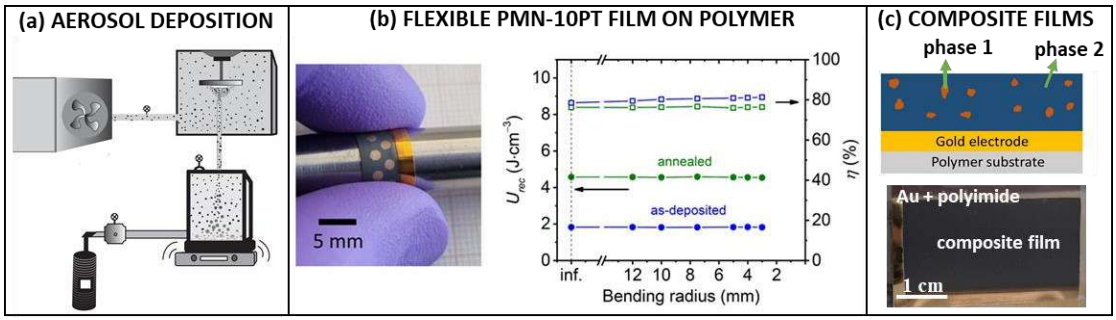

Figure 1: (a) Aerosol deposition process, (b) PMN–10PT thick film on a polymer substrate and their recoverable energy density (U_{rec}) and efficiency (η) versus bending radius measured at ~500 kV·cm^{-1} [2] (c) PMN–10PT/La- Fe-Si-based intermetallic alloy composite thick film on polymer substrate.

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IT 05

Dual Role of Microalgae in Wastewater Treatment for Bioproduct (Fish Feeds Alternative)

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ABSTRACT

Wastewater is heavily polluted water which rich in organic and inorganic matters depend on the source of the wastewater itself. The direct discharge of wastewater into water body is associated with eutrophication and spreading of the disease's phenomenon, despite exceed the standard limit for Sewage Characteristics and Effluent Discharge. Thus, treatment of wastewater before disposal shall be implemented and microalgae have potential to this treat wastewater by uptake of organic matters to produce biomass via phycoremediation process. Phycoremediation might be an alternative technology, because it is cheaper and more effective for removing nutrients compared to other physicochemical process. Microalgae biomass have high nutritional values in term of lipids, protein and carbohydrates as an alternative for fish feeds. Microalgae can adapt to harsh condition in wastewater to produce quality biomass depend on the light exposure, aeration, pH, temperature and also nutrient content such as nitrogen, carbon and phosphate in the wastewater. Microalgae biomass from treated wastewater may be an alternative to replaced traditional fish feeds production in aquaculture industry that expensive. This microalgae biomass from treated wastewater have potential to support fish growth, fish development, fish feeding efficiency, fish resistance to diseases, fish stress response and low cost compared to wild catch fish feeds from juvenile fish. Hence, this study aims to highlight the dual roles potential of microalgae to treat wastewater and produce biomass as an alternative to traditional fish feeds. The phycoremediation techniques for wastewater treatment and microalgae biomass as fish feed were reviewed.

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IT 06

Metal-Organic Frameworks Composites for Dye Degradation via Adsorption, Heterogeneous Photo-Fenton, and Photocatalysis.

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ABSTRACT

In this study, we explored two methods to improve the photocatalytic efficiency of titanium dioxide (TiO2). Firstly, we synthesized TiO2/MIL-100(Fe) composites to overcome TiO2's limited UV responsiveness and iron sludge formation in photo-Fenton processes. These composites efficiently removed organic dyes under simulated solar light. MIL-100(Fe) dispersed TiO2 and adsorbed dyes due to its high surface area. The composites absorbed visible light for photocatalytic and photo-Fenton reactions. Kinetic analysis showed pseudo-second-order dye removal. Secondly, we used carbon quantum dots (CQDs) and NH2-MIL-125 to enhance commercial TiO2 (P25) photocatalysis. CQDs expanded light absorption, while NH2-MIL-125 increased P25's surface area. The CQD/P25/NH2-MIL-125 composite utilized CQD up-conversion photoluminescence to improve photocatalysis by broadening light absorption and hindering electron-hole pair recombination. A 1wt% CQDs/P25/NH2-MIL-125 composite followed first-order kinetics with a rate constant of 0.0141. These approaches offer promising solutions for environmental remediation and energy conversion with TiO2 photocatalysts.

IT 07

Atmospheric pressure plasma deposition of interstellar dust analogues based on amorphous hydrogenated carbon and evolution after proton irradiation

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ABSTRACT

Natural or artificial carbonaceous particulate matter is of great current interest for e.g. atmospheric and environmental sciences, human health, engineering, and astrophysics. We present here our latest results on the synthesis and characterisation of hydrogenated amorphous carbon (a-C:H) products, deposited using low temperature plasma, at atmospheric pressure [1-2]. Dielectric Barrier Discharge (DBD) is a relatively new method for amorphous hydrogenated carbon (a-C:H) synthesis, and even more so for producing diffuse interstellar medium (DISM) dust analogues. The dust analogues were thoroughly characterized using a combination of analytical techniques such as Fourier-transform infrared spectroscopy (FTIR), micro-Raman spectroscopy, X-Ray photoelectron spectrometry (XPS), optical microscopy, scanning and transmission electron microscopy (SEM, TEM), or mass spectrometry.

In order to study the effect of cosmic rays on the disappearance of the carriers of 3.4 μm band in astrophysical environments, the dust analogues were irradiated with 3 MeV H^+. We observe morphological and chemical changes and evidence of the evolution of H/C, CH_2/CH_3, and sp^2/sp^3 ratios with increasing proton fluence. Using the observed 3.4 μm band decay with proton fluence we calculated the CH destruction cross sections and it was found that direct effects of cosmic rays are very likely responsible for the disappearance of the 3.4 μm band.

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IT 08

Molecular Design of Ion Pair Amphiphiles for Biomimetic Catanionic Bilayers with Designated Phase and Morphological Properties.

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ABSTRACT

Ion pair amphiphiles (IPAs) are molecular complexes formed by a pair of cationic and anionic surfactants. IPA can self-assemble into catanionic vesicles as potential liposome surrogates. Analogous to lipid bilayers, IPA vesicular membranes exhibit either a fluidic liquid-disordered phase or a solid-like gel phase above or below the main phase transition temperature (Tm), respectively. Hence, controlling the phase and morphological behaviours of IPA vesicles is crucial for controlled drug release. Here, we conducted series of molecular dynamics (MD) simulations to systematically explore the phase properties of IPA bilayers with different molecular designs. We correlated the membrane properties with various experimental measurements for characterizing IPA membrane phase transitions.[1,2] Furthermore, we examined various strategies for modulating the phase properties of IPA bilayers, including cholesterol additive, ethanol cosolvents, and amphiphile compositions. We constructed the phase diagrams via MD simulation for IPA membranes under the effects of cholesterol and ethanol. Additionally, we analysed the Tm response of the bilayers to IPA mixtures and the alkyl chain asymmetry. We observed Tm deviations from ideal mixing, arose partly due to the transition between tilted and non-tilted gel phases. Also, we characterized the dependence of membrane phases on the compositions of charged groups of IPAs. We identified the correlation the solvation free energies of ions and the association free energies of ion pairs via the law of matching water affinities (LMWA), allowing us to screen potential IPA membranes with pH-responsive potential. The combined results offer invaluable insights into the design of catanionic vesicles, innovating the novel drug carrier development.

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IT 09

Systematic Investigation to Enable the High-Efficiency Thermally Activated Delayed Fluorescence Emitter for OLEDs

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ABSTRACT

Thermally activated delayed fluorescence (TADF) emitters have evolved as a certifying candidate in light generation technologies for producing efficient organic light-emitting diodes (OLEDs) on account of their 100% internal quantum efficiency (IQE) via reverse intersystem crossing (RISC) and toxic metal free design. Fast rate of RISC (kRISC) is the ultimate requirement of an efficient TADF emitter which can be achieved by minimizing the singlet-triplet energy gap (ΔEST). Here, four donor-acceptor type TADF emitters namely 3BPy-mDCz, 3BPy-mDTA, 3BPy-mDMAC, and 3BPy-mDPT proposed based on benzoyl pyridine (3BPy) as an unaltered acceptor and varying the donor strength ranging from carbazole to phenothiazine. The ΔEST values decreased from 0.15 to 0.09 eV upon increasing the donor strength predicting their TADF nature. The maximum external quantum efficiency (EQE) of 18.7% for 3BPy-mDCz, 22.5% for 3BPy-mDTA, 13.8% for 3BPy-mDMAC and 2.1% for 3BPy-mDPT were obtained. These drastic difference in the performances of 3BPy-mDTA and 3BPy-mDPT is due to the locally excited 3LE(T2) intermediate state between the lowest singlet (S1) and triplet (T1). Among the 3BPy-mDMAC and 3BPy-mDPT, the efficiency of 3BPy-mDMAC outperforms as compared to the 3BPy-mDPT on account of high photoluminescence quantum yield (PLQY) due to less CT character. This work paves a new direction for efficient TADF molecular design by indicating the role of intermediate triplet state (3LE) despite possessing high ΔEST values.

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IT 10

Electro-oxidation of ethanol over IrO_x-Pt electrode surface: An approach to develop a CO tolerant catalyst

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ABSTRACT

Pt is widely acknowledged as an excellent catalyst to perform electrochemical oxidation of ethanol. But its activity often decreases over time due to irreversible adsorption of intermediate species, mainly, carbon monoxide (CO). To get rid of CO poisoning, a simple catalyst, IrO_x-Pt (iridium oxide film deposited on platinum electrode), was developed via cycling from 0 V to +1 V vs. Ag/AgCl (sat. KCl) in $Ir_2O_3.xH_2O$ colloidal suspension for 10 incessant cycles at scan rate of 0.1 V s^{-1}. Cyclic voltammetric analysis revealed that the activity of pure Pt catalyst in ethanol oxidation reaction (EtOR) was around 1.3 times higher than that on IrO_x-Pt but the CO-tolerant ability of Pt catalyst was around 3.5 times less than IrO_x-Pt. The stability test of Pt electrode also revealed that the activity of Pt electrode drastically decreased within 3 consecutive cycle. In case of IrO_x-Pt, the stability test revealed that the current density related to EtOR remained almost unchanged upon 500 incessant cycling, whereas almost 50% activity of Pt electrode dropped upon similar experimental condition (see **Fig. 1**).

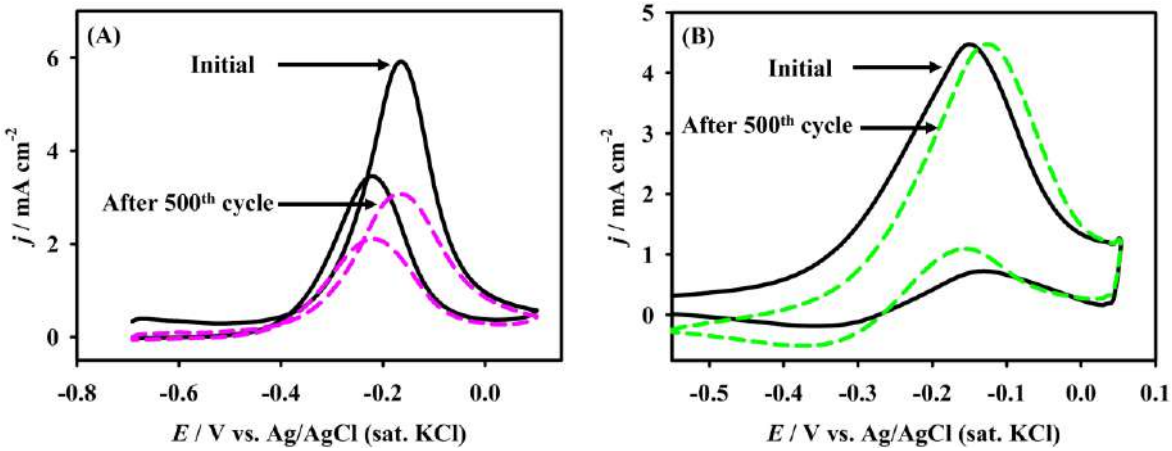

Fig. 1. (A) Comparative cyclic voltammograms of bare Pt in 0.1 M N_2-saturated NaOH solution having 0.25 M ethanol at 0.1 V s^{-1} recoded initially and after 500 incessant cycling in 0.25 M ethanol solution, (B) Comparative cyclic voltammograms of IrO_x-Pt in 0.1 M N_2-saturated NaOH solution having 0.25 M ethanol at 0.1 V s^{-1} recoded initially and after 500 incessant cycling in 0.25 M ethanol solution.

IT 11

Redox Cycling Amplification in Microgap-Based Bipolar Electrodes Using an Ion-Selective Membrane

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ABSTRACT

In conventional open bipolar electrode (BPE) systems, oxidation and reduction reactions proceeded on both poles of a BPE by generating a sufficient potential gradient in the solution[1]. However, the BPE is electrically floating, and the interfacial potential difference between the BPE and solution interface is not controlled. As the BPE is not connected to an external instrument, electrochemiluminescence (ECL) is usually employed to report information about the progress of redox reactions at the other pole of the BPE[2]. Utilizing an ion-selective membrane (ISM) on a part of a BPE can enhance the redox reaction on the electrode. With the ISMs, the potential difference at the membrane-solution interface changes depending on the concentration of analyte ions[3]. This technique will increase the redox reaction's performance on the BPE. Furthermore, the redox cycling principle applied in this study is an effective method for amplifying electrochemical signals generated by electrode reactions with a gap between two functional electrodes. This study involves the repetitive redox reactions inside a micrometer space between two functional electrodes. The performance of this device is further enhanced by combining it with an ISM, that can fix the interfacial potential between the electrode and the solution interface. The outcome of the redox cycling will be visually visible in the reporter chamber, where the ECL solution is located. It was observed that an ISM located near the anodic pole shows an increment in the ECL intensity, with an increase in the Na^+ concentration in the solution. Therefore, the interfacial potential differences at the cathodic and anodic poles varied with respect to the location of the ISM and/or the concentrations of the primary ions to be detected by the ISM, which can be independently regulated.

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IT 12

Novel multi-functional properties by magnetic metal-ceramics nano-granular films

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ABSTRACT

Magnetic metal-ceramic nano-granular thin films, in which nanometer-sized magnetic metal granules are dispersed in a ceramic matrix, have many For example, when the content of the magnetic metal composition is large (generally above 60%), high-frequency magnetic properties are developed. When the content of the magnetic metal composition is about a half (about 60 ~ 30%), a tunnel These properties have been studied for several 10 years and are now widely used in electromagnetic applications. These properties have been studied for several 10 years and are now widely used in electromagnetic applications. In our group, a new magneto-dielectric effect was discovered in granular nano-composites, and we named it the Tunneling Magneto-Dielectric (TMD) effect [1]. The TMD nanocomposites consist of magnetic granules with the size of several nanometers sparsely dispersed in an insulator matrix, making quantum tunneling possible as the tunnel barrier is thin enough. With applied AC field and magnetic field (H), the oscillation rate depending on the height of the tunnel barrier and relative magnetization orientation of the granules may coincide with the frequency of the AC field, thus producing a peak dielectric change $\Delta\varepsilon'/\varepsilon'0$ at a specific peak frequency. This presentation introduces the research background, TMD effect, thin film preparation, and characteristic improvement.

IT 13

Nano gold in immunosensing applications

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ABSTRACT

Immunosensors are a class of Biosensors that utilize antigen-antibody interactions for detecting pathogens. Typically, the immunosensor is a device that contains a transducer (Electrochemical, Optical, Mass sensitive device etc.,), an antibody or antigen for the recognition of the pathogen/ antibody, and a display device for displaying the results. A chemical can also be detected provided appropriate antibody is available. An immunosensor requires a material at the interface of the device and the antibody/antigen. The antibody is fixed to the material at the interface by immobilization techniques, such as physical, or chemical immobilization methods. The material used at the interface is normally gold, platinum, silver or metal oxides. On the other hand, gold is a well-known metal used in biosensor applications. The gold is non-corrosive, has good electrical conductivity and has good electrochemical properties. Hence finds applications in sensors. The nano gold displays a variety of properties such as variable colour, fluorescence, and conductivity. And high surface area. In addition, it is possible to immobilize the antigen/antibody on the gold by using a self-assembled technique. The gold nanoparticles were used in increasing the electrochemical surface area in electrochemical immunosensors. It is used in SPR-based instruments. In mass-sensitive devices like SAW devices and Cantilevers also it was used as a coating. In addition, it was used as a tag in which the gold nanoparticles were fixed to the antibody instead of using an enzyme as a tag. Nanogold offers more advantages over macro/mini/micro gold in realizing immunosensors. The nano gold can be made by chemical methods, physical evaporation method and electrochemical method based on the need. Various aspects of the use of nano gold in immunosensors from our research group and literature will be discussed. In general, the nano gold will enhance the sensitivity and ease of fabricating immunosensors.

IT 14

Nanomechanical metamaterials

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ABSTRACT

We overview our recent advances in plasmonic or dielectric nanomechanical metamaterials fabricated on elastic nanomembranes of silica or silicon nitride. Such metamaterials allow nanometric displacement of their building blocks under external forces and can be reconfigured with external stimuli to achieve optical modulation at high frequencies. Mechanical and optical resonances enhance the magnitude of actuation and optical response within these nanostructures, which can be driven by electric signals of only a few volts, microwatt optical signals or acoustical signals. This approach allows a range of functionalities to be achieved in the form of optical elements of sub-micron thickness including sensing, light modulation and nonlinear effects.

IT 15

Potential of Gold Nanobipyramids as an Antifungal Agent in Biomedical and Agricultural

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ABSTRACT

Fungal infections pose a critical challenge in biomedical and agricultural domains, prompting extensive exploration into effective treatment strategies. Traditional fungal treatment methods, encompassing chemical, physical, and biological, suffer from inherent limitations despite widespread usage. Chemical treatments such as amphotericin B are relatively toxic, while less poisonous and newer potent chemicals, fluconazole and itraconazole, still exhibit adverse effects on health. Physical treatments, including heat, ultraviolet radiation, and filtration, prove energy-intensive and demonstrate limited efficacy across diverse fungal strains. Furthermore, conventional biological methods employing fungal cultures and enzymes struggle to eliminate certain compounds, such as degradation-resistant wastewater pollutants. In response to these challenges, innovative fungal treatment strategies have gained prominence over the past decade, with nanoparticle-based methods emerging as promising alternatives. Thus far, silver nanoparticles have been extensively investigated but they have stability issues, which underscore the need for alternative nanoparticles. In light of this, gold nanoparticles are proposed as prospective antifungal agents, leveraging their unique characteristics to enhance therapeutic efficacy. The shape and size of gold nanoparticles influence their toxic effects on fungi, with anisotropic gold nanostructures demonstrating advantages in tunability and toxicity modulation compared to isotropic structures. The anisotropic gold nanostructure with a bipyramid shape, characterized by its unique geometric features and enhanced optical characteristics, has become a focal point in research and application. The geometric attributes, such as sharp tips and edges, contribute to increased surface interactions and catalytic activities, making nanobipyramids promising candidates for applications in fungi treatment. The intrinsic antimicrobial properties of gold nanobipyramids further enhance their efficacy against fungal pathogens. Additionally, the biocompatibility of gold nanobipyramids is critical in fungi treatment, ensuring minimal cytotoxicity and increasing their appeal for use in medical contexts. In our works, gold nanobipyramids showed inhibition against two fungi, namely Ganoderma and Dermatophytes fungus growth. It was proven that gold nanobipyramids have the potential to be innovative solutions against fungal infections.

Keywords: gold nanobipyramids, fungi treatment, metal nanoparticle

IT 16

Ab initio insights of 2D carbon lattices and doped analogues as alkali ion batteries materials

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ABSTRACT

Rapid increase in energy demand calls for sustainable and renewable energy sources. Li ion batteries are dominating the market for renewable energy sources. However, Li ion batteries have limited scope in foreseeable future owing to rare availability of Li, and high cost. The results of the ab initio study to design different 2D carbon lattices such as graphene and graphyne lattices where the carbon atoms are arranged in varied conformations and exist in different hybridization states for sodium ion batteries will be discussed. Si and N are doped in the carbon lattice to modulate the characteristic properties of parent lattice and systematically studied for structural, geometric, dynamic and thermal stabilities and established as effective anode materials in alkali ion batteries. The open circuit voltage for the proposed materials lies in the ideal voltage range. Based on these comprehensive sets of ab initio, and thermodynamic calculations, functionalized graphene and graphyne lattices are proven to be efficient anode materials in alkali ion batteries.

Design of LO Phase Shifter Based on Quadrature Hybrid Branchline Coupler for IQ Mixer in Synthetic Aperture Radar Applications

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ABSTRACT

Synthetic Aperture Radar (SAR) is a powerful instrument in microwave remote sensing because of its capability for all-weather and day-to-night time operation [1]. SAR has been widely used in many applications, particularly object detection, earth observation, agriculture, and terrain mapping [2]. SAR is constructed by the RF sub-system responsible for managing analog signals, with one of the important components being the IQ Mixer [3]. IQ Mixer mixes the base chirp signal with a carrier signal and increases the bandwidth of the transmitted signal to twice the base chirp signal. It is important because it can reduce the burden on the Field Programmable Gate Array (FPGA) that produces the base chirp signal and simultaneously increase the range resolution of the SAR system that depends on the bandwidth of the transmitted signal [4]. Therefore, to have a good performance of IQ Mixer, a steady supply of components, and demand to reduce cost production, we need to develop it independently. Three sub-parts construct the IQ Mixer: Local Oscillator (LO) Phase Shifter, Matched Mixer, and Power Combiner-Splitter. This paper proposes the design of an LO Phase Shifter based on a Microstrip Quadrature Hybrid Branch-line Coupler as a supporting component for IQ Mixer in Synthetic Aperture Radar Applications [5]. The measurement result from the fabricated coupler shows that all the specification requirement has been fulfilled. S11 has a low reflection of -26.54 dB, S41 has a high isolation of -32.27 dB, S21 and S31 have low attenuation with amplitude unbalance of 0.291 dB and phase unbalance of 2.17 degrees. The requirement bandwidth of 150 MHz at the center frequency of 5.5 GHz was also achieved. Therefore, this coupler can be considered to be used as an LO Phase Shifter.

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Fabrication of Electrode Materials for Sustainable Energy Applications

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ABSTRACT

The fabrication of electrode materials plays a crucial role in advancing sustainable energy applications, particularly in the development of energy storage and conversion devices. We have fabricated porous carbon nanosheet and nanostructured rhodium (Rh) thin film-based electrode materials for supercapacitor and water splitting applications, respectively. The electrode materials were characterized by FESEM, XPS, Raman, XRD and N_2 adsorption-desorption analysis. The constructed supercapacitor showed an operating potential window of 1.1 V in 1 M KCl neutral electrolyte solution. At 2.25 A/g the calculated specific energy was ~ 39.04 Wh/kg, along with a high specific power of ~ 1237.5 W/kg. The porous carbon material was able to retain specific energy of ~ 22.92 Wh/kg and specific power of ~ 41,250 W/kg at a high current density of 75 A/g. The porous carbon was used for making a coin cell prototype supercapacitor device and tested with a light emitting diode (LED). The Rh thin film electrode exhibited outstanding electrocatalytic activity for oxygen evolution reaction (OER). The effect of the supporting electrolytes on OER activity and the crystal planes of RhTF electrodes were analyzed using electroanalytical techniques and computational simulation methods. Tafel slope (TS) analysis revealed that electron transfer kinetics was slower for the NaOH compared to the KOH.

Keywords: Porous carbon, Rhodium, Electrocatalyst, supercapacitor, Oxygen evolution reaction.

Sn and Cr doped β-Ga_2O_3 Inter Digitated Electrode (IDE) gas sensors.

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ABSTRACT

This talk covers the enhancement of gas (or vapour) sensing capability of hydrothermally synthesized β-Ga_2O_3 at room temperature by introducing the suitable dopants. Here, we have chosen Sn and Cr as dopants. At the very first instance, a facile, surfactant-free hydrothermal synthesis route was employed to synthesize GaOOH at growth solution's pH = 7. These GaOOH powders have been thermally converted into β-Ga_2O_3 powder samples. By employing different material characterization tools, synthesized powder samples of GaOOH and β-Ga_2O_3 were well characterized. They were made into a thick film on top of the pre-printed silver inter digitated electrode (IDE) pattern on glass substrate by drop coating technique. Thus, prepared sensors have been utilised for the evaluation of gas sensing performance, towards the reducing vapours of ammonia, ethanol, methanol & acetone and oxidising gas of CO_2. It has been found that β-Ga_2O_3 showed higher sensing responses and sensitivities towards reducing vapours than oxidising gas which can be ascribed to its n-type conductivity. Based on these preliminary results, an attempt has been made to incorporate Sn into β-Ga_2O_3 at 2 mol% and 4 mol% concentrations by keeping pH = 7 by hydrothermal synthesis. It has been found that 2 mol% Sn incorporated β-Ga_2O_3 IDE sensors showed enhanced sensing responses, sensitivities and faster response-recovery processes compared to pure and 4 mol% Sn doped sensor owing to higher BET surface area (12.49 m^2/g), smaller crystallite sizes (26.36 nm) and lower bandgap (4.67 eV). Further, Cr was also introduced into β-Ga_2O_3 lattice at pH = 7 through hydrothermal method at 1 mol% dopant concentration. It has been observed that smaller crystallite size in Cr doped sample compared to pure one. The 1 mol% Cr incorporated sample exhibited cocoon shaped morphology with slightly higher aspect ratio with respect to the pure sample. The Cr doped β-Ga_2O_3 IDE sensor showed enhanced sensing responses and sensitivities of towards various reducing vapours at room temperature relative to the pure sample. Lower and upper limits of detection have been shifted to higher values in Cr doped β-Ga_2O_3 due to relatively higher aspect ratio.

IT 20

Multifunctional Pristine Magnetic Copper Ferrite ($CuFe_2O_4$) and $CuFe_2O_4$/rGO Binary Nanocomposites: Electrochemical Performance and Heavy Metals Adsorption

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ABSTRACT

This study unveils the fascinating potential of $CuFe_2O_4$/rGO nanocomposites, synthesized through a simple and efficient microwave method, by exploring their dual functionalities: remarkable electrochemical performance in supercapacitors and exceptional heavy metal adsorption capabilities for environmental remediation. As supercapacitor electrodes, the $CuFe_2O_4$/rGO composite shines with a stellar specific capacity of 800 C/g at a current density of 2 A/g, surpassing its pristine $CuFe_2O_4$ counterpart. This enhanced performance stems from the unique nanostructure formed by the synergistic integration of ferrite nanoparticles onto the rGO sheets. Furthermore, when incorporated into a hybrid supercapacitor device, it delivers an impressive specific energy of 18.3 Wh/kg and a power density of 455 W/kg, maintaining exceptional stability over a remarkable 3000 cycles. Beyond the realm of energy storage, the $CuFe_2O_4$/rGO composite unveils its prowess in environmental remediation by demonstrating a significantly higher capacity for adsorbing barium ions (Ba2+) compared to bare $CuFe_2O_4$ nanoparticles. The composite boasts a remarkable adsorption capacity of 161.6 mg/g, nearly double that of pristine $CuFe_2O_4$ (86.6 mg/g). This enhanced performance can be attributed to the increased specific surface area offered by the rGO, providing more sites for barium ions to interact with. Kinetic and thermodynamic studies suggest chemisorption as the dominant mechanism, highlighting the strong and selective interaction between the composite and the target pollutant. This work not only sheds light on the remarkable multifunctional nature of $CuFe_2O_4$/rGO nanocomposites but also opens exciting avenues for future exploration. The facile microwave synthesis method employed here paves the way for investigating other metal oxides with similar functionalities, potentially leading to a new generation of advanced materials with applications in both energy storage and environmental remediation. This study serves as a tool for the development of more sustainable and efficient solutions for addressing the ever-growing challenges in these crucial domains.

Keywords: specific capacitance, heavy metal adsorption, copper ferrite, microwave synthesis

Materials and Device Concepts of Large-area Perovskite Solar Cells

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ABSTRACT

Metal halide perovskite absorber based next generation solar cells (PSCs) reached a certified power conversion efficiency of 25.6%, a value comparable to that of first generation silicon photovoltaics. Defect tolerance, high optical absorption and long carrier diffusion length are few of the intriguing properties made halide perovskite potential material for low-cost, high-efficiency next generation photovoltaics. Although lab-scale PSCs with high efficiencies (> 20%) routinely fabricated by spin coating method, non-uniform solvent evaporation and crystallization over large area substrate limiting the PSC module efficiency around 15%. This talk will provide comprehensive insight and our approach on materials and device concept for the fabrication of perovskite solar module. The importance of interfaces and associated losses will also be discussed. Strategies to improve PSC module's efficiency and operational stability through rational design of device architecture and encapsulation will also be presented.

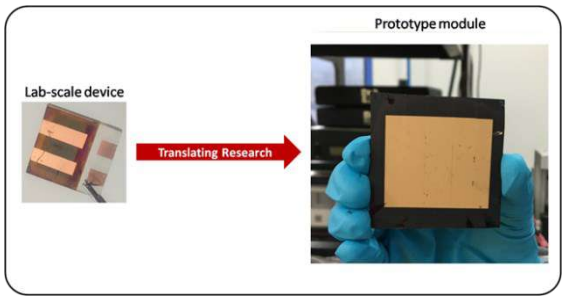

Fig. Up-scaling of perovskite solar cells

IT 22

Synergistic coupling {101}-{111} facet of N-doped TiO_2 film enhance spatial charge separation for methylene blue photodegradation

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ABSTRACT

The synthesis of N-doped TiO_2 film with co-exposed {101} and {111} facets via a one-pot facile hydrothermal method had proven to enhance the photocatalytic activity of TiO_2. The high-resolution transmission electron microscopy (HR-TEM) and X-ray photoelectron spectroscopy (XPS) data show the incorporation of N ions into the TiO_2 accomplishes the facet modification. The shifting of the N-doped TiO_2 photocatalyst adsorption bandgap toward a higher wavelength was identified as the TiO_2 band gap was reduced. Up to 66% methylene blue had successfully been degraded with the aid of N-doped TiO_2 as an active photocatalyst. The enhanced photodegradation of N-doped TiO_2 film is mainly attributed to the presence of {101} and {111} facets, leading to the efficient separation of carriers and lengthening the life of photogenerated carriers, consequently improving its photocatalysis potential.

The Challenge in Study of Topography Properties Using Atomic Force Microscope (AFM)

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ABSTRACT

The atomic force microscope (AFM) is entering its 4th decade as a primary technology for advanced materials research since its first discovery by Binnig, Quate, and Gerber in 1985. They originally studied AFM which contained a piece of diamond attached to a strip of gold foil. At that point, the diamond tip contacted the sample surface directly, and then the interaction mechanism occurred as a result of the interatomic van der Waals forces. AFM has been used to provide surface topography information for analysing countless area of disciplines and applications. AFM microscopes are one of the best solutions for measuring the nanoscale material surface and topography properties of samples. The maximum sample magnification and resolution of this AFM is approximately 1000x and 0.2 µm respectively. Theoretically, AFM contains various modes such as contact mode, non-contact mode, dynamic mode (tapping mode), magnetic mode, electrical/conductive mode, force mode, and nanoindentation mode. Among all, contact modes, non-contact mode, magnetic mode, and electrical/conductive mode will be discussed in this session on how it works, what possible sample can be scanned, and the challenge or difficulties while scanning some type of samples. For topography study, the selection of AFM modes is very crucial to obtain a clear image and accurate result of topology, this is due to the grain size and roughness for every sample is different based on its application. Usually, the rough sample is not suitable for contact mode because of the high risk and possibility for the cantilever to break while scanning throughout the sample. Therefore, non-contact mode quite favors for sample high roughness with bigger grain size.

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SPS Latest Technology/Application, Production System and New Model

Katsuhiko Nobeta

ABSTRACT

Our Spark Plasma Sintering Process & Equipment with latest and State of Art technology is designed for R&D of New Materials to Sinter various kinds of Materials from Metals to Ceramic in a wide range of Pressure & Temperature under controlled atmosphere. We have so far successfully manufactured and installed 465 SPS machines spanning the world. Progress of SPS Technology in our company evolved from Plasma Activated Sintering (PAS) in 1986 to developing Spark Plasma Sintering (SPS) in 1989 and progressed to successfully to a state of art SPS technology to challenge the needs of any R&D in this field, especially the Research Scholars worldwide. We are the only one having 60 years of experience in Dielectric and Induction Heating. The Newly developed SPS synthesis process employ On-Off pulse DC Voltage/Current has received considerable attention in the field of advanced new material development which was earlier not possible.

FUJI-SPS's Versatile Process and Potential are classified into

- Sintering
- Sinter-Bonding & Joining
- Surface treatment / Remove Oxidation - Plasma Cleaning
- Synthesis / Growth of single crystal

Technology and Applications

- Functionally Graded Materials (FGM)
- Nano-Phase Materials
- Thermo Electrical Materials
- Advanced Ceramic Materials
- Bio Materials
- The Fuji SPS configuration & Process can be discussed in detail at the exhibition hall booth where FUJI has a stall with their Indian counterpart M/s. MJ Enterprises, Chennai. You can inspect the sintered sample and discuss your requirement during this conference.
- FUJI-SPS Line up
- Desk Top
- Built-in Type
- Clove Box Type
- Batch-Type large sized SPS Manufacturing System

IT 25

Nano-dimensional Films for Novel Devices – Elucidating the Role of Hierarchy, Architecture and Doping Strategies

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ABSTRACT

Post pandemic situation we are increasingly relying on technologically advanced gadgets using a variety of functional and interactive devices. To realize smart, functional and cost-effective devices, utilizing combination of several materials in two-dimensional thin film form are inevitable. In this lecture I will be portraying the use of a variety of novel materials in the form of thin films, especially in nano-dimension with a focus on hierarchy, architecture and doping strategy making them suitable for applicability in several optoelectronic devices.

I will present and discuss results on three different types of thin films for appropriate applications. Firstly, I will elucidate the role of hierarchy to observe proximity effect in pulsed laser deposited oxide superconductors and half-metallic ferromagnetic (YBCO/LSMO & Bi-2212/LSMO) thin films. Secondly, the doping strategy of relevant donor elements into the SnO2 thin film coated by spray pyrolysis technique to make it an effective alternative transparent conducting oxide (TCO) electrode will be briefed. Finally, the importance of thin film multi-layer architecture at a thickness below the skin depth of several noble metals (Ag, Au, Cu & Pt) stacked in appropriate order by sputtering technique to serve as a flexible transparent conducting electrode (TCE) will be discussed along with their applicability in a couple of optoelectronic devices.

IT 26

Development of Bismuth-based Materials for Light-Driven-Assisted -Charging Supercapacitor

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ABSTRACT

Bismuth-based materials are interesting transition materials that are utilized for wide range of applications, especially photo-active materials, due to their characteristic features such as a suitable band gap to absorb visible light, reversible redox reaction, transparency, and photo-generated holes-electron. Herein, we conducted research on bismuth-based materials, emphasizing their potential in energy storage and electrocatalysis. In this work, the strategy to increase the photo-charge efficiency is purposed by crystal engineering, oxygen vacancy engineering, and heterojunction engineering. By crystal engineering the exposed [110] facets, BiOBr-pH 4 reaches the highest specific capacitance under LED of 209.32 F g^{-1} at 0.5 A g^{-1}, which is 1.45 times higher than that in the dark condition. Doping Ni atom onto the BiOBr structure can also enhance the photogenerated carrier separation efficiency, gaining 44.75% capacitance efficiency relative to the dark condition. More interestingly, composites bismuth-based materials with carbonaceous materials such as graphene can also improve photo-charge efficiency. Graphene can act as an electron acceptor, capturing the generated electrons from photon energy and synergistically enhancing their electrochemical performance. The mixed bismuth-iron oxide aligned on graphene surface can facilitate ion/charge transport and perform well-synergistic materials. This as-prepared hybrid electrode reveals the highest specific capacitance of 306.67 F g^{-1} at 1 A g^{-1} under UV irradiation, which is increased by 39.29 %.

Fabrication of Gas Sensors utilizing Semiconductor Heterostructures

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ABSTRACT

Heterostructure devices based on metal oxides and metal dichalcogenides have shown great potential in various fields, including electronics, photonics, and sensing. Semiconductor heterostructures were grown by physical & chemical vapor evaporation techniques. A variety of gas senors have been designed and fabricated with unique morphology exhibiting higher gas sensing response. The developed devices efficiently detect environmental pollutants gases. I'll discuss some of our recent findings in detail with possible mechanisms.

IT 28

Electric field control of magnetism: Energy-Efficient Spintronics for AI and IoT Applications

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ABSTRACT

The Internet of Things (IoT) and Artificial Intelligence (AI) devices need to process a vast amount of data at high speed for smooth interfacing with other supplementary devices on the network. However, the current computational architecture is not efficient for this purpose. One of the potential solutions to tackle this issue is to use spintronics devices. Spintronics-based memory devices conventionally use electrical current to manipulate electrons' spin direction and dynamics, which is elegant but comes with higher energy costs and lower device endurance. To meet the demands of faster, smaller, and ultra-low-power electronic devices, recent research has focused on voltage control of magnetism, which promises to deliver non-volatile memory solutions with ultra-low-power consumption for next-generation computing systems. Our recent efforts in this field involve voltage-controlled magnetism using different approaches, including voltage-controlled magnetic anisotropy (VCMA), voltage-controlled exchange coupling (VCEC), and multiferroic-based magnetoelectric coupling (MEC) for spintronics applications. Through these studies, we have made several new findings. For example, we achieved large perpendicular magnetic anisotropy (PMA) tunability by inserting heavy metallic layer at the MgO/ferromagnet interface. We also demonstrated the modulation of interlayer exchange coupling using non-ionic liquid gating, such as MgO. Additionally, we showed the modulation of magnetism by utilizing the magneto-electric coupling effect in a bismuth ferrite-based multiferroic system. These findings provide various pathways to modulate the resistance states of spintronic devices at low power and offer exciting possibilities for developing next-generation energy-efficient computing devices.

Keywords: Spintronics, MRAM, AI, IoT, Voltage-Control of Magnetism

IT 29

Thermoelectric Energy Harvester for Floating System Application

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ABSTRACT

Many countries face increasing challenges in meeting its energy requirements while minimizing environmental impact and promoting renewable energy sources. In addition, sectors involving energy production are the main greenhouse gases emitters. In order to tackle this issue, this study discusses the utilization of waste heat from water body surfaces as a viable source for generating zero carbon electricity. The process involves capturing waste heat from the water surfaces of ponds, lakes or reservoir and utilizing it to generate electricity through energy harvester system based on thermoelectric devices. In this study, we investigated the ability of the thermoelectric module to generate electrical power from the waste heat by evaluating its electrical power output under the fluctuating temperature. The power output was evaluated from simulated heat distribution and output voltage of a thermopile with several different structures, materials and heat sinks. It is found that a single thermopile consisting of $Bi_2Te_{2.7}Se_{0.3}$ and $Bi_{0.5}Sb_{1.5}Te_3$ as n- and p-type legs, respectively, produces a total power output of 0.85 mW at ten specific times for a day. A higher temperature difference within a thermopile can be obtained with a combination of Cu and water with a specific thickness as the heat sink materials resulting in a higher power output of 216 mW of a thermoelectric module. Consequently, the abundance of water body presents a significant opportunity for harnessing this untapped energy resource by implementing the proposed thermoelectric system.

IT 30

Earth abundant nitride thin films for energy applications

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ABSTRACT

Semiconducting materials based on II-IV-N_2 Nitrides, in particular, Zn–IV–N_2 display outstanding optoelectronic behavior and gained popularity in development of new nitride materials for thin film solar cells and light-emitting devices. Zn-IV-N_2 family semiconductors represent a potential nontoxic earth abundant element alternative to GaN, InGaN and the incumbent thin film photovoltaic absorber materials for both light generating and light harvesting technologies. Zinc Tin Nitride ($ZnSnN_2$) has been discovered as a new potential solar absorber for energy applications since its properties are similar to group III nitrides. But the main challenging issue for this material is to reliably synthesize films with carrier density 10^{17} to 10^{18} cm^{-3}. In this regard, $ZnSnN_2$ thin films were successfully developed by radio frequency (RF) magnetron sputtering and a systematic in-situ post growth annealing was performed in order to study its effect on the optoelectronic properties towards p-type conductivity. But at 500°C, in-situ post growth annealed film possesses good crystalline nature (69 nm) and also exhibits low carrier concentration ($3.97\text{-}2.42\times10^{18}$ cm^{-3}) and high mobility in the range of 14.5-11.1 cm^2 V^{-1} S^{-1}. However, alkaline-earth metallic dopants can improve the performance of Zn-IV-N_2 semiconductors. In view of this, Ba acceptor was successfully doped into $ZnSnN_2$ crystal lattice with various dopant concentrations (~0-7%) by reactive RF magnetron co-sputtering at 450°C. The orthorhombic structured Ba doped ZnSnN2 (Ba:ZTN) films with preferential orientation along (002) plane were obtained. Hall measurement studies revealed that the type of conduction is changed from the conventional n-type to p-type via Ba doping. The deposited Ba:ZTN films exhibited high hole concentration in the range of 1018-1019 cm-3 with low resistivity of ~10^{-1} Ωcm and a reasonable mobility of ~0.5-5 cm^2 V^{-1} s^{-1}. The doping of Ba at either Zn or Sn site would be responsible for the p-type conductivity in Ba:ZTN films. The variations in the surface properties such as morphology and topography of $ZnSnN_2$ on Ba doping were described by FE-SEM and AFM analysis. Further analysis by UV-Vis-NIR and X-ray photoelectron spectroscopies were also performed in order to reveal the optical performance and chemical bonding composition of Ba:ZTN thin films. The existence of Ba^{2+} ions in Ba:ZTN was confirmed by the obtained binding energies from XPS analysis. From the collective results, it is suggested that Ba:ZTN could be employed as effective p-type earth abundant layer in thin film solar cells.

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IT 31

Manipulation of polar topology

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ABSTRACT

The intricate configurations of topology provide a fertile ground for delving into emerging phenomena and exotic phases in condensed-matter physics. The recent discovery of polarization vortices, their intricate phase coexistence, and response to applied fields in ferroelectric oxide superlattices have inaugurated a new era of investigation into topology, emergent phenomena, and techniques for manipulating such features through the application of electric fields and temperature.[1,2] Here, we unveil the discovery of room-temperature chiral polar skyrmions within a lead-titanate layer, constrained by strontium-titanate layers through the manipulation of epitaxial constraints.[3] These nanoscale polar skyrmions serve as the electric counterparts to magnetic skyrmions, holding the potential to elevate ferroelectrics to unprecedented levels of functionality. This includes features such as motion of the skyrmion, manipulation of skyrmion boundary/core, and topological phase transitions through temperature and electric fields. [4-6] The integration of such functionality anticipates substantial advancements in high-frequency electronic applications, ferroelectric racetrack memory[6].

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IT 32

Electrocatalysts for Sustainable Carbon-Free E-Fuels

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ABSTRACT

The increasing demand for energy and environmental concerns has induced global efforts to find and explore alternative energy sources for fossil fuels. Electrocatalysts have been key in various electrochemical energy devices, such as Polymer electrolyte fuel cells and electrolyzers [1]. As an ideal candidate, hydrogen from water splitting is an attractive green approach for next-generation energy conversion devices. Design for highly efficient and durable catalysts has been considered. Replacing noble metal or metal oxides is a promising approach to overcome high-cost and elemental scarcity, greatly hindering their widespread applications. First, I will describe our recent research on developing low-cost, efficient, and robust electrocatalysts catalysts for water splitting to store sustainable energy resources. The new transition metal-carbon (TM@NC) electrode shows the OER overpotential of 330 mV with an ultra-stability over the noble electrode. The long-term water electrolysis cell stability testing using alloy core-carbon shell catalysts shows over 760 h stable activity (voltage loss of 4%) and outperformed the commercial (noble) catalysts [2]. Electrochemical ammonia synthesis by N2 fixation has proven to be a promising alternative to the energy-consuming, befouling Haber-Bosch process. Considering the low faradaic efficiency and sluggish kinetics of nitrogen reduction reaction (NRR), designing a robust and selective catalyst is significant. A hybrid nanocatalyst fabricated by a single-step in-situ nitridation method is a potential cost-effective electrocatalyst for NRR will be discussed [3. In addition, we demonstrate a room-temperature approach to transform pollutants into value-added e-chemicals with high selectivity and efficiency. The electrochemical reduction of nitric oxide to ammonia using a membrane electrode assembly electrolyzer over a core-shell catalyst in which Ni nanoparticles are wrapped by a porous nitrogen-doped carbon shell (Ni@NC) will be discussed [4,5].

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IT 33

Silicon-on-Insulator Photodiode with SP Antenna and Its Applications to Advanced Light Detection

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ABSTRACT

After the Ebbesen's discovery of extraordinary transmission through sub-wavelength hole array [1], the sub-wavelength optics have been applied to many optical fields because it can provide the transmission efficiency greater than predicted by the standard aperture theory, and overcome the fundamental diffraction limit. The phenomenon utilizes the optical near-fields of the surface plasmon (SP) waves that are strongly localized along the surfaces of periodic metallic grating. In the field of photodetector, SPs have been used to enhance the light sensitivity via SP excitation around the grating arranged near semiconductor photodetectors [2], [3]. We have applied SP antenna composed of metallic grating structure to silicon-on-insulator (SOI) p-n junction photodiode (PD). SOI substrates have been used for high-performance microprocessors in servers and gaming machines, because the isolation distance between devices can be made much smaller than that of bulk silicon (Si) counterpart, and parasitic capacitances can also be reduced largely. However, the SOI thickness for such high-performance integrated circuits is usually less than the gate length, and it becomes very difficult to integrate sensitive photodetectors due to the thickness being not large enough as a light absorber. In order to improve the light sensitivity in thin SOI, we have developed the SOI PDs with gold (Au) line-and-space (L/S) grating type SP antenna [4]. The L/S grating structure can excite a diffracted light from incident light, and then the diffracted light efficiently couples with the waveguiding mode in the SOI layer. Furthermore, two types of the applications using our SOI PD with SP antenna have been already proposed. The first one is an angle-sensitive pixel (ASP) which is an essential component in the field of computational imaging technology [5]. The second one is a refractive index (RI)-based optical biosensor [6]. The above details will be introduced in the presentation.

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IT 34

Mechanistic Investigation on the Capacity Loss in Phosphonated Anthraquinone Based Redox Flow Battery

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ABSTRACT

Continuous addition of renewable energy, such as solar photovoltaic and wind, to the grid requires an energy storage platform to maintain the resilience of the electric grid. A continuous decline in installation cost and a friendly policy allows rapid expansion of renewable energy installations. Complications associated with the seasonal and diurnal fluctuations of energy production can be handled effectively having an energy storage option attached to the grid. One of the promising approaches to manage energy efficiently is storing the energy in redox flow batteries. Although matured technologies such as vanadium redox flow batteries are available, their entry into commercial space is prohibited by the cost of vanadium. This situation calls for cheaper local content in place of redox active material. Our group explores various organic redox active molecules/scaffolds for aqueous and non-aqueous redox flow battery chemistries. Besides, our interest is in exploring various degradation pathways contributing to the capacity decay of the redox flow battery. Once the degradation pathways were identified either by molecular engineering or suitable means, we could stabilize the capacity of the battery.

Hydrothermal optimization of one-dimensional zinc oxide Nanostructure arrays for resistive based biosensors

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ABSTRACT

This study aims to investigate the influence of precursor concentration, reaction time and temperature on the growth of 1-D ZnO array via hydrothermal process through response surface methodology (RSM). One-dimensional zinc oxide (1-D ZnO) with high nanostructure density and smaller diameter size was created for better performance of DNA sensing. That morphological feature is strongly dependent on synthesis parameters. Herein, the Box-Behnken design was used to model and optimize the two independent synthesized parameters, which were successfully have been determined. The optimized parameter to produce high nanostructure density with a smaller diameter size of 1-D ZnO included a precursor concentration of 0.055 M, a reaction time of 5 hours and a temperature of 120 ℃. The experimental results indicated that the nanostructure density was 84.9 %, as confirmed by EDX analysis, which was close to the predicted result. In addition, the FESEM image also demonstrated that the actual and expected result of diameter size for the optimized sample were closely the same at 150.04 nm and 144.70 nm, respectively. Another essential finding in DNA sensing application is at least 30 minutes of incubation time and 40 minutes of drying time under 50℃ required for optimal hybridization process to get the accurate result. The proposed resistive biosensors lead to a good response toward DNA sensing as its sensitivity calculated was 1.98 MΩ/µM.cm2 with a wide linear range of 10 fM to 1 µM and the detection limit attained was 100 fM. The distinctive feature of these experiments is the fact that the samples were obtained to achieve two optimum parameters at the same time. This can be especially interesting for the development of biosensors based on nanostructures.

IT 36

Structural, magneto-caloric and unusual magnetic behavior in the nanocrystalline manganites

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ABSTRACT

Structural, magnetic, magneto-caloric and magneto-transport properties of nanocrystalline manganites were studied. The samples were prepared using sol–gel method and their morphology, particle sizes were confirmed by various microscopy measurements techniques. Field-cooled and zero field-cooled magnetization protocols with temperature span of 2 K–300 K, confirm the paramagnetic (PM) to ferromagnetic (FM) phase transition. The complete investigation of isothermal magnetization, Arrott plots, and magnetocaloric effect as well as quantitative analysis of second-order phase transition were discussed. The criticality at the PM-FM transition was examined for the samples, and the obtained critical exponents were verified for their reliability through the utilization of the scaling hypothesis and Kouvel-Fisher plot. We observed a large magnetic entropy change (~7 J-Kg^{-1}K^{-1}) for an applied magnetic field of 5 T. Above the metal–insulator transitions the electrical resistivity shows a small polaron hopping conduction mechanism, however, at low temperatures scattering mechanism dominates and the whole range was explained by the universal percolation model. The colossal value of negative MR was found for the studied samples. As a result of our experimental data, we can grasp the intuitive understanding of magnetic as well as electrical transport properties in Bi-doped manganite systems.

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Low lattice thermal conductivity of novel nivsn compound with 19 valence electron count

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ABSTRACT

Previous research on half-Heusler (h-Heusler) materials, such as MCoSb, and MNiSn, are primarily focused on 18 Valance Electron Count (VEC) per unit cell as it is thermodynamically more stable since all their bonding states are filled. In contrast, all of its antibonding states (conduction band) remained empty, resulting in the semiconductor behavior. As a result, most of the h-Heusler materials with 18 VEC have been considered the best candidate for thermoelectric (TE) materials. Further, stoichiometric h-Heusler composition XYZ with 18 VEC typically exhibits superior TE performance due to their closed shell configuration. However, understanding the variability of VEC impact on thermal and electrical transport is crucial for broad-based optimization of TE characteristics on the h-Heusler compound. Hence, in the current study, novel pristine compounds of VEC of 18 (NiVAl & NiAlSb) along with VEC of 19 (NiVSn) materials were synthesized via arc-melting followed by hot-pressing at 1073 K. The measured carrier concentration for all the compounds was found ∼ 10^{20}-10^{21} cm^{-3}. Further, NiAlSb, NiVAl, and NiVSn half-Heusler (HH) compounds displayed n-type semiconductor behavior, with maximum Seebeck coefficients (S) of −50.2 μV/K, −40.5 μV/K, and −14.5 μV/K at 723 K. As a result of the measured S and electrical conductivity, the estimated power factor for NiVSn (0.20 $mWm^{-1}K^{-2}$), NiAlSb (0.41 $mWm^{-1}K^{-2}$), and NiVAl (0.65 $mWm^{-1}K^{-2}$) at 723 K. The NiVSn lattice thermal conductivity (κl) was reduced to ∼ 79.8 % and ∼ 76.7 % when compared to NiAlSb and NiVAl 18 VEC compounds. The lower κl was mainly due to weak chemical bonding caused by lower phonon group velocity, resulting in increased anharmonicity in the lattice. Therefore, NiVSn of VEC 19-based compound opens a new avenue and can be considered as a potential candidate TE material with doping modulations when compared to traditional 18-VEC h-Heusler compounds.

Keywords: Thermoelectric; Anharmonicity; Phonon; Thermal conductivity; Electrical conductivity

IT 38

Visible light-driven Z-scheme photocatalyst of $sns_2/g\text{-}C_3N_4$ for dye decomposition.

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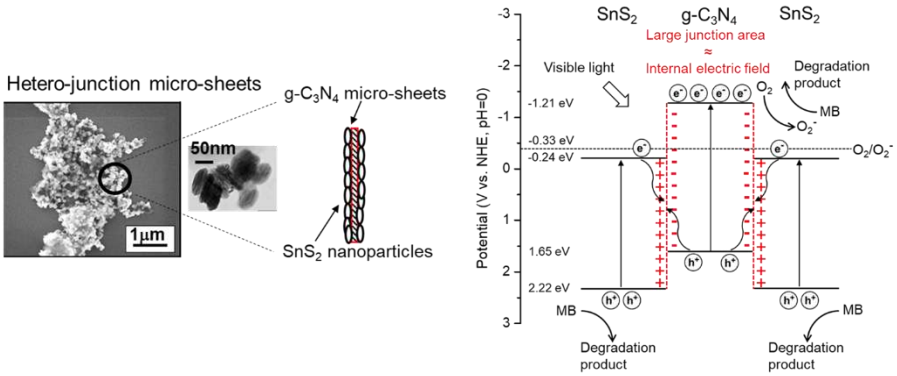
ABSTRACT

The stable formation of heterojunction composite and the enlargement of the junction area has been regarded as an effective approach for realizing highly efficient photocatalysts [1,2]. This study proposed a simple fabrication method for forming a stable heterojunction composite of $SnS_2/g\text{-}C_3N_4$ and aimed for a beneficial coupling of $g\text{-}C_3N_4$ and SnS_2 at the interfaces to increase the heterojunction area to the maximum degree. The synthesized $SnS_2/g\text{-}C_3N_4$ photocatalyst showed sufficient enhanced photocatalytic degradation of methylene blue (MB) dye under low-powered visible LED irradiation. Based on the X-ray photoelectron spectroscopy (XPS) analysis and the MB adsorption curves, a pseudo-double Z-scheme photocatalytic mechanism was proposed to explain the enhanced photocatalytic efficiency.



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IT 39

Development of high performance thermoelectric material in mid-and high temperature regime for viable power generators

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ABSTRACT

Thermoelectric materials can convert thermal energy to electricity via the Seebeck effect, and they are attractive because this conversion can be achieved with a compact solid state semiconductor device. There are two increasingly important applicative directions in which thermoelectric materials can play a large and critical role. One is the urgent necessity for energy saving to contribute to the recent carbon neutral/zero emission goals for the environment, and the other is energy harvesting to dynamically power the myriad necessary sensors for the Internet of Things (IoT) future society. In this talk, I will discuss recent developments and current research in high performance bulk thermoelectric materials (573-1273) K, comprising nanostructuring, mesostructuring, band alignment, band engineering and synergistically defining key strategies for boosting the thermoelectric performance. To date, the dramatic enhancements in the figure of merit achieved in bulk thermoelectric materials have come either from the reduction in lattice thermal conductivity or improvement in power factors, or both of them. Here, I'll summarize these relationships between very large reduction of the lattice thermal conductivity with all-scale hierarchical architecturing, large enhanced Seebeck coefficients with intra-matrix electronic structure engineering, and control of the carrier mobility with matrix/inclusion band alignment, which enhance the power factor and reduce the lattice thermal conductivity. The concept of hierarchical compositionally alloyed nanostructures to achieve these effects will be presented. Systems based on SnTe and SiGe in which spectacular advances were obtained will be given emphasis. A discussion of future possible strategies is aimed at enhancing the thermoelectric figure of merit followed by the development of viable power generators.

IT 40

Search of Band Bending Potential Curve Consistent with the Observed Electronic States

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ABSTRACT

Band bending, induced by electric field penetration into semiconductors, is a semiconductor property essential for field-effect transistors to operate. Recently, the realistic shape of band bending has attracted much attention because it is necessary to predict device performance, especially when the device size reaches the nano level[1-3]. In our previous study, we reported that the electronic states observed in Si(111) subsurface[4] (Fig. 1(a)) are inconsistent with the conventional band bending potentials in some cases. To explain the observed electronic states, a band bending potential consistent with the experimentally obtained electronic states was proposed through a time-consuming try-and-error search (Fig. 1(b)). The unconventional shape was attributed to the confinement of valence electrons into nano space [5]. This talk presents a more effective search of the band bending potential employing an artificial intelligence approach.

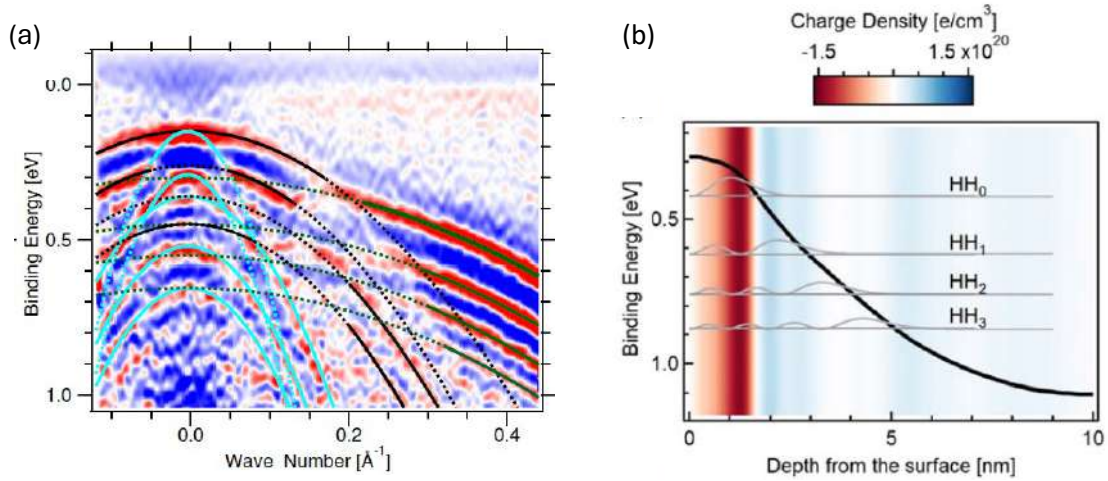

Fig. 1 (a) Electronic states in Si(111) p-type inversion layer obtained using photoelectron spectroscopy[4]. (b) Band bending potential consistent with one of the observed electronic states[5].

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Flash Joules Heating Methods with High Voltage Capacitor for Lab-Scale Graphene

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ABSTRACT

Flash joule heating (FJH) is a process where a material is heated to a very high temperature (3000°K) in a fraction of a second, turning electricity to heat using a capacitor. This treatment is commonly used to produce some types of carbon allotropes, such as Graphene [1–3]. In this research, the FJH components is consisted of one 450V 6000μF capacitor, 450VDC power supply, quartz pipe, copper wool, flash chamber, resistor, switch, cable, and storage tube. Figure 1 shows FJH methods.

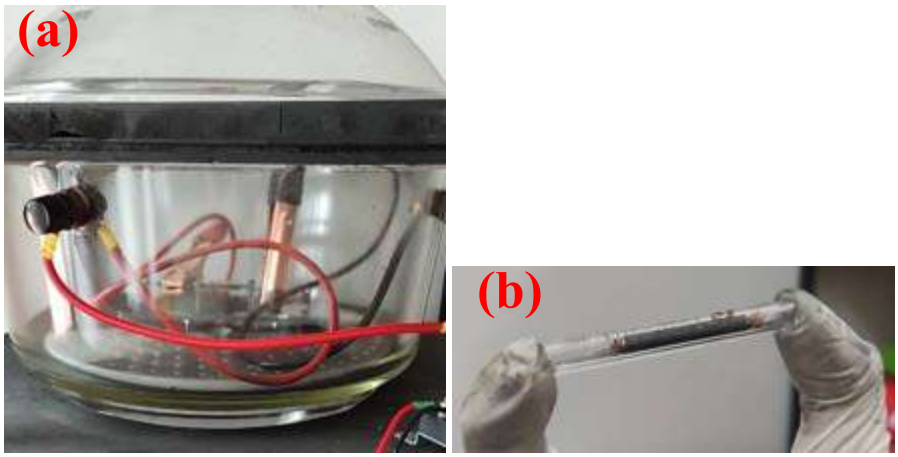

Figure 1. (a) FJH Chamber. (b) Carbon materials.

The resistivity of the material treated by the procedure will be measured, and Raman analysis will be performed. Variables of the process, that is the cable differences in the flash circuit and the types of FJH carbon material will be analyzed to determine the optimal FJH process. From the analysis, we can conclude that the parameters of the experiment are correlated to the FJH, and the process can be optimized.

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IT 42

Synchrotron-based Characterizations of Electrocatalytic Metal-Organic Frameworks and Covalent Organic Framework-based Solid Electrolyte Interphase for Stabilizing Anode of Rechargeable Batteries

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ABSTRACT

Considering energy-related technologies including rechargeable batteries and water electrolysis, effective catalytic materials play a crucial role in the rise and unceasing development. Metal-organic frameworks (MOFs) have drawn attention due to their abundant and identical catalytic sites along the periodic network with tunable catalytic functionality and stability. Herein, structural information, catalytic sites, and their corresponding mechanistic pathways have been investigated by employing synchrotron-based X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS). The framework stability, the accessible active sites related to pre-designed metal clusters, the alteration of oxidation state of, and the coordination geometry around the active metal centers evolving along the electrochemical oxygen evolution reaction (OER) are thoroughly revealed. In addition, aqueous zinc-ion batteries (AZIBs) are promising energy storage systems due to their cost-effectiveness and eco-friendliness. However, there are some limitations restricting their practical utilizations such as the high activity of water leading to Zn corrosion and hydrogen evolution, along with the formation of dendrites on the Zn surface during repeated charge–discharge cycles. To limit parasitic side reactions, an artificial solid electrolyte interphase (ASEI) protective layer made of a covalent organic framework (COFs) is an effective strategy. Herein, grazing-incidence XAS was employed to specifically characterize the Zn speciation on the electrode surface. According to XAS results, the protective COF-ASEI layer can retard the coordination of water at the electrolyte–Zn interface, improve Zn plating/stripping kinetics, and increase the stability of the Zn anode. This presentation highlights the significance of synchrotron characterizations in energy-related technologies.

IT 43

Fabrication of CeO2 and Cu2O Films for Humidity and Bending Sensors by Using Solution Processes Based on Thermochemical Calculations

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ABSTRACT

Functional oxide films such as CeO2 and Cu2O are generally fabricated by dry processes or thermal decomposition of starting material solutions. These processes need high temperature, and the required temperature is above about 300ºC in the case of the CeO2 films. However, both of CeO2 and Cu2O can be formed from Ce3+ and Cu+ ions below 100ºC according to the thermochemical calculations as shown in Fig. 1. The films fabrication below 100ºC by the solution process opens the way to fabricate the films on low heat-resistant resin substrates such as polyethylene (PE) and polyethylene terephthalate (PET), and on porous substrates such as foams with maintaining their original structure. CeO2 and Cu2O films were fabricated on the conductive PE foams and the flexible PET substrates by the G-LPD process1 and the spin-spray process2, which were developed by our group. The PE foams coated by CeO2 layers kept their original structure and perform humidity sensor properties1. The PET substrates coated by Cu2O films showed bending sensor properties with high resolution covering a wide curvature range2. Other than CeO2 and Cu2O, many kinds of oxides can be formed by the solution process. Our research enables to fabricate the functional oxide films on the porous and flexible resin substrates with maintaining their original structure.

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IT 45

Effect of Carbon Electrode Annealing Temperature on Perovskite Solar Cells

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ABSTRACT

Perovskite solar cells (PSCs) have shown an outstanding performance improvement since their first introduction[1]. Currently, high-performing PSCs still utilize gold, silver, or platinum as their counter electrode which can hinder the path of commercialization. Thus, carbon is introduced as an alternative counter electrode for PSC. Usually, to utilize a carbon counter electrode, carbon powder was made into a paste and then deposited onto the substrate. The substrate is then heated to evaporate the solvent and become a solid carbon layer. Research related to carbon annealing temperature was already conducted by another researcher, but their structure was mesoscopic where the carbon layer was deposited before the perovskite layer[2]. In this research, we investigate the effect of the annealing temperature of carbon counter electrode in PSC. The PSC was constructed on a fluoride-doped tin oxide (FTO) glass substrate. The FTO/compact TiO_2/mesoporous TiO_2/Perovskite/CuSCN/carbon structure was used. Carbon annealing temperature was varied to 80ºC, 100ºC, and 120ºC. It was found that as the annealing temperature was increased, the PSC's performance decreased. The notable decrease factor was from the open-circuit voltage (V_{OC}) parameter where it was 0.90 V at the annealing temperature of 80ºC, then steadily decreases to 0.81 V and 0.71 V at 100ºC and 120ºC, respectively. Short circuit current density (J_{SC}) also gives a similar decreasing trend. This might be caused by the change in perovskite crystal[3]. Even though the perovskite crystal formation was completed since its deposition process, exposing it to high temperatures during carbon layer deposition changed its characteristics and decomposed the perovskite material. It also noticed that the hysteresis of the PSC increases when exposed to high temperatures. Until now, the hysteresis issue in PSCs is under debate, but one factor is from defect in perovskite material which induced trap-assisted charge recombination[4]. High annealing temperature might induce a defect in the perovskite material. From the experiment, a carbon annealing temperature of 80ºC gives the best PSC performance with V_{OC} of 0.90 V, J_{SC} of 9.44 mA/cm^2, fill factor of 0.40, and efficiency of 3.36%. These results provide consideration on the preference of annealing temperature of a layer that deposited after perovskite, especially for carbon counter electrode.

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IT 46

Thermoelectric Metrology: A Comprehensive Review from a Manufacturer's Perspective

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ABSTRACT

Thermoelectric metrology, situated at the intersection of thermoelectricity and metrology, plays a pivotal role in optimizing thermoelectric materials as well as ensuring the accuracy and reliability of thermoelectric devices across various applications. We want to provide a comprehensive overview of recent advancements and challenges within thermoelectric metrology, from the perspective of an established commercial manufacturer and partner of the scientific community. Beginning with elucidating the state-of-the-art techniques and methodologies employed in the characterization of thermoelectric bulk materials and devices, including Seebeck coefficient measurement, thermal conductivity determination, and figure of merit evaluation. Furthermore, this overview highlights established setups for characterizing nano-scaled thermoelectric films, such as a unique chip-based system, utilizing the three-omega technique, as well as a FDTR setup, which is optimized from a commercial perspective. Analogous to an academic project progress, after the material characterization, a brief insight into the state-of-the-art characterization of thermoelectric devices will be provided. Finally, attention is drawn to open questions in measurement technology, underscoring areas ripe for further exploration and potential collaborations within the field of thermoelectric metrology.

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IT 47

Functional Nanomaterials for Theranostic applications

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ABSTRACT

Functional nanomaterials have emerged as a promising class of materials for theranostic applications, which refers to the integration of diagnosis and therapy into a single platform. These materials offer unique properties that make them well-suited for this purpose. Due to its high surface area, it allows for the attachment of multiple imaging and therapeutic agents, enabling multimodal theranostics. Because of its ability to tune size and shape, properties can be controlled to optimize the interaction of the nanomaterials with biological systems. The Biocompatibility of many functional nanomaterials can be designed to be biocompatible, meaning they can interact with biological systems without causing harm. For example, Gold nanoparticle can be functionalized with targeting molecules to specifically deliver drugs to diseased cells. Quantum dots are used for imaging (e.g., fluorescence, bioluminescence) and drug delivery. Mesoporous silica nanoparticles can be functionalized with targeting molecules to specifically deliver drugs to diseased cells. On the whole, Functional nanomaterials have the potential to revolutionize the diagnosis and treatment of diseases. They offer a unique combination of imaging and therapeutic capabilities that can lead to more effective and personalized treatments.

IT 48

Computational Insights into Multi-Donor-Acceptor Design for High Performance Thermally Activated Delayed Fluorescence Emitters

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ABSTRACT

Thermally Activated Delayed Fluorescence (TADF) is an exciting mechanism in the field of organic optoelectronics, offering the potential for efficiently converting triplet excitons into emissive singlet excitons. This property has significant implications for enhancing the quantum efficiency of applications such as organic light-emitting diodes (OLEDs). Our research is dedicated to exploring the design and development of efficient TADF molecules by investigating different arrangements of donor (D) and acceptor (A) connections. Specifically, our study will examine the D-A, D-A-D, A-D-A, D-A-D-A, D-A-A-D, and A-D-D-A connection configurations and their effects on the ground and excited state properties of TADF molecules. Through this study, we aim to establish a connection between donor-acceptor architecture and TADF properties by evaluating both ground and excited state characteristics of the newly designed molecules.

IT 49

Analysis of Performance Degradation in Single-Layer OLEDs Fabricated Using Vacuum-Free Lamination Methods

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ABSTRACT

Since efficient OLEDs were successfully demonstrated in 1987 [1], Organic Light-Emitting Diodes (OLEDs) have attracted significant attention for their promising applications in display [2] and lighting technologies [3]. Among various fabrication methods, solution-based polymers using the lamination method are promising since they offer a much lower cost and enable large-area device fabrication [4,5]. However, using lamination techniques in OLED fabrication has presented challenges in maintaining optimal performance. This study aims to analyze the factors contributing to the decline in the performance of laminated OLEDs. The research employs a comprehensive approach, integrating experimental investigations and theoretical analyses to identify and understand the causes behind the diminished performance. Key factors such as device structure, lamination process parameters, and environmental influences are explored to assess their impact on OLED functionality. Device structure emerges as a critical aspect affecting OLED performance, as improper interactions between layers can lead to reduced fabrication success rate and efficiency and compromised device integrity. The study investigates the effects of double Kapton taping to enhance fabrication success rate, to be used in mitigating performance degradation. Lamination process parameters, including temperature, pressure, and spin coating speed, are scrutinized for their influence on OLED performance. Variations in these parameters can affect the uniformity of layers and alter the overall device characteristics. Furthermore, environmental factors, such as moisture and oxygen ingress during the lamination process, including bias application, are considered potential contributors to performance decline. This analysis draws on a comprehensive review of relevant literature and experimental results, offering valuable insights into the challenges associated with laminated OLEDs.

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IT 50

Li-ion Capacitors and Recycling Li-ion batteries

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ABSTRACT

Recycling lithium-ion batteries (LIBs) are gaining attention in the recent past since the short lifetime of ~3 years in electronic devices and ~5-10 years in EVs could generate a mammoth volume of spent LIBs, with 2 million metric tonnes expected by 2030, which encourages the development of effective recycling technologies. With environmental concerns, spent LIBs has triggered massive interest in emerging various crystal structures of metal oxides and different kinds of carbon materials that provide the opportunities to replace commercial materials beyond the energy storage and conversion applications cost-effectively. Finally, the requirement for the workhorse anode, graphite, is also demanding. The discovery of graphene, also driving a graphite demand, further upsurges the global graphite market, paving the search for new battery-grade graphite sources. The existing spent LIBs industrial recycling technologies overlook that graphite should be recycled to meet the global demand, creating an opportunity for reuse in the LIB manufacturing process and reducing the burden of resource dependency. The recovered graphite anode renders excellent performance in Li-ion capacitors with activated carbon as the counter electrode. The performance has been compared with commercial graphite, hard carbon, synthetic graphites, semi-crystalline carbon, etc.

IT 51

Fabrication of Magnetic Nanoclusters Modified Gold Electrode for the Impedimetric Detection of Serum Albumin

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ABSTRACT

Albumin is the most abundant protein in blood. Human serum albumin (HSA), with a molecular weight of 66.5 kD, is produced in liver. Serum albumin has essential physiological functions such as to maintain the osmotic pressure between blood and tissues and to transport those species such as hormones, fatty acid, etc. Therefore, albumin is a very important biomarker indicating the physiological condition of one□s body. Additionally, iron oxide magnetic nanomaterials have been widely investigated because of their superparamagnetic property upon subjected to an external magnetic field. Consequently, we propose an Au electrode modified by iron oxide magnetic nanoclusters (MNCs) for the electrochemical detection of serum albumin. Thermal decomposition was applied to prepare uniformly distributed iron oxide nanoparticles. Afterwards, iron oxide magnetic nanoclusters (MNCs) were successfully prepared. The hydrophobic surfaces of the nanoclusters were turned into hydrophilic by appropriately chosen ligand. The hydrophilic nanoclusters were further conjugated with sulfo-SMCC (sulfo-N-succinimidyl 4-(N-maleimidomethyl) cyclohexane-1carboxylate). Vi which, the electrode coated with SMCC conjugated MNCs (MNC@SMCC) were able to capture albumin. Impedance analysis on the electrodes at different stages was carried out. Thus, the calibration curve of impedance change against albumin concentration spiked in serum was established with excellent linearity. Detection of albumin concentration in the range of 1~10 g/dL is feasible by the as-prepared MNC@SMCC coated Au electrode. For stability test, the as-prepared sensor can maintain reproducibility for at least 30 days. To the 60 serum specimens received from NCKU hospital, the average recovery of 82% is achieved by the measurements from the as-prepared sensor.

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IT 52

A visible light wide angle optical divider based on III/nitride for under water application

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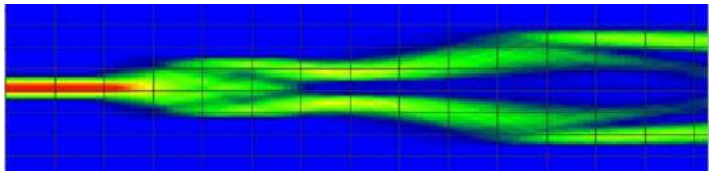
ABSTRACT

In this paper, we propose the design of a wide-angle 1×2 optical power divider using gallium-nitride (GaN) semiconductor on sapphire, suitable for underwater optical wireless communication. The design comprises six rectangular waveguides based on mode coupling phenomena. Numerical experiments reveal that optimal results are achieved with a width of 4 µm for the input and output waveguide ports, and a 15 µm distance between output ports.

The design analysis employed the beam propagation method (BPM). Optimization was carried out using the 3D FD-BPM method with an optical signal input at the maritime application wavelength of λ=0.45 µm. The optical signal was injected into the central input waveguide. Results indicate that at a propagation length of 860 µm, the optical power divides into two output beams with an excess loss of 0.75 dB and equal power output. This proposed design holds promise for further development and application in underwater communication technology.



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IT 53

Langmuir-Blodgett technique: a versatile method to prepare high quality and ordered ultra-thin films for various applications

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ABSTRACT

Lately, numerous low dimensional materials, such as carbon nanomaterials (CNs), layered transition metal dichalcogenides (TMDs), oxides (TMOs) and conducting polymers, have been investigated for various applications owing to their chemical and thermal stabilities as well as environmental friendliness. It has been suggested that the quantum confinement as a result of reducing the dimensions of these materials may induce many improved properties such as thermoelectricity, mechanical flexibility, metal-to-insulator transition[1,2]. Various techniques, such as chemical vapor deposition, Radio-frequency (RF) sputtering, thermal evaporation, laser pulse deposition, atomic layer deposition (ALD) and molecular beam epitaxy (MBE) have been employed to prepare these ultra-thin films. However, present techniques to prepare films have following disadvantages (i) necessity of corrosive precursor or co-reactants (ii) requirement of high vacuum and high deposition temperature, so difficulty in deposition on conventional flexible substrates (iii) high consumption of materials, (iv) high cost and (v) scalability. Langmuir-Blodgett (LB) technique, on the other hand, is very simple, environmental-friendly, and versatile method to prepare ordered multilayers of controlled thickness on all kind of substrates. However, the use of this technique to prepare films of materials, such as CNs, TMOs, TMDs, conducting polymers etc is hindered by lack of amphiphilic character in the material. In order to overcome this difficulty, generally a suitable surfactant is mixed to the spreading solution, but this approach results in inferior electrical properties of the deposited material. In this regard, we have extensively used LB technique to develop highly ordered, pure (without surfactant) and uniform ultra-thin films of various materials such as PEDOT, MEH-PPV, WO_3, TiO_2, PdO, CeO_2 on various substrates[3]. The morphology and compactness of the films was optimized through suitable manipulation of spreading solution, subphase pH, barrier speed, deposition speed, and post-transfer treatments etc. The prepared films were thoroughly characterized to optimize properties such as structure, energy levels, morphology, and conductivity. In this talk, a review of the efforts made along these directions will be presented and their applications for various practical devices will be discussed.

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IT 54

Nanostructured Manganese Oxide based Two-Dimensional Nanocomposites for the Removal of Organic Pollutants

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ABSTRACT

Nanostructured manganese oxide-based two-dimensional (2D) nanocomposites have emerged as promising materials for the removal of organic pollutants. These materials combine the advantageous features of low cost, high surface area, wide potential window, high theoretical capacity, and rich valence states. Nanostructured manganese oxide-based 2D nanocomposites were synthesized via an electrostatic self-assembly method. These novel materials exhibit great potential for the removal of organic pollutants. The nanocomposites were confirmed to possess a cubic structure and the structural insight is crucial for understanding their properties. The morphological characterization like SEM, FESEM, and TEM analyses revealed an intriguing architecture: accordion-like multilayer graphene and Ti_3C_2Tx MXene sheets adorned with 1D Mn_2O_3 nanorods and $NiMnO_3$/$NiMn_2O_4$ materials. This unique arrangement enhances surface area and active sites. The synthesized nanocomposites exhibited excellent performance in the photodegradation of both single and mixed dyes. Its efficient removal of organic pollutants makes it a promising candidate for environmental applications. A scavenger test confirmed the active involvement of radicals in the photodegradation process. These findings contribute to the growing field of advanced materials for environmental remediation and underscore the potential of Nanostructured manganese oxide-based 2D nanocomposites in addressing pollution challenges.

IT 55

Growth of $Si_{1-x}Ge_x$ ($0 < x < 1$) alloy semiconductor under rapid cooling

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ABSTRACT

$Si_{1-x}Ge_x$ alloy semiconductor is a potential material for electronic applications since its band gap and lattice constant can be tuned by varying the composition. Moreover, it is a well-known material for thermoelectric applications especially at elevated temperatures. However, the thermoelectric properties of the alloys are drastically varied with composition. Therefore, compositionally homogeneous $Si_{1-x}Ge_x$ alloy semiconductor is highly imperative for thermoelectric applications. Understanding the growth mechanism is useful for controlling the compositional variations. On the other hand, regarding the fundamentals of crystallization, some phenomena during the growth process have not been clarified completely. Dendrite growth is a well-known phenomenon, which appears during the solidification processes of various materials. However, the details of dendrite growth in $Si_{1-x}Ge_x$ ($0 < x < 1$) melts have not yet been investigated in detail. It is attempted to observe dendritic growth in $Si_{1-x}Ge_x$ ($0 < x < 1$) melts over a wide range of composition by an in-situ observation technique [1, 2]. It was found that twin-related dendrites appear in $Si_{1-x}Ge_x$ ($0 < x < 1$) melts [2]. It was also found that faceted dendrites can be grown in directional solidification before instability of the crystal/melt interface occurs, when a growing crystal contains parallel twin boundaries.

Keywords: In-situ observation: $Si_{1-x}Ge_x$ alloy semiconductor; Crystal Growth

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IT 56

Nanomaterial Applications in Ultrafast Photonics

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ABSTRACT

Nanomaterials, distinguished by their exceptional optical, mechanical, and electrical attributes, have become pivotal in advancing fields such as optoelectronics, sensors, biomedicine, and ultrafast photonics. Their nonlinear optical properties, rapid recovery times, and wide-ranging operational capacities uniquely position nanomaterials as highly effective saturable absorbers in ultrafast pulsed lasers. Over the past decades, a diverse array of nanomaterials has emerged as saturable absorbers, contributing to the development of lasers with outstanding performance characteristics. This review aims to provide a comprehensive overview of the integration and applications of nanomaterials in ultrafast photonics, serving as a landmark for current cutting-edge developments. The exploration covers the utilization of nanomaterials in ultrafast photonics, with a detailed examination of carbon-based materials (carbon nanotubes and graphene), typical 2D materials (topological insulators, transition metal dichalcogenides, black phosphorus, and MXenes), and metal-based nanomaterials (gold, silver, copper, and metal oxides). Each nanomaterial's ultrafast applications are systematically summarized, highlighting major parameters of ultrafast lasers and distinctive features of individual nanomaterials. This presentation offers insightful perspectives on the potential trajectory of nanomaterials for further advancements in ultrafast photonics, encouraging ongoing research endeavours in this dynamic and rapidly evolving field.

IT 57

Growth and Defects challenges of Wide bandgap Electronic Materials: Applications

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ABSTRACT

GaN and ZnO are the well-known wide bandgap (~3.4 eV at room temperature) with large exciton binding energy semiconducting materials for Electronic device applications. Their optical bandgap can be tune from UV to IR regions of electromagnetic spectrum by alloying. Hence, they can be used for various applications. Especially III-nitride semiconductors have been using for making high temperature, high frequency and high-power devices. However, a reverse leakage current due to unintentionally added dislocations/deep level defects in the materials during their growth time or at processing is remain a big challenge. In this talk, I will first demonstrate on method to identify the deep level defects in GaN Schottky barrier diode and InGaN/GaN quantum well-structured LEDs and explore possible reverse leakage current mechanism such as Poole-Frenkel (PF) emisión via deep defects in these devices. Secondly, growth challenges involved to obtain 0D, 1D, 2D and 3D of ZnO nanostructures. In our work, various nanostructures of ZnO such as nano-rod, nano-disc, nano-flakes and core shell hetero structures were found while doping ZnO in synthesis process and studied their applications. Particularly, ZnO nano-rods studied for polymer LED applications. It was observed that, luminance of ZnO nanorod/MEH-PPV LED increased by 20 % as compared to PLED without rods due to single waveguide effect in ZnO nano-rods. Finally, I will talk about how the core-shell structured SmO/ZnO hetero nano-junction will be used to remove methyl green dye molecules from water.

Research on the Energy Conversion Devices: Focusing on Solar Cells and Mechanoluminescence

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ABSTRACT

Energy can be converted from one form into another. Solar cell is a well-known example of the energy conversion device that converts light energy to electrical energy. We have been engaged in the researches on dye-sensitized and perovskite-type solar cells, and mechanoluminescent materials, the latter is the material which convert mechanical energy to light energy. In the present talk, I introduce two topics regarding to the title: Firstly, novel fluorine-doped tin dioxide (FTO) nanostructures as a transparent conducting layer for the dye-sensitized solar cells. Secondly, color controllable novel organic mechanoluminescent materials. Various nanotechnological architectures of FTO layers have been formed on a glass substrate by using an advanced spray pyrolysis deposition (SPD) technique. The technique allows the perfect control of morphology of nanotechnological architectures of FTO, which can be achieved simply by controlling spray condition. As such, 0-D nanocrystallites, 1- D uncapped nanorods and 1-D capped nanorods; all in 2-D thin layers, and extensively cross-linked 3-D nano- technological architectures of FTO can be prepared, on soda lime glass surfaces. This is the first report on kinetically-controlled growth of different nanotechnological architectures of FTO, using the same technique. Furthermore, the technique is versatile and is not limited only to fabricate FTO nanostructures, but, it can also be used to fabricate thin layers of nano-technological structures of different dimensionalities of various materials on various substrates, which is capable to withstand required pyrolytic temperatures. Mechanoluminescence (ML) is a phenomenon that light emission is induced by a mechanical action on a solid. Europium-doped dibenzoylmethide triethylammonium (EuD_4TEA) has been known as an organic ML material. We have succeeded to synthesize EuD_4TEA at a very low temperature of 70 °C using controlled slow cooling method. An addition of polyvinylpyrrolidon has enhanced the emission intensity. Orange light emission is demonstrated in the talk. We have also synthesized organic mechanoluminescent material based on a 1,10-phenanthroline and an acetylacetone. The synthesized material shows a green-color mechanoluminescence by doping of a terbium (Tb). Furthermore, we have investigated an effect of co-doping of Tb and europium (Eu) or dysprosium (Dy) on the luminescence property.

IT 59

Spatial Representation of Multi-Energy 3D X-ray CT Using Mixed Reality for Nondestructive Testing

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ABSTRACT

Augmented reality (AR), virtual reality (VR), and mixed reality (MR) are increasingly applied in non-destructive testing fields. Multi-energy 3D X-ray CT has gained prominence for specific functions for its material discrimination based on energy information[1]. This study explores mixed reality (MR) technology for spatially representing internal object structures using multi-energy X-ray CT data in material discrimination segmentation. A spatial representation that overlays two-dimensional DICOM images on a surface-rendered model to visualize both the object's surfaces and internal structures using motion capture has been proposed. The system transfers X-ray CT data to a high-performance PC, which performs surface rendering and data conversion into 3D format. Unity is employed to superimpose DICOM data onto the model's cross-section and match the coordinate positions in virtual and real space. Leap Motion Controller facilitates gesture-based interactions. A Spatial Reality Display represents data in three dimensions. The system has been demonstrated by imaging a lithium-ion battery, displaying its internal structure and control board using multi-energy X-ray data in red and blue on the spatial reality display. MR representation enabled the observation of the lithium-ion battery's substrate structure. Boundary surface manipulation through hand gestures allowed dynamic exploration. Users could enhance specific areas of interest by superimposing 10-70KeV data in red and 70-150KeV data in blue at 50% density. This study successfully showcased MR's application in material discrimination using multi-energy X-ray data. MR representation in three dimensions offers flexible observation angles. Boundary surface manipulation and data compositing provide versatile tools for exploring internal structures, enhancing the information extracted from multi-energy X-ray imaging.

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IT 60

Upgraded Recycling of Cast-Iron Scrap Chips towards Fe-based Thermoelectric Materials for Waste-heat Energy Harvesting

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ABSTRACT

In this research, an environmentally friendly and cost-effective production process involving the upgraded recycling of cast-iron scrap chips into thermoelectric materials based on iron (Fe) was proposed. The thermoelectric performance of Fe-based materials, including iron-silicide (β-$FeSi_2$) and Heusler alloys (Fe_2VAl), utilizing cast-iron scrap chips was thoroughly examined across temperatures ranging from room temperature to 800°C. The study identified an optimal dimensionless figure of merit, ZT (0.22 for n-type at 700°C and 0.17 for p-type at 700°C), making it a favourable starting material for producing β-$FeSi_2$ thermoelectric materials [1]. The development of n-type and p-type β-$FeSi_2$ modules was achieved, and the coefficient of thermal expansion was evaluated. Isothermal oxidation tests were conducted at 800°C in air for 14 days using an electric furnace to assess the oxidation behaviour of β-$FeSi_2$ prepared from cast-iron scrap chips [2]. The results indicated that β-$FeSi_2$ derived from cast-iron scrap chips exhibited a promising long lifetime at high temperatures (around 800°C) in air, showcasing excellent potential for stability in high-temperature thermoelectric devices when utilizing cast-iron scrap chips as a starting material. Furthermore, the thermoelectric performance of Fe_2VAl, prepared using cast-iron scrap chips, demonstrated positive outcomes. The p-type Fe_2VAl exhibited the highest power factor (PF) value of 1604$\mu Wm^{-1}K^{-2}$ at 200°C. Additionally, undoped Fe_2VAl, prepared from cast-iron scrap chips, showed a substantial improvement, with a PF value of 967$\mu Wm^{-1}K^{-2}$ at 200°C, approximately twice that of previously reported values [3]. Unfortunately, the fabrication of n-type Fe_2VAl specimens from cast-iron scrap chips was hindered by impurities present in the scrap chips' composition [4]. Despite this limitation, the use of cast-iron scrap chips for producing undoped and p-type Fe_2VAl alloys holds potential for contributing to eco-friendly and cost-effective production processes. Ultimately, the research delves into comprehensive guidelines aimed at enhancing recycling processes, with a specific emphasis on esteemed intermetallic compounds. This exploration occurs within the broader framework of elevating the recycling of cast-iron scrap chips, representing a significant endeavour to mitigate the abundance of waste and advance toward a more environmentally friendly and cost-effective production paradigm.

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IT 61

Indigenous Materials for Energy Storage Applications: From Lab Innovations to Semi-Pilot Scale Production

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ABSTRACT

Lithium-ion batteries (LIBs) are currently used in most electric vehicles (EVs) due to their high energy density, better nominal voltage, enhanced temperature stability, low maintenance, eco-friendliness, long cyclic stability and low self-discharge. Among the cathode chemistries used in LIBs, Lithium ferrous phosphate (LFP) cathode material has a safer chemistry because it avoids self-oxidation and thermal runaway due to strong covalent bond between P and O in PO4 structure of LFP. The first part of the presentation highlights the development of. Indigenous electrode materials technology that are essential for the manufacturing of Li-ion batteries within the country. ARCI has developed an innovative and low-cost high energy milling process for the synthesis of in-situ carbon modified LFP for Lithium-ion batteries. In continuation with the effort to synthesize large quantities, 15-20 Kg C-LFP/batch has been successfully carried out in collaboration with Indian Powder Metallurgy Industry. The electrochemical performance of large-scale synthesized C-LFP exhibits a capacity of 1.75 Ah and 1.45Ah at the formation and 1C current rate respectively. An Indian patent and foreign applications are filed related to this invention.1 Technology Know-how for the production of LFP has transferred to M/s. Allox Minerals (within India), and M/s. ALTMIN (Global), and the technology has successfully demonstrated. M/s. ALTMIN established a LFP semi-pilot plant of 50kg/day production capacity at ARCI campus. Further, ARCI also developed a simple, economical scalable, and energy-efficient process for the production of lithium titanium oxide (LTO) anode material with a performance at par with commercial LTO. Subsequently, LTO-based 1.5Ah 26650 cell as well as 0.45Ah Pouch cells have been fabricated and demonstrated. A large-scale demonstration of ARCI's developed LTO process has been initiated in collaboration with Industry. 15 kg batch of LTO has been synthesized and the resulting LTO delivers a superior rate capability of 145 mAh/g at 4C with good cyclic stability. The LTO innovation has been filed in National and worldwide2 and technology transfer is in progress

The second part of the presentation will focus on the development of graphene-like activated porous carbons3 by a low-cost chemical activation process using petcoke, a by-product of the oil refining process. Petcoke is a rich carbon source material but contains a significant amount of sulfur as an impurity making it unsuitable as fuel in cement and steel industries due to the emission of CO2 and SO2. Its alternative use in supercapacitors can abate the emission problem while finding a high-value addition to it. Herein, we report the synthesis of activated graphene like structured carbon carbon with a surface area of 2394 m^2/g by chemical activation process, and demonstrate beyond the coin-cell level, i.e. by fabricating a 1200 F cylindrical supercapacitor (60 mm dia & 80 mm height using the indigenously developed petcoke derived carbon. Then, an indigenous Supercapacitor device with the specifications of 1200 F, 2.7V, and with a stored energy of 1.22 Wh and a gravimetric energy density of 5.05 Wh/Kg has successfully fabricated using petcoke-derived carbon.4 16 numbers of 1200F indigenous Supercapacitors were connected in serial to assemble the module with specifications of 75F, 43V, 19.2 Wh for E-Bicycle demonstration. The developed supercap-Bike have been successfully demonstrated for the driving range of 1 km range with charging time of >5 min.

Template assisted sol-gel synthesis of $BiFeO_3$ hollow tubes

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ABSTRACT

Bismuth ferrite ($BiFeO_3$) is one of the most prominent perovskite materials well known for its multifunctional properties and related applications. The recent research on this material includes the synthesis of hollow-structured $BiFeO_3$ using various methods and exploring their applications in photocatalysis and sensing. In this study, we introduce a facile method for the synthesis of $BiFeO_3$ hollow tubes using the sol-gel method, where kapok fiber collected from Ceiba Pentandra is used as a biotemplate for the first time. In the procedure, the annealing path was modified by introducing intermediate holding steps besides varying the final annealing temperature. The structural analysis was carried out using x-ray diffraction (XRD) and Raman analysis, whereas the formation of hollow tube morphology was confirmed with the help of FESEM analysis. The complete decomposition of the kapok fiber template during the annealing process was confirmed with the help of Fourier transform infrared spectroscopy. The XRD analysis indicated that monitoring both the annealing pathway and the final annealing temperature is pivotal in attaining the formation of phase pure $BiFeO_3$. The proposed method eliminates the requirement for additional procedures for extracting the synthesized hollow tubes from the parent template, in addition to providing a less expensive strategy for the synthesis of $BiFeO_3$ hollow tubes.

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IT 63

Development of Chemical Vapor Deposition Technology for the Synthesis of Carbon Nanotube and Nanofiber Forest

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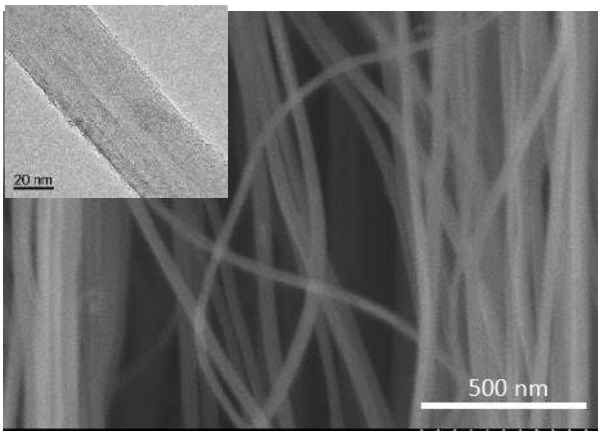
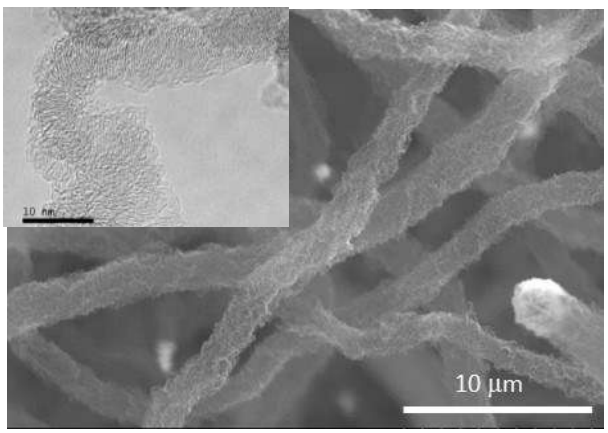
ABSTRACT

Chemical Vapor Deposition (CVD) is a process where a solid material is synthesized through the chemical reaction of vapor near or on a substrate surface, typically heated, within a controlled environment such as a vacuum or inert atmosphere. Carbon precursor gases, when passed over the heated substrate (which may include a catalyst deposition), undergo chemical reactions leading to the formation of a solid phase, deposited onto the substrate. The growth conditions, choice of carbon feedstock, and catalyst selection are critical factors influencing the occurrence and kinetics of various reactions, ultimately determining the carbon structures synthesized. Here, we introduce a newly developed multifunctional chemical vapor deposition system used for the synthesis of spinnable carbon nanotubes and carbon nanofibers using Cu and Fe catalysts. Spinnable carbon nanotubes were produced utilizing acetylene as the carbon feedstock and $FeCl_2$ as the catalyst. Continuous spinnability was achieved by introducing Cl_2 gas into the acetylene stream, with chamber conditions set at a pressure of 3 torr and a temperature of 800°C. The resulting spinnable carbon nanotubes were utilized to create CNT yarns and sheets, forming single-direction aligned networks for various applications.

Furthermore, substituting Fe catalyst with Cu catalyst in the form of CuI led to the growth of carbon fiber forests using acetylene gas under chamber conditions set at a pressure of 3 torr and a temperature of 750°C. SEM and TEM analysis revealed a unique structure of carbonrods where thousands of carbon nanorods constituted each microcarbon rod. To the best of our knowledge, though there are studies about carbonaceous-based nanomaterials using Cu catalysts, this is the first study to use CuI as the catalyst for the synthesis of carbon nanofibers by the floating catalyst method. The figure below illustrates the spinnable carbon nanotube forest and carbon nanofiber forest grown using $FeCl_2$ and CuI catalysts, respectively.





IT 64

Synthesis mechanisms of chalcogenide nanostructures via aqueous based reflux method for enhanced room temperature thermoelectric performance

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ABSTRACT

Current research on thermoelectric (TE) materials is focused on improving the power factor with a drastic reduction of thermal conductivity (κ) using mixtures of multiphase nanostructured materials and hence the nanostructured TE materials have attracted much attention for achieving enhanced figure of merit (ZT) for practical applications. Among the available class of TE materials, group V chalcogenide materials have attracted as good TE materials known to exhibit very high ZT values around room temperatures. In this work, we discuss a simple, cost effective, and a systematic study of surfactant assisted aqueous-based low-temperature chemical method for the synthesis of (Bi,Sb,Sn)-Te nanostructures. Again, thermoelectric properties of the developed nanostructures are investigated. An in-depth understanding of the chemistry involved in the reaction mechanism and decomposition of Ethylenediamenetetraacetic (EDTA) acid is proposed for different precursors of Bi, Sb and Sn where possibilities of aqueous based low temperature synthesis of phase pure Bi_2Te_3, SnTe, and Sb_2Te_3 will also be discussed in detail.

IT 65

3D printed Phase Retarders

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ABSTRACT

Form birefringence is important in photonics because it allows one to control polarization state of light using non-birefringent, optically isotropic materials. Here we report on realization of form birefringent phase retarder structures operating atvisible wavelengths by the 3D laser printing technique. The structures use 3D photonic crystal architecture modified to enhance their structural anisotropy, leading to strong birefringence and phase retardation exceeding a full wavelength, while their total thickness remains less than about ten full wavelengths. As far as 3D laser printing is concerned, the 3D form birefringent structures are easier to realize and offer much better performance compared to the simple form birefringent 1D sub-wavelength gratings (SWG). The finely patterned 3D structures remain self- supporting and mechanically stable, which enables one to control their thickness and achieve the required high phase retardation levels, whereas mechanical stability of laser-printed SWGs becomes poor when their period becomes shorter than the visible wavelength, which limits their maximum thickness and the achievable phase retardation. We demonstrate laser printing of 3D form birefringent structures exhibiting the quarter- and half-wave phase retardation levels needed in many applications as well as fabrication of spatially-variant Q-plate structures having a half-wave retardance, and a radially-variant orientation of the optical axis. Fast prototyping of such structures using 3D laser printing technique may help to realize compact polarization-sensitive optical elements for integrated photonic devices.

IT 66

Metal-Organic Framework Derived 3D Hierarchical Metal Oxides for High Energy Density Supercapacitor Application

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ABSTRACT

Metal-organic frameworks (MOFs) have been considered a vowing class of advanced materials for supercapacitors, sensing, gas adsorption, and catalysis due to their crystalline structure, high porosities, and tuneable chemical composition. With their unique porous structure with large surface areas, MOFs are ideal sacrificial templates to derive various porous materials, like metal oxides, carbonaceous materials, and metal/carbon composites. Typically, these derivatives possess the same structures as those of their parent MOFs, as well as higher surface areas and porosity compared to those produced by other synthesis methods. These are beneficial for supercapacitors since they can provide many active sites, shorten the ion diffusion length, and increase the wettability of the electrode material. In the present work, the 3D hierarchical Co_3O_4@NF electrode is fabricated by simple thermolysis of a cobalt-based metal-organic framework which was grown on nickel foam (NF). The electrochemical properties of Co_3O_4@NF studied in mixed electrolyte solution contain LiOH and KOH with different ratio. The electrolyte with 0.2 M LiOH and 3 M KOH provided better ionic transportation to the Co3O4@NF electrode and exhibited a specific capacity of 630.4 Cg^{-1} at 1 Ag^{-1}. We fabricated an ultrahigh energy density asymmetric supercapacitor (ASC) having metal-organic framework derived Co_3O_4@NF as a positive electrode, commercial activated charcoal (CAC) as a negative electrode, and mixed cationic electrolyte of potassium hydroxide (KOH) + lithium hydroxide (LiOH). The ASC gives an energy density of 61.84 W h kg^{-1} at a power density of 775 W kg^{-1} with 72.3 % capacity retention over 10,000 cycles at 10 Ag^{-1}.

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IT 67

Wearable Thermoelectric Power Generator for Self-Powered Physiological Sensor

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ABSTRACT

For long-term monitoring of patients, we have developed a novel wireless sensor with self-power generation using wearable thermoelectric devices, in which there are two viewpoints. One is a study on the optimal wearable device structure [1], and the other is the improvement of flexible thermoelectric materials [2,3]. In this presentation, with the aim of realizing high-efficient flexible thermoelectric materials appropriate for wearable devices, the results of the crystallographic property of ZnO nanorods grown on conductive NiCu fabrics by microwave-assisted solvothermal synthesis are mainly explained.

ZnO nanostructures were formed on a NiCu fabric substrate using two-step microwave-assisted solvothermal synthesis. Dense seeds of ZnO were grown on the fabric as a first step, and then, ZnO nanorods grew up in the second step. The microwave was used in both steps.

From scanning electron microscope (SEM) images of ZnO morphological structures grown on a NiCu fabric for microwave power 100 W with an irradiation time of 3 min in the crystal-growth step, it was found that the fabric surface is fully covered with dense nanorods with a diameter of about 10 nm although there are large protrusions locally. In the case of conventional solvothermal synthesis with a furnace, it spent several hours for ZnO growth, and ZnO nanosheets and nanopillars were frequently observed [2,3]. Therefore, the microwave has effects of shortening the synthesis time and of making ZnO nanorods.

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IT 68

Nanotechnology Advancements for Sustainable Energy: Addressing Critical Materials Challenges

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ABSTRACT

This study delves into nanotechnology's pivotal role in advancing materials sustainability for energy applications, addressing concerns surrounding the depletion of critical technology metals. The paper advocates the use of nanostructured materials and nanotechnology-based systems to tackle issues in the supply of crucial materials for clean and renewable energy technologies. Strategies proposed encompass the exploration of new nanostructured materials, leveraging quantum effects, and employing nanotechnology for efficient separation and recovery of critical materials from non-traditional sources like mine tailings and electronic wastes. For thin-film solar cells, which rely on critical materials like Tellurium and Indium, the suggested sustainability strategies involve discovering alternative nanostructured absorbing materials, utilizing quantum confinement, and incorporating advancements in nanophotonics to reduce the demand for these critical elements. Similarly, for LED devices and phosphors in lighting technologies dependent on Gallium, Indium, and Rare Earth Elements (REEs), the proposed strategies include harnessing nanoparticles, quantum confinement, and transitioning to LED lights to significantly decrease phosphor usage. In the realm of solar fuel generators using catalysts such as Platinum and Palladium, the sustainable approach involves developing catalysts with nanomaterials based on earth-abundant elements and optimizing grain size to enhance catalytic activity. Colloidal route synthesis of quaternary compound CZTS (Cu_2ZnSnS_4) has been anticipated with an inimitable combination of coordinating ligands and solvents using the Hot Injection technique. CZTS is recognized as one of the worthiest materials for photo-voltaic/catalytic applications due to its exclusive properties (viz., non-toxic, economical, direct bandgap, high absorbance coefficient, etc.). This work also demonstrates the formation of crystalline, single-phased, monodispersed, and electrically passivated CZTS nanoparticles using a distinctive combination of ligands viz. Oleic acid (OA)-trioctylphosphine (TOP) and Butylamine (BA)-trioctylphosphine (TOP). Detailed optical, structural, and electrochemical studies were done for all CZTS nanoparticles, and the most efficient composition was found using ligands Butylamine and TOP. CZTS nanocrystals were rendered hydrophilic via surface-ligand engineering, which was used for photocatalysis studies of organic pollutants and textile effluents for waste water remediation. Malachite-green (MG) and Rhodamine-6G (Rh) for water remediation and has great commercial prospects. This work seeks to replace costly noble-metal co-catalysts with economical, transition-metal alternatives. CZTS nanocrystals exhibit effective photoluminescence quenching, demonstrated by notable Stern-Volmer quenching constants (K_{sv}), signifying efficient charge transfer for one dye, alongside energy transfer phenomena for another dye, evident through spectral overlap and FRET efficiency. The study also explores nanotechnological parameters for next-gen photovoltaics, emphasizing the synthesis of bulk heterojunction solar cells, low-cost production of inorganic thin films, self-assembly techniques for nanorod structures, and the use of chemically synthesized quantum confined structures. From a global and Indian perspective, the study underscores the need for improved scientific infrastructure, increased research investment, and refined implementation strategies to drive sustainable energy development.

IT 69

Nanostructured antimonides for waste heat harvesting

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ABSTRACT

Thermoelectric materials have gained increasing recognition as a sustainable source of electric energy that can meet a wide range of applications. The energy conversion efficiency of the thermoelectric (TE) materials is determined by the dimensionless figure of merit (ZT), which depends on the thermal and electrical conductivity, the Seebeck coefficient, and the temperature gradient. However, the major barriers to mainstreaming the use of TE devices in the practical application are their low ZT and high cost. Cobalt antimonide ($CoSb_3$) based skutterudites and layered magnesium antimonides (Mg_3Sb_2) are preferred for thermoelectric (TE) applications due to their advantageous fabrication process and cost effectiveness. Chemical substitution and filling in these materials have garnered significant attention for automotive TE modules, as they exhibit stable TE properties within the temperature range of 573 to 773 K. This has led to the innovation of novel filled/doped antimonides, demonstrating improved ZT values at intermediate temperatures. Our focus lies in the cost-effective development of TE materials for applications in the intermediate temperature range. Utilizing the powder metallurgy route allows for the efficient production of antimonides in large quantities within a shorter time frame. Additionally, thermo-mechanical treatments further enhance the mechanical properties of these materials [1]. A noteworthy achievement is the attainment of the highest ZT value, approximately 1.85, in n-type singleelement filled skutterudites [1]. Furthermore, our research indicates that codoping of monovalent atoms (such as Li-Ag and Na-Ag) at the Mg site of Mg_3Sb_2 results in a synergistic effect, boosting electrical conductivity and enhancing the thermoelectric properties of p-type Mg_3Sb_2. It's worth noting that Ag prefers the Mg_2 site, while Li and Na are favourable at the Mg_1 site of the Mg_3Sb_2 lattice [2]. In understanding the mechanisms at play, our investigation confirms the dominance of the three-phonon scattering mechanism and the four-phonon scattering process in monovalent atoms doped Mg_3Sb_2 [3]. Our work on a constructive approach to enhancing ZT through potential doping as well as the significance of optical phonons in antimonide-based thermoelectric materials will be presented.

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IT 70

Designing High Efficiency Bi-Te Thermoelectric Power Generators: Challenges and Approaches

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ABSTRACT

Worldwide the waste heat distribution of temperature in environment from various energy resources is concentrated in the temperature range of 373-573 K. Thermoelectric Generators (TEGs) can directly convert heat into electrical energy, and thus are very promising towards fuel efficiency (η) enhancement and developing self-sustained power sources for remote applications. To develop efficient thermoelectric generators (TEGs), a prerequisite is to couple high figure-of-merit ($zT=\alpha^2\sigma/\kappa$) n- and p-type thermoelectric materials through metallic interconnect, with low specific contact resistivity (ρc). The realization of low ρc involves several critical factors as the chemical stability, mechanical strength, sharpness of interfaces etc. which should be carefully optimized to achieve consistent output performance under long-term operation. Owing to the emerging concepts and strategies in material designing, compatible high zT (~1.2) n/p-type Bi-Te materials are developed. Using the electrically conducive Ni interface layers mechanically stable low contact resistivity (< 10 μΩ-cm^2) is realized in n-type and p-type Bi-Te material. Designed TEG shows the η of ~8%, at temperature gradient of ~240 K, which is at par the best report value in Bi-Te material at lab scale.

IT 71

Atomic layer deposition of oxide layers for efficient passivation of silicon solar cell surface

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ABSTRACT

High-efficiency silicon solar cell technologies such as PERC, TOPCon, etc., rely on the reduction of charge carrier recombination at the surfaces, which is known as surface passivation. This is achieved using dielectric surface passivation layers such as HfO_2, Al_2O_3, SiO_2, etc. Traditionally, silicon surface passivation involves the formation of a thin SiO2 layer, which requires a high-thermal budget process for longer periods. In order to mitigate the issues with high-thermal budget processes, considerable efforts have been made to develop low-temperature surface passivation methods. Among these methods, atomic layer deposition (ALD) has proven to be an efficient process for developing high-quality dielectric layers for silicon surfaces. It is a self-limited reaction mechanism by chemisorption of multiple precursors pulsed into the reaction chamber alternately. However, the interface quality of oxide-silicon plays a crucial role in reducing the surface recombination losses, which in turn depends on the method used to develope the oxide dielectrics. In the present talk, the development of oxide films using the ALD method is being elaborated for the efficient passivation of silicon. The oxide (HfO_2/Al_2O_3) thin films have been grown on Si substrates by two different ALD methods, such as thermal (T-ALD) and plasma-enhanced (PE-ALD) modes. The films were deposited using metal-organic precursor, while water vapor was used as an oxygen reactant in the case of the T-ALD process, and it is oxygen plasma during the PE-ALD process. A systematic study has been carried out for both the ALD methods, and the influence on their physical properties as well as the quality of the interface with silicon has been evaluated using appropriate evaluation methods. The T-ALD method demonstrated state-of-the-art quality surface passivation with a minority carrier lifetime exceeding 3 ms at the temperatures < 400 ºC. Alhough good quality films have been deposited using PEALD (200 ºC), the layers are more defective, i.e., with vacancies promoted by the electric field of the plasma sheath. The effective surface recombination velocity (Seff, max) ~ 10 cm/s is achieved at intermediate bulk injection levels using T-ALD layer within the thickness range, < 10 nm. The role of field and chemical passivation is investigated in terms of fixed charge and interface defect densities. It is concluded that uniform films could be grown using T-ALD at a relatively higher temperature in comparison with the PE-ALD, and effectively passivate silicon surface due to their low interface defect density and moderate fixed oxide charges.

IT 72

Effect of Gravity on the Growth of InGaSb Alloy Semiconductor Crystals

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ABSTRACT

InGaSb is a ternary alloy having tunable lattice parameter (6.096 ~ 6.479 Å) and wavelength (1.7 ~ 6.8 μm) in IR region. The dissolution and growth processes are strongly influenced by gravity because the transportation of the solute is affected by convection. Microgravity (μG) is a good condition to suppress the complex convective heat and mass transports and to make deeper insight into transport phenomena. InGaSb ternary alloy semiconductor crystals were grown at International Space Station (ISS) and 1G condition on Earth to elucidate the factors affecting the crystal growth of a bulk ternary alloy semiconductor. GaSb single crystals and InSb poly crystalline crystals were grown by Czochralski method and a sandwich structure of ampoule GaSb(seed)/InSb/GaSb(feed) was prepared. It was used to grow InGaSb crystals by vertical gradient freezing method at a temperature gradient 0.6 ˚C/mm. Heat pulses were introduced during growth for every 2 h to calculate the growth rate and interface shape of the grown crystals. It was found that the interface shape was highly concave towards solution and more amount of seed crystal was dissolved than feed crystal even though the seed temperature was lower than the feed temperature under 1 G. On the other hand, the interface was nearly flat and more amount of feed crystal was dissolved than seed crystal under μG. It indicated that gravity affected dissolution and growth processes. The detailed results on the microgravity experiment and related numerical simulation would be presented.

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IT 73

Intermittent Spray Pyrolysis Deposition for Thin-Film Formation and Its Applications to Various Functional Film Makings

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ABSTRACT

A spray pyrolysis deposition (SPD) for thin-film formation is performed under atmospheric pressure using simple system consisting of two-fluid type atomizer, air compressor, solution reservoir, and well temperature-controlled heater. Starting raw materials-containing solution is atomized towards a heated substrate by a pneumatic system not consecutively but intermittently to hold well a substrate temperature prescribed, because mists of starting solution after atomized with compressed air lets the substrate temperature reduce immediately. Inorganic and organic metal compounds having any adapted solvent are all available as raw materials for SPD. Original component and composition of starting solution are surely reflected in deposited film except for easily evaporated additives; namely, this method gives neatly thin-film with expected component and composition. Deposition process is probably divided into four stages of ①mists from atomizer wet substrate surface to make liquid film and the surface temperature is kept at the boiling temperature of solvent until its evaporation according to the Gibbs' Phase Rule, ②solute left behind on a substrate yields metal clusters throughout thermal decomposition and/or chemical reaction, ③metal clusters convert instantly to compound-clusters by reacting with negative ion existed in solution, and ④condensation and cohesion of these compound-clusters yield solid film finally. To start with fluorine-doped tin oxide (FTO), many examples of functional thin-films formation using SPD will be introduced variously including metal, oxide, double oxide, sulfide, oxy-sulfide, etc.

IT 74

Nanoplasmonic micro- structured chip for single cell sensing application

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ABSTRACT

Protein secretion monitoring provides intercellular cell activity information that can be used as early indication of infectious diseases in the human body. It is common to use average response from bulk cell as primary cell activity observation. However, this standard method does obscures any individual cell momentous response over large population of cell, hiding any important signal to highlight. Therefore, it is necessary to isolate cell into single cell position, reducing cell to cell contact arrangement before observeits intercellular activities. To address this issue, we developed label free new sensing platform that combine micro – structure microwell array that able to isolate individual cell with nanoplasmonic sensing capacity that can be used to observe real time intercellular activity. Clean Aluminum oxide electrode undergoes two-step anodizing procedure. Specific design was developusing Su8 photoresist forming 60µm diameter disk on this surface. Prepared mould was used to emboss 188µm thickness Zf-14 cyclo olefin polymers (COP) with high pressure. Finally, gold layer was sputtered forming micro and nano structure on its surface. Imaging observation reveals mushroom look-alike nano-structures with average diameters of 190nm and micro-structured microwells with diameters of 70µm in single chip. The sensitivity prepared plasmonic device was further evaluated over various surrounding refractive index environments. This plasmonic device shows red-shifted behavior with sensitivity calculated at 274nm/RIU. Next, trapping capacity of prepared microwell design was calculated by allowing 20um beads solution (~1200 beads) to sediment for 30minutes before number beads isolated in each microwell was determined. It is found that, 14% of total microwell was showing single cell isolation phenomena.

IT 75

Current Scenario of Dye-sensitized Solar Cells - Modifications and Large-Scale Production

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ABSTRACT

Dye-sensitized solar cells (DSSCs) are gaining much attention mainly because of the ease of fabrication and the materials employed are low-cost, and environmentally friendly. Modification of key components of DSSCs and large-scale production is in progress nowadays. Replacing Pt electrodes in conventional DSSCs by 2D transition metal dichalcogenides (TMDCs) are of MX2 type semiconducting materials where M denotes Mo, W, or Zr and X denotes S, Se, or Te have been discussed in this lecture. Further, migration from DSSCs towards perovskite solar cells has also been highlighted here

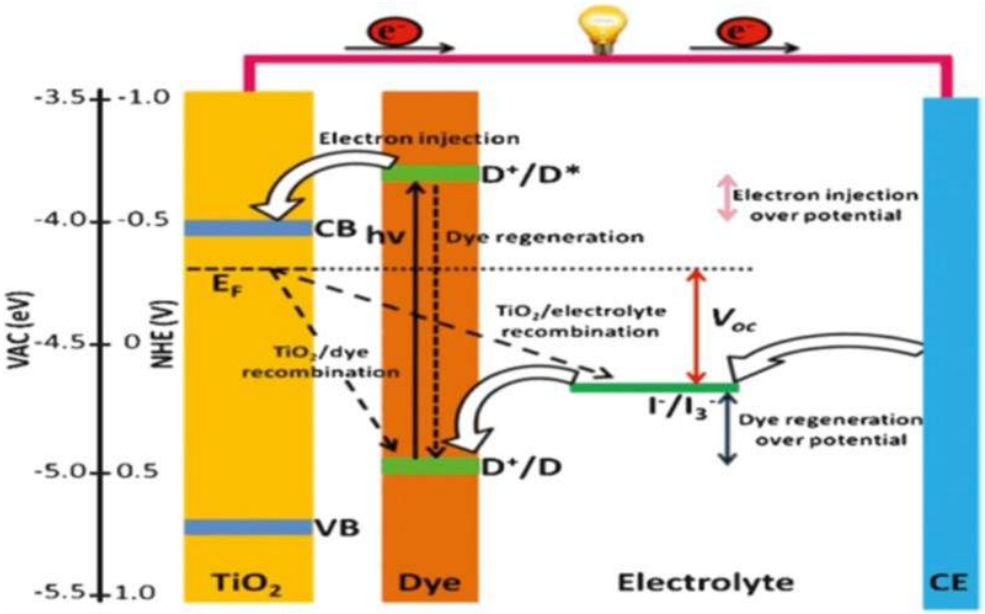

Figure: Diagram showing DSSC's energy levels

IT 76

Synthesis and Versatile Applications of Cu-Based Delafossite Compounds

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ABSTRACT

Cu-based delafossite compounds such as $CuCrO_2$, $CuFeO_2$ and $CuAlO_2$ have attracted much attention as a p-type transparent conductive oxide(TCO) used for several applications such as transparent diodes and solar cells. Related studies on delafossite oxides are interested not only in examining the TCO properties but also in exploring their applications as photo catalysts for hydrogen evolution, removal of divalent metal ions, reduction of cadmium, magnetics, and thermoelectric devices. One method for improving the catalysis efficiency is to decrease the size of the catalyst to increase the surface area and adsorption ability. Synthesizing Cu-based delafossite powder can therefore be expected to improve the performance of catalytic applications, and controlling the valence state of Cu to 1+ and Fe to 3+ is the key to synthesize delafossite successfully. We not only successfully synthesized Cu-based delafossite powder[1] but also synthesized a lot kind of composite such as $CuCrO_2$-TiO_2, $CuCrO_2$-CeO_2 nano powder using glycine nitrate process[2]. Employed electrospinning method to prepare $CuCrO_2$, $CuFeO_2$, $CuCrO_2$-TiO_2, $CuCrO_2$-CeO_2 nanofiber[3] and $CuAl_2O_4$, $CuCrO_2$ nanotube[4]. We prepared various shaped 0D nanoparticle, 1D nanofiber, 2D thin films, 3D porous powder of delafossite compound to examining their potential applications such as p-type TCO[5], antibacterial coating[6], photo catalyst for heavy metal reduction[7], steam reforming of methanol[8], catalyst for CO_2 reduction[9], electrochemical sensor[10], etc.

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IT 77

Recycling of polyethylene terephthalate wastes for prosthetic applications

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ABSTRACT

With the increasing usage of polyethylene terephthalate (PET) wastes polluting the environment, the recycling of PET wastes has become a crucial issue to be overcome. PET has been extensively used for broad applications due to its durability, strength, non-toxic, and lightweight characteristics. Because of the limitations possessed by the current recycling methods, a variety of ideas have also been suggested and experimented with by reinforcing nanofillers with recycled plastic wastes to enhance the mechanical strength as well as the dimensional stability of recycled products. This can be done using solvent-based method, which will reduce the damage to the mechanical and other properties of the final products. However, there was scarcely any research reported that studied the reincorporation of nanofillers with PET using solvent-based means and its effect on the respective thermo-mechanical properties of the final composites. Therefore, the presented research study will produce an optimum PET-Zinc Oxide (ZnO) nanocomposite specifically for the application of prosthetic sockets. To date, the PET matrix has been successfully reincorporated with the ZnO at different concentration loadings and their chemical analysis have been analyzed. Future work for the rest of the study will involve investigation of different ZnO concentrations towards the morphology, mechanical, thermal behavior, and antimicrobial properties. The PET- ZnO nanocomposites obtained will then be utilized for the fabrication of a prosthetic socket. The results that will be obtained from this study are aid the future development of prosthetic socket as an alternative material with a more affordable cost. It also helps to extend the study of the PET recycling method using a solvent-based method without damaging the molecular structure of PET and degrading its properties.

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CL 01

A 920 MHz RF-to-DC Rectifier Circuit as Radio Frequency Energy Harvesting Module for Agriculture Applications

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ABSTRACT

Agriculture 4.0, which is the future of agricultural technology, symbolizes a revolution in farming through the integration of advanced technologies such as the Internet of Things (IoT), precision agriculture, and many more. One method for involving the next-generation IoT implementation in proactive energy replenishment and next-generation wireless network is Radio Frequency (RF) energy harvesting. As a tool for energy harvesting, a rectenna (rectifier and antenna) is proposed in LoRA frequency of 920 MHz, which consists of a receiver antenna, matching network, RF-to-DC Rectifier, storage element, and a load. By exclusively capturing the LoRa frequency characterized by narrowband features, the selectivity of RF signal energy targeting and extraction from particular sources is heightened. This optimization aims to maximize the potential for energy harvesting while minimizing vulnerability to interference from undesired noise sources. The two-stage voltage multiplier based on the Greinacher voltage doubler is adopted for rectifier and combined with dual-band E-shaped patch antenna. According to the simulation results, the proposed circuit has an output voltage of 3.3 V, an output current of 2.2 mA, and an efficiency level of 73.31%. This circuit is constructed in a PCB with a 4 x 2.4 cm dimension.

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CL 02

Electrical Properties of Polymer Blend Electrolyte on Dye-Sensitized Solar Cells (DSSC) Application

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ABSTRACT

Polymer blend electrolyte (PBE) based on poly-methyl methacrylate (PMMA) and polyvinylidene fluoride (PVdF) polymers have been prepared using a solution casting technique [1]. Prepared PBE has been investigated using various ratios of PMMA and PVdF polymers. The Electrical Impedance Spectroscopy (EIS) shows the optimum conductivity value is PMMA:PVdF (70:30) with 3.82×10^{-5} Scm^{-1}. The temperature dependence conductivity has been performed in the 300–373 K range, which is observed to obey the Arrhenius behaviour [2]. The dielectric constant (ε') and loss (ε") increases with temperature at lower frequencies and approach negligible values at higher frequencies. This behaviour can be explained based on electrode polarization effects [3]. The plot of the real, M_r and imaginary part, M_i versus frequency, indicates that the systems are predominantly ionic conductors. DSSC's performance's efficiency value is impressive by using PBE, standing at 0.06%. The interaction between these two polymers influences the performance of DSSC.

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CL 03

High-Performance Etched-TiO_2 rod Nanophotocatalyzer for Methelyne Blue Degradation

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ABSTRACT

Titanium dioxide (TiO2) is widely known as a good catalyst for photocatalysis to treat dyes. However, the degradation of methylene blue (MB) using TiO2 rods comes to a standstill at 50-55%. Hence, high-crystallinity TiO_2 rods are etched with hydrochloric acid (HCl) to improve their catalytic efficacy. The etching treatment assists by increasing charge transfer and improving surface area by transposing the blunt tip of nanorods to nanocaves. The photocatalytic analysis was conducted to study and compare the ability of as-deposited and etched TiO_2 rod to degrade the MB. The degradation percentage of MB is plotted against time to observe the photocatalytic efficiency. With fixed reaction time of 10 hours, it resulted in a degradation increase of 52.48%. Nevertheless, TiO_2's photocatalytic activity is also greatly influenced by other factors, including pH, and pollutant loading. The results reveal that the MB degradation is at the highest at 99.39% which favour pH 12 and 5ppm concentration. The experiment was conducted to prepare rutile phases of TiO2 in the presence of UV light irradiation. This work shows that optimizing the conditions for the catalyst and pollutant places a role in improving the photocatalytic activity.

Keywords: *TiO2, Photocatalysis, Methylene Blue, Thin Film*

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CL 04

Formation of Calcium-Alginate Microbeads Encapsulated Gold Nanorods and its Potential for Long-Term Fungal Treatment

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ABSTRACT

Anisotropic gold nanoparticles (GNPs) colloids have stability issues maintaining their size and shape for a long time. In fungal treatment, controlled release is crucial to ensure optimal functionality and overcome lifetime limitations. Hence, encapsulation of GNPs was proposed to stabilize and protect the particles from unwanted chemical interaction and simultaneously extend the use time with controlled release. In this study, gold nanorods (GNRs) were encapsulated with varied sodium alginate (SA) ratios and calcium chloride. The GNRs were synthesized using seed-mediated growth methods (SMGM), which comprised the preparation of seed solution for 2 hours and a 20-hour ageing growth period. The formation of encapsulated gold nanorods (EGNRs) was done using an extrusion method, in which the mix of centrifuged GNRs and SA was dropped into CaCl2 solution at a flow rate of 1 mL/min. The optical response of GNRs shows two plasmon peaks after the centrifuge process at 528 nm and 699 nm, whereas the structural results exhibit two XRD peaks on the (111) and (200) planes, confirming the formation of GNRs. The synthesized GNRs have an average surface density of 74.81% and an aspect ratio of 4.23 ± 0.36. The encapsulation process suggests increased SA concentration causes larger Ca-Alg microbeads EGNRs. The characterization of EGNRs resulting in the 3:1 ratio of SA to CaCl2 is the most optimal for encapsulation and potential for controlled release application. The optimum sample shows an excellent hydrophilic surface with an angle of 39.30° and a good response to the control release test. Therefore, the EGNRs were proposed for long-term fungal treatment due to their exceptional ability to control the release of the anisotropic GNPs colloids.

CL 05

Development of LSPR-Based Glucose Sensor Using Short-Term Period Thiol-Functionalized Gold Nanobipyramids

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ABSTRACT

Glucose is essential for human health because it serves the primary function of providing energy for the body's cells. The low glucose level can cause hypoglycemia with dizziness, confusion, weakness, sweating, trembling, and even loss of consciousness. On the other hand, a high glucose level can increase the risk of developing type 2 diabetes, a long-term disorder that interferes with the body's control of blood sugar levels. This may result in numerous consequences, such as nerve damage, renal disease, and cardiovascular disease. Therefore, it is crucial to detect and keep track of glucose to ensure that it stays within the usual range. An alternative glucose detection method is proposed using a Localized Surface Plasmon Resonance (LSPR), called a plasmonic sensor, to improve several areas from conventional methods, such as invasive, needing an expert for the result analysis and needing long-time detection. The gold nanobipyramids (GNBPs) are chosen as a sensing material due to their advantage, such as being inert, slow to react with other chemicals, conducting electricity well, and safe as catalysts. Also, they produce higher electric field enhancement, increasing sensitivity and selectivity compared to other structures. The GNBPs are synthesized using the seed-mediated growth method (SMGM), divided into seeding and growth processes. Then, GNBPs are functionalized by thiol groups for a short period, i.e., 3 hours, to improve the sensor performance. The short-period thiol-functionalized GNBPs (t-GNBPs) with a length of 117.99 ± 10.37 nm, a width of 43.64 ± 4.13 nm, and an aspect ratio of 2.72 ± 0.34 are tested in the glucose medium with a 100 – 106 µM concentration. The result shows that a plasmonic sensor using short-period t-GNBPs for glucose detection performs a high sensitivity factor of 40.116 nm/RIU for t-SPR and 13.080 nm/RIU for l-SPR and high linearity through R2 over 0.9; an excellent selectivity towards three different analytes; good stability with a low error value of 0.58 ± 0.0008 a.u for the t-SPR peak and 0.74 ± 0.000033 a.u for the l-SPR peak; and good repeatability with a low CoR value of 0.00544 and 0.00886 for the t-SPR and l-SPR peak, respectively. In addition, the limit of detection for this system is 1 µM. This result shows that short-period t-GNBPs perform a better sensing parameter than long-period t-GNBPs. Hence, the plasmonic sensor using short-period t-GNBPs to detect glucose is successfully developed with promising performance for practical application.

Keywords: *functionalization, glucose detection, plasmonic sensor, thiol*

CL 06

Electron Transport Properties Analysis of Titanium Dioxide Dye-sensitized Solar Cells (TiO_2-DSSCs) based on Ratio (TiO_2 powder-P25) using Dye Gambier as Sensitizer

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ABSTRACT

The depletion of fossil fuel supplies and their impact on climate change has led to an energy crisis. Scientists have developed a third-generation solar cell technology called dye-sensitized solar cells (DSSCs) to address this issue. DSSCs have many advantages, including low cost, simple production, good performance in low illumination levels, and the ability to use multi-color dye options. However, the efficiency of DSSCs is still low compared to thin film-based solar cells. The two components that have a significant impact on DSSC performance are the semiconductor (as the working electrode) and the dye (as the sensitizer). For the semiconductor, titanium dioxide (TiO_2) is used because it has a band gap of 3-3.2 eV, which allows electrons to be transferred from the HOMO to the LUMO. Meanwhile, the dye is one of the primary components influencing cell performance. The use of natural dyes is a promising strategy since natural sources are plentiful, and the extraction process is simple and non-polluting. For this investigation, Gambier dye was chosen because it has numerous capabilities that can be used to increase the performance of DSSCs. The optimal ratio of TiO_2 was determined based on the electron transfer and dye absorption, which can be examined electrically and optically.

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CL 07

A Novel Composite Coating of SiO_2 and PVDF for Daytime Passive Radiative Cooling

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ABSTRACT

Passive radiative cooling (PRC) technology can reflect sunlight and radiate excess heat through the atmospheric window to outer space by utilizing the material's inherent properties without requiring any energy input or generating any pollution[1]. PRC can effectively reduce the use of traditional air conditioning, thereby reducing the energy consumption and greenhouse gas emissions associated with industrialization, effectively palliating energy crises and global warming. Therefore, passive radiative cooling technology has become a novel cooling technology[2].

In this study, we employed the Stöber method[3] to synthesize SiO_2 particles and modulated their surface morphology and particle size by adding cetyltrimethylammonium bromide(CTAB), thereby improving the solar reflection of silica capability and thermal radiation performance. According to the experimental results, it has been confirmed that the addition of CTAB can effectively control the surface morphology and particle size of SiO_2 particles, resulting in higher solar reflectivity and excellent selective emissivity. By blending SiO_2 particles with polyvinylidene difluoride (PVDF), which has high thermal radiation performance, we successfully prepared a passive radiative cooling paint and used a simple blade-coating method to fabricate a radiative cooling coating.

As the result of the outdoor experiment, our radiative cooling coating can achieve a cooling performance lower than the ambient temperature under high solar irradiance and high humidity conditions unfavorable for daytime radiative cooling, proving the radiative cooling coating has an excellent radiative cooling ability.

Keywords: *Passive radiative cooling coating, SiO2 particles, PVDF, CTAB*

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CL 08

Overcoming Performance Evaluation of Hysteresis-issued Perovskite Solar Cells with a Maximum Power Point Tracking (MPPT)

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ABSTRACT

The rapid research and development of perovskite solar cells (PSC) for practical applications are driven by both global warming concerns and industrial demands. However, the unique power generation behavior of PSC, including hysteresis, presents challenges in standardizing the evaluation methods. This urgent issue necessitates the development of accurate evaluation techniques. In this study, we present an equipment system designed to address this requirement. Hysteresis in I-V measurements, caused by capacitance components in stacked PSC, can lead to overestimation or underestimation of the performance[1]. PSC exhibiting hysteresis in the I-V curve manifests two distinct maximum power points in the forward and reverse I-V curves, which depend on the scan speed, starting point, and direction of the scan. By implementing maximum power point tracking (MPPT), the genuine maximum output power of PSC can be promptly determined[2]. Our newly developed device enables both I-V tracing and MPPT for PSC. The system continuously plots the light intensity and temperature data alongside the maximum power point, allowing each sample to handle up to 10 V and 1 A capacity. With a programmable electronic load integrated into the analyzer, the MPPT algorithm maintained a sample at its maximum power point, ensuring efficient power generation. This MPPT-integrated PV power analysis system offers a comprehensive solution to the evaluation challenges faced in PSC research and development. It makes accurate and efficient assessment of PSC performance, contributing to the advancement of practical applications and standardization of evaluation methods. Additionally, novel PSC fabrication process consisting of spray pyrolysis deposition, ink-jet printing and dispensing will be introduced instead of predominantly used spin-coating.

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CL 09

Comparative Evaluation of X-ray Backscattered Energy Spectrum for Subsurface Material Characterization

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ABSTRACT

X-ray backscattering emerges as a pivotal technique in the realm of subsurface exploration, offering a non-invasive approach to material characterization beneath the soil. This method is significant due to its ability to provide detailed insights into the composition and structure of buried materials without direct physical contact, a feature crucial in fields like geology and environmental science.

Central to this research is the integration of wavelet technology with X-ray backscattered energy spectrum analysis. This synergy enhances the method's effectiveness in delineating the unique spectral signatures of different subsurface materials, such as metals, and ceramics. Wavelet technology, known for its proficiency in signal processing, significantly improves the resolution and accuracy of X-ray backscattering data. It effectively addresses challenges like signal attenuation and noise, enabling a more precise and detailed analysis.

Looking forward, the use of X-ray backscattering, augmented by wavelet technology, is set to become a key technique in subsurface material characterization. Its capacity to provide high-resolution data paves the way for breakthroughs in understanding subsurface structures. Looking ahead, the utilization of X-ray backscattering is poised to become a cornerstone in subsurface material characterization, revolutionizing our approach to exploring and interpreting the hidden layers beneath our feet.

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CL 10

Predicting Synthesis Conditions of ZnO-nanorods from SEM Images using Persistent Homology

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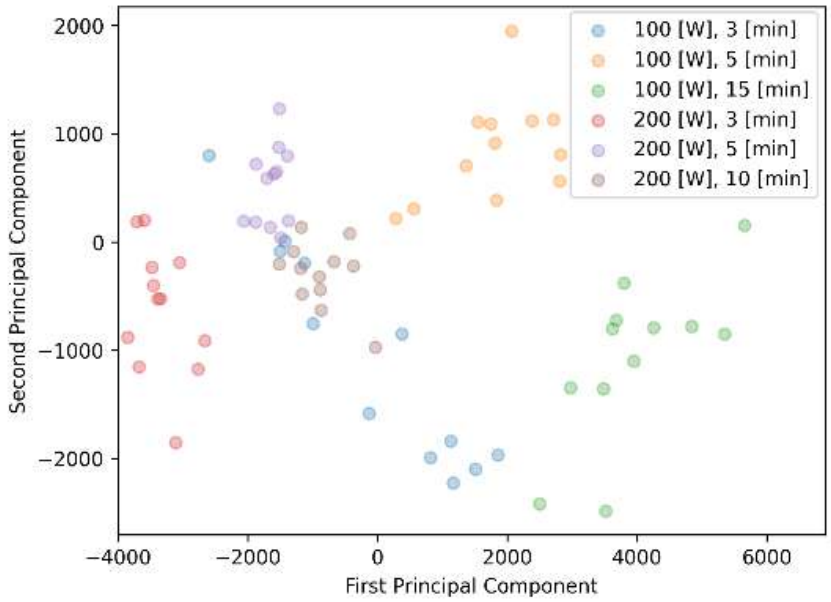
ABSTRACT

ZnO-nanorods on conductive NiCu fabrics made by microwave-assisted solvothermal synthesis are a candidate of high-efficiency flexible thermoelectric devices. However, the relationship between the synthesis condition the characteristics of the product is unclear and thus we need experiments to optimize the condition. To reduce the cost and time of the experiments to clarify it, we propose a machine learning method to predict characteristics from SEM images of ZnO-nanorods that are easier to obtain. As a first step of optimizing the condition, we developed a method to predict the synthesis condition from SEM images in this study.

To see the structure of nanorods, we used Persistent Homology (PH), one of the topological data analyses for point clouds. We applied PH to images by using thresholding and succeeded to show that SEM images include the information of the synthesis condition.



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A 001

Study of Embedded Metal Nano-disc Arrays and rings as Plasmonic back Reflector for High Performance Thin Film Amorphous Silicon Solar Cell

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ABSTRACT

In this work, a new arrangement of nanodisc arrays and rings is used to enhance theefficiency of thin-film a-Si solar cell with a thickness of 110 nm. The designed metal nano disc arrays plasmonic back reflector can improve the photocurrent and hence the efficiency. At first,a double layer SiO_2/Si_3N_4 as the antireflection (AR) was analyzed. The study was carried out by a 3D finite difference time domain method and the optimized parameters were calculated toobtain higher efficiencies. We analysed the results over a wide range of wavelengths (300- 1200 nm) using plane wave Source. We have also compared the results with different metal nano disc arrays with increasing height and metal nanorings. We found that Tungsten metal nanostructure gives good results in both types of structures (16.24 mA/cm^2 for dual metal nanorings and 18.36 mA/cm^2 for metal nano disc arrays with 20 nm thickness). As we increasethe thickness of the nanostructure we found the optimized value of short circuit current density i.e. equal to 41.15 mA/cm^2 for dual nano rings and 44.17 mA/cm^2 for nano disc arrays for tungsten. We also observed the average absorbance in the Visible and near IR range (400- 1000 nm) is greater than 95% and plotted it. Finally, a relatively higher photocurrent and conversion efficiency of 44.17 mA/cm^2 and 35.12% were achieved for the optimized structurewith nano disc arrays back reflector respectively.

Keywords: *Optical absorbance; nano-Silicon film; Nano metal disc-disk arrays; Lumerical FDTD.*

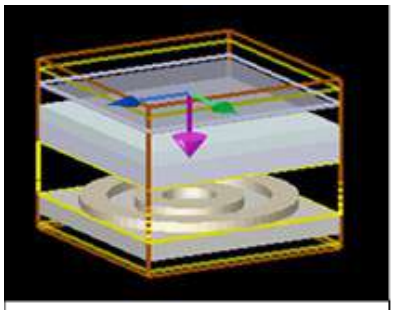

Fig. 1. Modelled structure of dual metal nano-rings without Silicon.

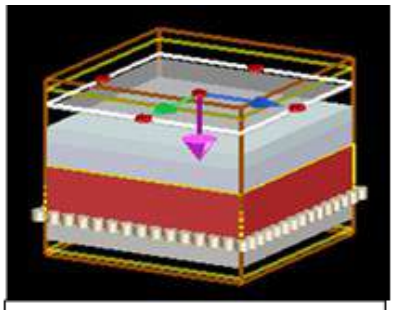

Fig. 2. Modelled structure of metal(W) nano-disc array with Silicon.

A 002

Dual Dopant Ce-Sn:Cd Thin Films as Interfacial Layer of Cu/Ce-Sn:Cd/*n*-Si Schottky Diode for Photodiodes Application

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ABSTRACT

In the current investigation, we fabricated a highly photosensitive Schottky barrier diode based on dual soak Ce-Sn:Cd (1, 3, 5wt%) thin films. The thin films were capped on a transparent plate and silicon substrate by low-cost jet nebulizer spray pyrolysis method at constant substrate temperature of 450 °C. The films structural, optical, morphological and electrical properties were observed through XRD, AFM, UV-Vis's spectroscopy, electrical and I-V characteristics of diode. The XRD pattern exposed that all stoned thin films are the cubic structure. The atomic force microscopy [AFM], exposed a smoother surface and an improved surface roughness of them thin film while varying the Cd concentration. The UV-VIS spectroscopy based on optical absorbance and band gap energy 2.86 eV. The electrical conductivity increases Cd concentration of films corresponding activation energy decreased. The current voltage [I-V] characteristics, photodiode parameters of the Cu/Ce-Sn:Cd/n-Si diodes were evaluated under dark and light conditions. The maximum barrier height (Φ_B) for the diode fabricated was found to be 0.69 eV, as well as minimum ideality factors (n) 2.57 of the diode parameters. As a consequence, the 5wt% of Cd parade greater device performance than other diodes.

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A 003

Synthesis And Photoluminescence Properties of the Rare Earth Ions (Eu^{3+}, Dy^{3+}, Tb^{3+}, Pr^{3+}, And Sm^{3+}) Doped Lithium Strontium Vanadate Phosphors for WLED And Thermometric Applications

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ABSTRACT

WLEDs are expected to be the next generation of lighting, because of their significant features, such as low energy consumption, enhanced luminous efficiency, extended lifespan, and environmental friendliness. LED lights are up to 90% more energy efficient than the incandescent (glowing) light bulbs and last much longer than the conventional light sources, making them much more economical and environmentally friendly. On this basis, the rare earth ions doped phosphor materials are synthesized via solid state reaction technique. The phase formation and the crystal structure are confirmed via powder XRD. The morphological and the elemental analysis are done using SEM with EDAX mapping. The band gap values are evaluated via diffuse reflectance spectroscopy. The 'room temperature photoluminescence and decay time' and 'variable temperature photoluminescence and decay time' measurements are carried out. The room temperature PL shows the characteristics of the dopant rare earth ions and their decay time values are obtained to be in the millisecond range. The variable temperature dependent PL and the decay time give the thermal stability and the sensitivity of the prepared phosphors respectively. In addition, the CIE coordinates, color purity, and the CCT values are evaluated. These findings validate their use as one of the components for WLEDs.

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A 004

Swapping Conventional Doping with Novel White Light Emission from La_2O_3: Clitoria Ternatea Extract

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ABSTRACT

White light emitting La_2O_3: Clitoria ternatea extract complex is studied and deemed as a potential replacement for conventional rare-earth doping. The common flower Clitoria ternatea extract is prepared by boiling the floral part in the de-ionized water and the remnants are removed. The La_2O_3: extract complex is formed by mixing and vaporizing the excess water resulting in a greenish white powder. The luminescence property is investigated for different heating conditions and extract concentrations. The successful complex formation is verified through the XRD and Raman spectroscopic patterns. The complex shows broad emission peaks centered at 444 nm and 592 nm. The emission peaks are due to the presence of organic dyes present in the floral extraction namely anthocyanin delphinidin and betalains betacyanin. Even though the extract shows emission in its solution state the intensity of emission reduces rapidly owing to the high decay rate of organic compounds. The complex formation helps in reducing the decomposition in appreciation of the antioxidant properties of La_2O_3. Here the host as such is inert to excitation and has a band gap of 4.5 eV. Up on complex formation, the optical band gap is reduced to 2.798 eV. Unlike the conventional rare-earth doping which only provides a sharp peak, this method gives a broad emission band in the visible blue-green and red regions which makes it a potential white light source.

Keywords: *Clitoria ternatea; Photoluminescence; La_2O_3; White light emitting diodes*

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A 005

Improving Optoelectrical Properties of Ga_2O_3 Photodetector by Reduced Graphene Oxide (rGO) Decoration for Deep UV Photodetection

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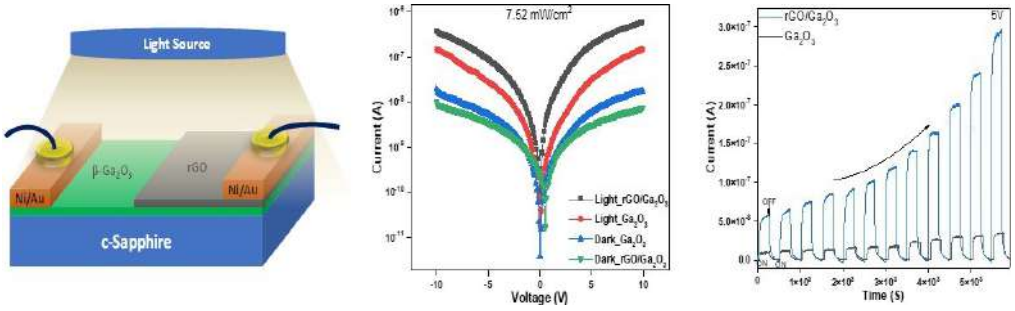
ABSTRACT

Deep ultraviolet (200-280 nm) photodetectors have received much attention in the fields of biology, industry, military, etc. The promising optical and electrical properties of wide bandgap, *n*-type gallium oxide (Ga_2O_3) make it quite suitable for deep UV photodetection. Our work shows that decorating reduced graphene oxide (rGO) can further enhance the photoresponse of the Ga_2O_3 photodetector (PD). rGO - a 2D material has received a lot of interest recently because of its distinctive qualities. In this work, we fabricated rGO/Ga_2O_3 heterostructure for deep UV photodetection where Ga_2O_3 thin film was deposited on c-plane sapphire substrate using Pulsed laser deposition, and rGO was synthesised by modified hummers method followed by thermal reduction, which was then drop casted on Ga_2O_3 film. The photoresponse of the rGO/Ga_2O_3 PD illuminated under 250 nm light was found to be substantially higher than the Ga_2O_3 PD, indicating an improvement of photoelectric properties for the UV photodetector based on Ga_2O_3 thin film. The dark current was found to be lower for rGO/Ga_2O_3 PD, and the illumination-to-dark current ratio ($I_{illumination}/I_{dark}$) was increased to 78.31 from 7.30 for Ga_2O_3 PD at a voltage of 5 bias and power density of 12.83 mW/cm^2. Thus, it can be concluded from the results that rGO/Ga_2O_3 PDs have great promise for photodetection applications.



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A 006

Tunable WORM Memory Performance of Donor/Acceptor End-Capped Phenanthroimidazoles

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ABSTRACT

The organic resistive memory devices can achieve multi-level data storage, which can be modulated with different donor and acceptor structural arrangements in the molecular backbone. Here, we have designed and synthesized donor-acceptor (D-A) based compounds for multi-level data storage. The imidazole core was substituted with triphenylamine, carbazole, pyrene, dibenzothiophene, and dibenzofuran unit to get a binary/ternary write once read many (WORM) memory. The optical investigations revealed an absorption maximum of 348 nm in pyrene-substituted imidazole. Besides, the electrochemical study exhibited the irreversible anodic peak in the range of (1.05-1.08 V), ensuring the one-electron oxidation of the triphenylamine unit. The well-connected network in the film facilitates the charge transport between the donor and acceptor units. All the fabricated devices exhibited the binary/ternary WORM memory characteristics. The compound substituted with pyrene and triphenylamine in the imidazole core showed a current ON/OFF ratio of 10^8 with a low threshold voltage of -0.99 V. Notably, the compound with dibenzofuran and triphenylamine attached with imidazole moiety displayed the ON/OFF current ratio of 10^6 with the low threshold voltage of -1.32 V. The stability of the devices was measured with retention and endurance characteristics up to $4x10^3$s and 100 cycles. The molecular simulations unveiled the plausible mechanism for binary/ternary memory with charge transfer and charge trapping. The charge traps in the molecular backbone confirm the electron-withdrawing nature of imidazole, dibenzofuran, and dibenzothiophene units. These insights into molecular architecture and memory performance can clarify the role of substituents in multi-level data storage.

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A 007

Isatin-Based D-A Systems for Non-Volatile Resistive Switching WORM Memory Devices

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ABSTRACT

Organic memory devices have recently gained much attention due to their potential for flexible electronics, affordable manufacture, and compatibility with large-scale integration. A series of new compounds with D-A architecture were synthesized employing different donor groups and the isatin moiety as the acceptor utilizing Suzuki-Miyaura coupling reactions. Strong intramolecular interactions were observed in the synthesized compounds, further corroborated by an optimal bandgap. The SEM investigation confirmed the compounds' improved molecular ordering and superior thin film surface coverage. All the compounds demonstrated notable binary WORM memory behavior. The switching threshold voltage for these D-A systems ranged from -0.79 to -2.37 V, with the compound having isobutyl substituent showing the lowest threshold voltage and maximum ON/OFF ratio of 10^2, thus outperforming others. The combined effects of charge transfer and charge trapping are responsible for the resistive switching mechanism prevailing in these systems. The alterations in D-A molecules that affect molecular packing, thin film morphology, and, finally, the memory performance of the active layer are highlighted in this work.

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A 008

Mechanistic Insight into the Optoelectronic Properties of $Cs_2AgInCl_6$ Compounds by Y^{3+} Rare Earth Substitution

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ABSTRACT

Recently, halide double perovskites (HDPs) with the chemical formula $A_2B'B''X_6$ (where A = Cs, B' = Ag^+, Na^+, K^+, B'' = In^{3+}, Bi^{3+}, Sb^{3+}, and X = Cl^-, Br^-, I^-) have gained more attention in the field of optoelectronic devices due to their non-toxicity, high stability in ambient atmosphere and their remarkable optoelectronic properties. Among various HDPs, $Cs_2AgInCl_6$ (CAIC) has been the study of interest because of its direct bandgap, high carrier lifetime, and broad emission[1]. Herein, our main strategy is to improve the photoluminescence quantum yield (PLQY) of CAIC as it has low PLQY arising from its inversion symmetry-induced parity-forbidden transition[2]. According to Laporte's selection rule, thereby creating Jahn-teller distortion in the octahedral site ($InCl_6^-$) it is possible to break the forbidden transition and achieve the allowed transition. Therefore, the replacements of In^{3+} ions with different concentrations of rare-earth ions (Y^{3+}) in $Cs_2AgIn_{1-x}Y_xCl_6$ compounds have been successfully synthesized. The substitution of Y^{3+} rare-earth ion, which has higher ionic radii compared to In^{3+} ion will be able to break the dark transition by contributing to the optical transition and thus inducing allowed transition (odd-even) as per Laporte's rule[3,4]. To support our findings, XRD data reveals that the diffraction peak shifted with Y^{3+} substitution confirming the distortions that occur in the substituted samples. Likewise, we have also carried out the UV–visible, photoluminescence, and photophysical studies to understand the proposed mechanism and their results will be further discussed in detail.

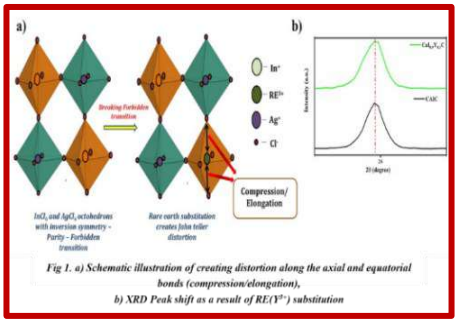

Fig 1. a) Schematic illustration of creating distortion along the axial and equatorial bonds (compression/elongation), b) XRD Peak shift as a result of RE(Y^{3+}) substitution

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A 009

Profound Investigation of Photoluminescent Characteristics of $BaCeO_3:Sm^{3+}$ Perovskite Synthesized Through Both Combustion and Solid-State Reaction Techniques

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ABSTRACT

Samarium doped barium cerates phosphorus has potential application in the production of Amber LEDs and can also be used as solid electrolytes for intermediate temperature solid oxide fuel cells. The present study focuses on comparing two different methods for photoluminescence analysis of samarium doped barium cerate perovskite, conventional solid - state reaction method and gel combustion technique followed by calcination at high temperature. $BaCeO_3:Sm^{3+}$ was synthesised successfully using both methods. Structural and optical properties of the both samples were studied using X-ray diffraction method and Photoluminescence spectroscopy. The Photoluminescence properties were carried out over the range of 500 - 650 nm and UV - Visible spectrophotometer is analysed in the wavelength range 200 - 800 nm for both samples. On excitation at 348 nm, peaks in the emission spectra are observed at 616 nm (orange), and 574 nm (yellow). It has been found that samples prepared using gel combustion techniques exhibit better photoluminescence properties than those prepared using the solid-state reaction method.

Keywords: *Barium cerate; luminescence; Samarium doping; gel combustion; solid state method; Amber LED; Solid oxide fuel cells*

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A 010

Charge transport mechanism and fractional order capacitive behavior in PVDF/PVDF-HFP- 2D MoS_2 nanocomposite films

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ABSTRACT

We have reported the solid-state fractional-order capacitor (SSFOC) behavior of PVDF-2D MoS_2 and PVDF-HFP -2DMoS_2 nanocomposite films. The samples have been synthesized by the wet chemical route and are characterized by using X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), thermogravimetric analysis (TGA), Raman and Fourier transform infrared (FTIR) spectroscopy. The ac electrical properties of the samples have been studied in the frequency range of 100 Hz $\leq f \leq$ 8MHz and by varying the measuring temperature from room temperature (RT) to 423 K. Identification of the constant phase zone (CPZ) and its relative change with different weight percent of nanosheets inclusions have been studied from the phase angle (θ) versus frequency (f) variation. The impedance spectroscopy data have been fitted with a proposed electrical equivalent circuit (EEC). We have elucidated further, the role of the segmental motion of the ferroelectric polymer chains and its interaction with the MoS_2 nanosheets on the charge transport mechanisms and the origin of CPZ in the SSFOCs. Activation energies and barrier heights for the pristine and the nanocomposite films have also been calculated and compared in this context.

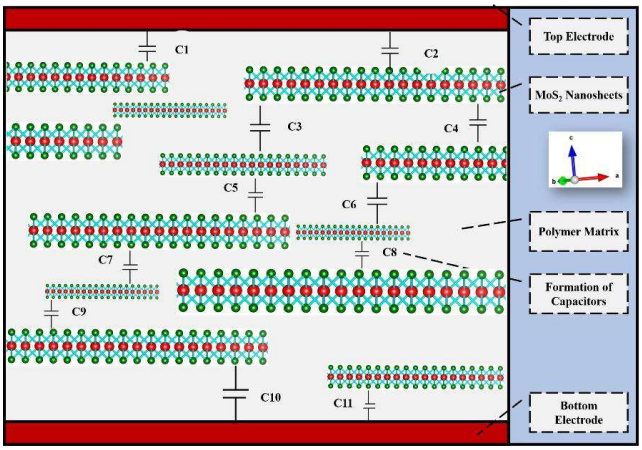

Figure 1: Schematic of the polymer nanocomposite films between two electrodes. C1, C2, C3….C11 represent the typical micro electrostatic capacitors that may form inside the nanocomposite while thepolymer matrix may also offer resistive behavior. It may be considered a random resistors-capacitorsnetwork.

A 011

Nonlinear Optical Studies of Benzil-PEO Nanofibers for Laser Safety Applications

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ABSTRACT

Benzil-Polyethylene Oxide (PEO) nanofibers were synthesized by electrospinning technique with optimization of various spinning parameters. The nanofiber sheet obtained was pale yellow coloured. The preliminary morphological analysis using optical microscope showed that the single fibers had diameter in nano range and using the SEM images with better resolution the diameter was found to be around 250 nm and it is also found to be smooth which means that there had been no outside crystallisation. The sharp peaks obtained in the X-ray diffraction studies confirmed that benzil has been crystallised inside the PEO nanofiber. Linear optical studies showed that the fibers exhibited an absorption peak at 385 nm which yielded a bandgap energy of 3.22 eV. Nonlinear absorption studies had been conducted using open aperture Z-scan technique utilizing an Nd:YAG laser of wavelength 532 nm, pulse rate of 9 ns and repetition rate of 10 Hz at input intensity 2.46 x 10^{12} Wm^{-2}. The sample was found to exhibit reverse saturable absorption which occurred due to two photon absorption and the nonlinear absorption coefficient was found as 1.4 x 10-10 mW^{-1}. The optical limiting threshold value obtained was 3.21 x 1012 Wm^{-2}, this certified that benzil-PEO nanofibers show suitable application as an optical limiter in laser safety devices.

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A 012

Optoelectrical Performance of Thermally Evaporated Orthorhombic $SnS_{(1-x)}Se_x$ Thin Films

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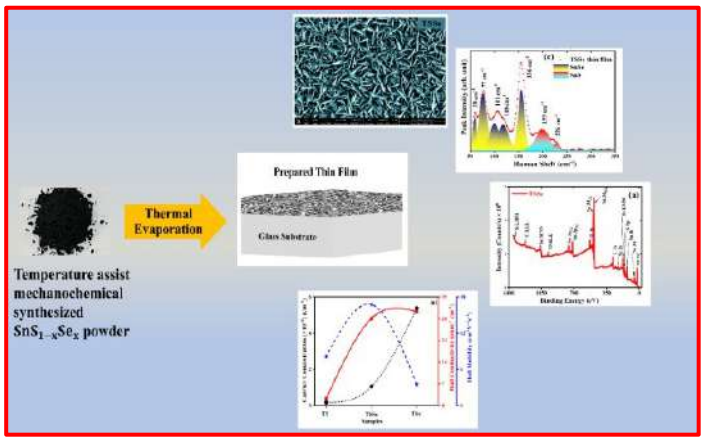
ABSTRACT

2D tin chalcogenides are a promising material for thin-film solar cells due to their excellent characteristics. Researchers have garnered attention for $SnS_{1-x}Se_x$ alloy films over the last few decades due to their tunable physical features. Here, we report the successfully preparation of $SnS_{1-x}Se_x$ powder using a temperature-assisted mechanochemical process and its subsequent deposition on glass substrate via thermal evaporation. X-ray diffraction (XRD) and Raman spectroscopy were used to extensively analyses $SnS_{1-x}Se_x$ thin films, elucidating their structural characteristics. The presence of a ternary alloy has been verified by both energy dispersive X-ray spectroscopy (EDAX) and X-ray photoelectron spectroscopy (XPS). Absorption spectrum shows that TSSe thin film has great potential for absorbing wide range of visible light. Hall measurement revealed that n-type TSSe thin films have shown great promise with the highest hall mobility up to 16.7 $cm^2V^{-1}S^{-1}$. Our study demonstrates that TSSe has excellent potential as a 2D material for cutting-edge photovoltaic applications.



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A 013

Effect of Trivalent Transition Metal Ion (Cr^{3+}) Substitution on the Optoelectronic Properties of Halide Double Perovskite $Cs_2AgInCl_6$ Compounds

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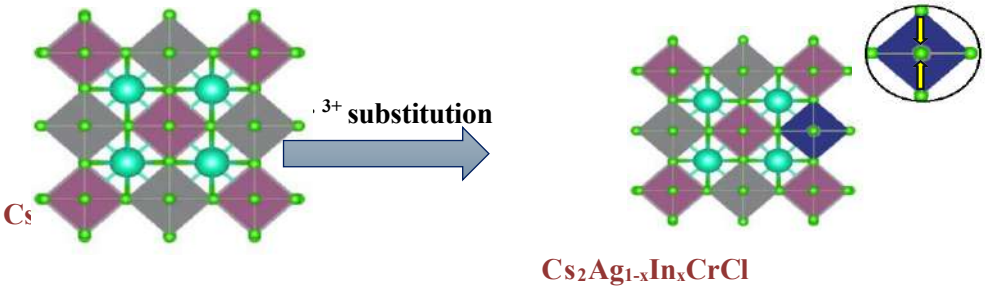
ABSTRACT

Recently, lead-free halide double perovskites (LFHDPs) materials have shown significant interest in optoelectronic applications due to their non-toxicity, tunable bandgap, broad photoluminescence spectra, and high stability under ambient conditions. Herein, considering direct bandgap nature of $Cs_2AgInCl_6$ (CAIC) compound as compared to other LFHDPs compounds (Cs_2AgBiX_6(X=Cl, Br)), we chosen CAIC compounds for this study. However, the direct parity-forbidden transition of CAIC has lowered the photoluminescence quantum yield which makes them unsuitable for practical applications.[1]In this work, we employ systematic studies to break the forbidden transition of CAIC through the introduction of lattice distortion into the $InCl_6$ octahedra.[2]To achieve allowed transition, Cr^{3+} anion (ionic radii 0.615Å) has been substituted in $Cs_2AgInCl_6$ compounds at the site of In^{3+}(ionic radii0.80Å), which may lead to notable lattice distortions in the crystal structures.[3]This lattice distortions will break the inversion symmetry resulting in an optical transition from dark (even-even) to bright (odd-even) transition as per Laporte's rule.[2] Herein, we have successfully synthesized the various concentrations of Cr^{3+} in $Cs_2AgInCl_6$ compounds by hydrothermal method. The diffraction peaks of the XRD pattern indicate cubic crystalline structures with space group $Fm\bar{3}m$ of CAIC compound and also show no sign of impurity phase. By substitution of Cr^{3+}, the observation of XRD peaks shifted with respect to the pristine compound, which is a clear indication of lattice distortions that occurred in the samples. In addition, we have also carried out UV-visible, photoluminescence, and FTIR studies to confirm our findings and their results will be discussed in detail.



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A 014

Novel White Phosphor Bi^{3+} Co-Doped $SrCeO_3$: 2 Wt% Sm^{3+} Synthesized Via Fuel Excess Gel Combustion Synthesis for wLED Applications

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ABSTRACT

The current study focuses on the production and analysis of white phosphor Bi^{3+} co-doped $SrCeO_3$: 2 wt% Sm^{3+} perovskite material, by varying the concentrations of bismuth (x=0.5 wt%, 1 wt%, 1.5 wt%, 2 wt%). The perovskite material was synthesized using a low-temperature fuel excess gel combustion method, utilizing citric acid as the fuel and ammonium nitrate as an extra oxidizer. By co-doping $SrCeO_3$: 2 wt% Sm^{3+} with Bismuth, we aimed to enhance its functional properties, such as structural, and photoluminescence. We explored the impact of changing concentration levels on both the development of crystalline phases and the luminescent properties of ceramic powders. This investigation was conducted through the application of X-ray diffraction and Photoluminescence characterization methods. Also, studied the morphological, and vibrational modes using FESEM and Raman spectra analysis. Our experimental findings reveal that achieving a single-phase perovskite formation necessitates a lower calcination temperature of 1223 K, in contrast to the higher temperatures required in conventional solid-state reactions. The X-ray diffraction and photoluminescence spectroscopy, allow us to identify the optimal amount of co-dopant required to maximize these functional properties. The optimized sample was subjected to morphological and vibrational spectra studies for its application in wLED applications. Thus, a bright white light emitting perovskite nano phosphor $SrCe_{0.97}Sm_{0.02}O_3$: 1wt% Bi^{3+} acts as an inevitable direct phosphor coating the near UV chip in LEDs, which can be a great revolution in energy savings applications

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A 015

Fabrication and Characterization of Illumination-Dependent Cu/*n*-Si Schottky Barrier Diodes with P(VDF-TrFE)-Ho_2O_3Nano composite as interfacial insulating Layer

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ABSTRACT

Metal insulator semiconductor (MIS) structured Schottky Barrier diodes are inevitable for a wide range of opto electronic devices and applications. Holmium oxide embedded Polyvinylidene fluoride Tri fluoroethylene [P(VDF-TrFE)] is used as the interfacial insulating layer in the present study because of its high work function, wide band gap, optical, thermal stability etc. Ho_2O_3 nano particles are synthesized by wet chemical method. The structural, morphological, optical and electrical properties of nanoparticles are studied. The prepared Holmium oxide nano particles are dispersed in P(VDF-TrFE) and are spin coated on *p*- Si wafer. Structure and morphology of the thin film is studied using X-ray diffraction analysis and Scanning electron microscopy (SEM). From UV visible spectral analysis band gap is found out using Tauc method. Vibrational spectral analysis is carried out using Fourier transform infrared spectroscopy. DC sputtering technique is employed to deposit Cu electrode over the thin film thus forming Cu/P(VDF-TrFE)- Ho_2O_3/p-Si metal- insulator-semiconductor structured Schottky barrier diodes. Silver paste is coated on both the surfaces of this MIS structure for better Ohmic contact. Current - Voltage (I-V) measurements are analyzed in both dark and illuminated conditions for Cu/P (VDF-TrFE)- Ho_2O_3/*p*-Si Schottky Barrier diodes.The electronic parameters such as ideality factor and barrier height are calculated.

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A 016

Saturable Absorption of 4-Nitroaniline (4NA) Embedded in Poly Methyl Methacrylate (PMMA) Electrospun Nanofibers

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ABSTRACT

Due to their advantages of high beam quality, low cost, efficient structure, alignment-free compact design, and excellent compatibility, passively mode-locked ultrafast fiber lasers based on saturable absorbers (SA) have become one of the most powerful techniques to develop ultra-short pulses [1,2]. This work reports the study of the nonlinear absorption of optically nonlinear 4NA molecules embedded PMMA fiber matrix synthesized by electrospinning technique. Confirmation of fiber formation and calculation of average diameter (900 nm) was done with optical microscope and Scanning electron microscope (SEM). The incorporation and orientation 4NA Nano-crystals inside the polymer with average crystallite size 29 nm, were analyzed by XRD technique. Further linear optical studies and vibrational studies were performed with UV- VIS and FTIR spectroscopy. The nonlinear absorption properties are investigated by Z-scan technique in open aperture configuration with Q-switched Nd: YAG laser source (532 nm, 10Hz,9ns). Measurements show that 4-NA-PMMA nanofibers exhibit saturable absorption with nonlinear absorption coefficient (β) equal to -0.34×10^{-10} W/m^2. The saturable absorption behavior of 4NA-PMMA nanofibers ensures their application in the fields of ultrafast lasers for mode-locking, which enables the generation of ultra-short laser pulses [2].

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A 017

Electron beam Irradiation-Induced Modification of Dielectric Properties in Nano ZnS–Natural Rubber Disks

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ABSTRACT

ZnS is a wide bandgap semiconductor material which have potential optical and optoelectronic applications. ZnS nanoparticles were synthesized via coprecipitation technique and is coated with natural rubber to prepare ZnS-NR disks. The impact of electron beam irradiation on the dielectric and conductivity properties of nano ZnS–natural rubber (NR) disks was investigated in this study. It was found that electrical properties such as AC conductivity, dielectric constant, and loss tangent of the irradiated samples exhibited significant improvements compared to the non-irradiated samples, and these improvements were associated with defects in the composites. The total number of dipoles generated within the polymer matrix upon irradiation depended on the dislocations formed inside the matrix. Experimental results indicate that electron beam irradiation in the amorphous region results in both crosslinking and breakdown simultaneously. The enhancement of dielectric and conductivity properties suggests that nano ZnS–NR disks hold great promise for applications in the optoelectronic industry. Furthermore, the study also examined the influence of temperature on the electrical conductivity of the irradiated samples.

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A 018

Modified Anode/Semiconductor Interface by Multiple Plasmonic Resonance Bands: Experimental and Simulation Study

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ABSTRACT

For the highly efficient photovoltaic performance, all the photo-generated carriers in the active layer should be collected at the electrode. Before reaching the electrode these photo-generated charge carrier undergoes various loss mechanisms. These types of losses have a direct consequence on the PV efficiency. To reduce such losses transport path should be low resistive and trap free. This can be achieved by maintaining the balanced electron and hole mobility of active layer and high conducting transport layers. Additionally making the Schottky and Ohmic contact closer to the ideal barrier condition will reduce the carrier losses. In this work, various combination of dual nanoparticles (Al:Ag, Ag:Cu, Cu:Al) and triple nanoparticle (Al:Ag:Cu) were embedded in HTL to study the PV efficiency. Metal nanoparticle in the HTL manipulate dynamics of charges as well as light in the device. Metal nanoparticles in anode buffer layer offer percolation path to the carriers. Percolation pathways provides multiple states between energy level offset of semiconductor and electrode interface which favors easy carrier transport. Presence of these metal particles also improves the light confinement near the active layer/hole transport layer. This work provides some insight in the organic photovoltaics using metal nanoparticle at the anode interface. Primary objective of using metal nanoparticle in the polymer photovoltaics arises due to its plasmonic properties where it can support in improving light absorption of the active layer. And the second role of it is to improve the conductivity of the buffer layer. The novel idea behind this work is to step down the energy offset for charge carriers to reach anode. From the obtained result it is noted device with triple nanoparticle loaded HTL showed high PCE than dual nanoparticle and neat devices. It is observed the PCE of triple metal particles device exhibits the highest PCE than dual metal particle and neat devices. Resultant PCE exhibits the following order, triple particle device > dual particle device > neat device. It is found that addition of triple metal nanoparticles of different work function helps in the interface charge transport by means of step down the energy offset.

Key words: *Polymer solar cell, Plasmonic effect, Al, Cu, and Ag nanoparticles.*

A 019

Highly Efficient Orange Phosphorescent Organic Light Emitting Diodes Using Carbazole and Acridinone Based Host Materials

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ABSTRACT

Phosphorescent organic light-emitting diodes (PhOLEDs) are important for commercial OLED displays and lighting, though, high device efficiency with long operational lifetime hosts designed based on orange PhOLEDs are limited. Herewith, a new xanthene conjugated carbazole and acridinone substituted hosts (XANPh-Cz and XANPh-Ac) were synthesized and utilized for yellow PhOLEDs. The two materials are appropriate hosts for yellow emitters in electroluminescent devices, because it possesses deep highest occupied molecular orbital (HOMO) and shallow lowest unoccupied molecular orbital (LUMO) levels as well as higher triplet energies (2.50-3.90 eV) and thermal stability (390-420 °C). The optimized yellow PhOLEDs device structure was constructed by Bis(2-phenylquinoline) (acetylacetonate) iridium (III) ($Ir(pq)_3$ used as an emitter with hosts materials (XANPh-Cz and XANPh-Ac). Both host materials display higher external quantum efficiency (EQE) of 22.3% for XANPh-Cz and 20.5% for XANPh-Ac with Commission Internationale de l'Eclairage (CIE) coordinates of (0.53:0.46) and (0.54:0.45). In addition, both device shows lower turn on voltage (2.5 V) and high-power efficiency of 60.0 l m W^{-1}, which are the highest values for orange PhOLEDs.

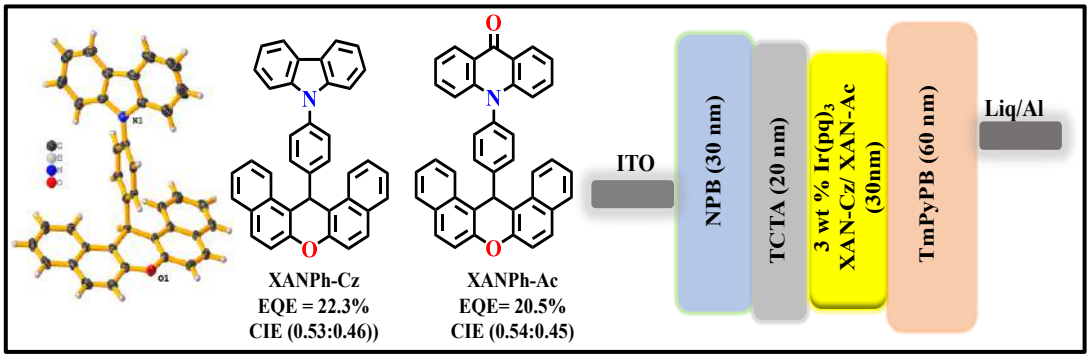

Figure 1. Molecular structures of host materials and optimized PhOLED device structure.

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A 020

Gold-Copper-Nanoclusters-Based Pure Red Light-Emitting Diode (LED) with High Efficiency

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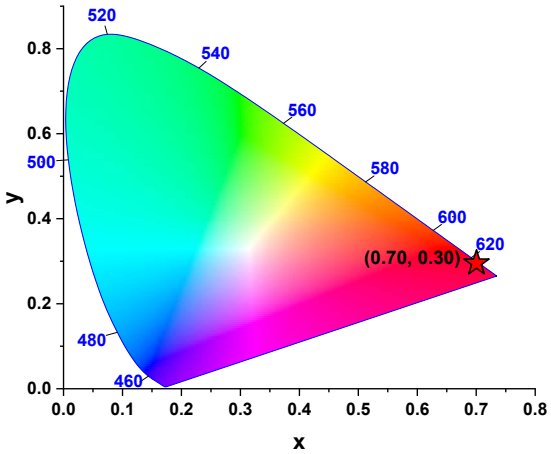
ABSTRACT

Light-emitting diodes (LEDs) are promising for lighting applications over incandescent lamps due to their high energy efficiency, low power consumption, low cost, and longer operational lifetime. In recent years, the efficiency of LEDs has revolutionized due to the use of nanostructures as an emissive layer. These nanostructures with reduced dimensions improve the radiative recombination efficiency by confining electrons. Our work involves the fabrication of a highly emissive, monochromatic, pure red-colored LED using Gold-copper nanoclusters (NCs). The maximum external quantum efficiency (EQE) of 12.57% is obtained with these Gold-copper NCs. The CIE coordinates of (0.70, 0.30) were obtained, which indicate the emission of the most saturated pure red color from the fabricated Gold-copper NCs-based LED device. The turn-on voltage of the NCs-based LED was 3V at 1 cd/ m^2. These results show that Gold-copper-based NCs LED have great promise for the monochromatic, pure red-colored light-emitting diode.



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A 021

One Pot Synthesis of 1-Phenylimidazo[1,5-a] Pyridine–Anthracene Luminophore for Fabrication of Yellow Organic Light Emitting Diode

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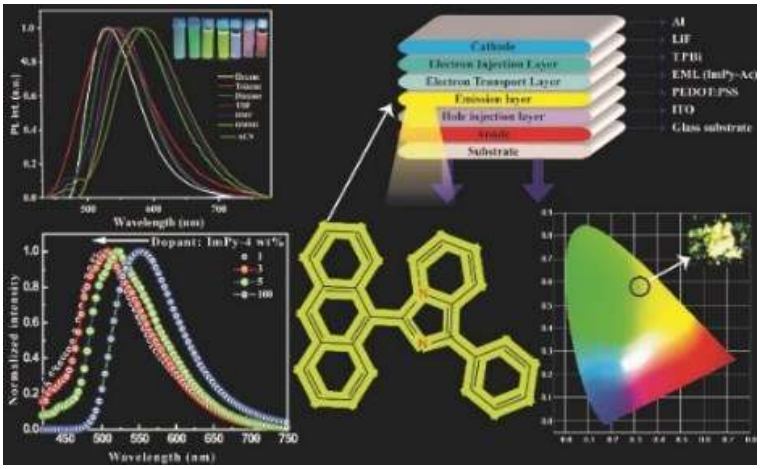
ABSTRACT

In recent years, significant emphasis has been given to organic light-emitting diodes (OLEDs) devices constructed from small organic luminophores via solution-process. The method offers the advantages of using small organic fluorophores, exhibit substantial morphological homogeneity with polymers, and also inexpensive. Here, a one-pot condensation reaction was used to synthesize the imidazole [1,5-a] pyridine (ImPy) derived fluorophore that is embellished by an aromatic π-system, anthracene which is attached at the C_3 position of ImPy. The synthesized compound is characterized through NMR, HRMS, single crystal XRD (SCXRD) and different spectroscopic techniques. From the theoretical study, the energy difference between HOMO and LUMO (band gap) is found to be ~3 eV. The molecule shows excellent thermal stability as well as electrochemical stability. Electrochemical investigation demonstrates that the emitter exhibits appreciable oxidation and reduction characteristics. The OLEDs made of this emitter as the emissive material displayed good device performance. It exhibited a luminous efficiency of 4.4 cd A^{-1}, a power efficiency of 2.2 lm W^{-1}, and an external quantum efficiency of 3.2%. Additionally, this OLEDs emitted greenish-yellow light and possessed a low turn-on voltage of 7V.



A 022

Investigating the Doping Effects of Nano-Size Semiconducting Materials on Electrochromic Devices

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ABSTRACT

The aim of this study is to investigate the doping effect of nano-size semiconducting materials on the performance of electrochromic devices. An electrochromic device (ECD) controls optical properties such as optical transmission, absorption, reflectance and/or emittance in a continual but reversible manner on the application of voltage [1] and it has vast applications in smart glass, charge storage indicators, energy-efficient buildings, automobile industries. The reasoning behind selecting semiconducting materials is that it has a wide band gap and the advantages associated with a wide band gap include higher breakdown voltages, the ability to sustain large electric fields, lower electronic noise, and high-temperature and high-power operation. The wide band gap of material will only allow the diffusion of ions from the electrolyte to the electrode surface after a certain potential which helps in increasing the electrochromic performance such as color contrast, switching time and coloration efficiency as the ions will be diffused simultaneously. For this purpose, nano-sized [2] ZnO semiconducting material has been synthesized using co-precipitation method. Prior to device fabrication, ZnO powder will be studied electrochemically using Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) to confirm the nature of the material. Ethyl viologen (EV) will be mixed with the synthesized ZnO powder as an n-type material. Poly 3-hexylthiophene(P3HT) will be selected as a p-type material. The device consists of a layer of P3HT-coated ITO, a layer of (EV+ZnO) gel, and a layer of bare ITO, stacked on top of each other [3]. The electrochromic performance of the device will be studied using bias-induced in-situ UV-Vis spectroscopy. The study will also provide information on the suitability of P3HT with ZnO as an electrochromic material.

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A 023

Effect of Bismuth Doping on the Structural and Optical Properties of Gadolinium-Based Ceramics Synthesized Via Solid State Reaction Technique

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ABSTRACT

Recent developments in the mobile and satellite communication demands portable, affordable, and loss-free microwave equipment, which opens the door for their usage in microwave communication systems. Ferrites are identified to be a perfect choice for microwave applications since they combine the qualities of an electrical insulator and a magnetic substance. Rare earth iron garnets, $RE_3Fe_5O_{12}$, have a cubic symmetry and are well-known for its outstanding performance in microwave devices. One of the main practical issues with this area of material science is the reduction of the sintering temperature. Glass addition, chemical processing and fine-particle starting materials have been proved to play a vital role in reducing the sintering temperature. In the present work, Bi is substituted in $Gd_3Fe_5O_{12}$ ceramics to lower the sintering temperature. The Bi substituted Gadolinium Iron Garnet (Bi:GIG) samples having different compositions (x = 0,1) of $Gd_{3-x}Bi_xFe_5O_{12}$ are prepared using the solid state reaction route. Crystal structure and phase purity of the prepared samples are investigated using X-Ray Diffraction technique. Further investigations are performed to elucidate the optimum temperature corresponding to the highest density. The chemical characterisation of the prepared samples is studied using the EDS analysis technique. FTIR patterns confirm the shifting of the main vibration modes of Gd up on Bi doping. The SEM micrographs of the Bi:GIG ceramics are observed to be composed of grains having size below 5 µm. Due to the effective incorporation of Bi^{3+} into GIG, the sintering temperature is found to be considerably reduced and the densification improved significantly.

Keywords: Ceramics, Gadolinium Iron Garnets, Sintering temperature

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A 024

Conquering the Quantum Barrier in Tunnel Junctions

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ABSTRACT

Molecular Electronics belongs to an active research field due to its unraveled charge transport mechanism through molecular junction[1]. Quantum tunneling is one of accepted mechanisms for chargetransport in molecular junction when molecule length (or thickness of molecules inside junction) is lessthan 2 nm for alkanes and 5 nm for conjugated molecules. But it is still not clear *"what happens to its charge transport mechanism beyond the tunneling limit."* Recently this problem was identified by David et al[2]. which challenged all the existing models reported for charge transport. Here we are proposing photon as probe first to identify the height of potential barrier if any (figure1) and later to overcome the barrier by illumination the junction by light. By careful analysis of relative IV characteristics in the presence and absence of photons one can identify the properties of the barriers present in the junction as well as differentiate underlying charge transport mechanism.

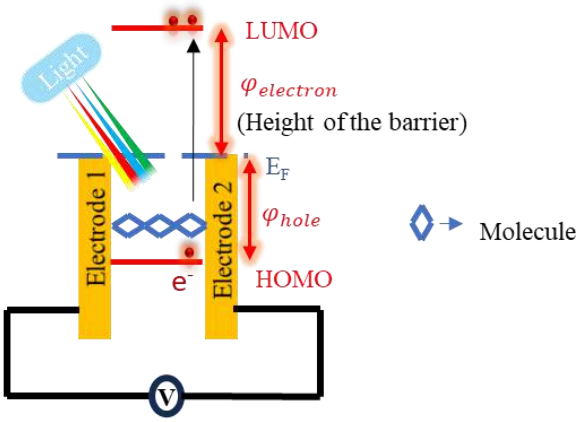

Figure 1. Schematic of molecular junction under illumination.

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A 025

Ambiguity between Band Gap and Photoluminescence in Silicon Nanowires

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ABSTRACT

Silicon Nanowires (SiNWs) are the one-dimensional nanostructured materials holds the potentials for optoelectronic applications[1] such as solar cell, LED etc. The quantum confinement effect is very well accepted mechanism for its visible luminescence. But here we demonstrate the discrepancy between band gap energy and photoluminescence in SiNWs fabricated by metal induced etching process[2]. The band gap energies are found to be increasing with decreasing in silicon nanowire (porous silicon nanowire) size which is good agreement with quantum confinement in contrary to this photoluminescence (PL) peak positions are observed at same position irrespective of the size of silicon nanowires. This paper elaborates the visible PL mechanism in silicon nanowire.

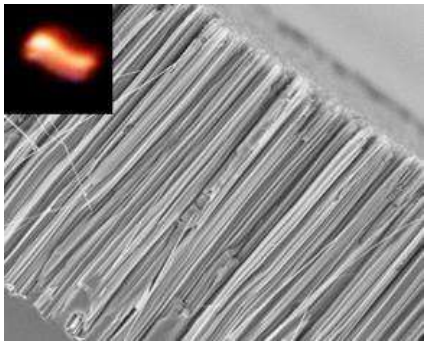

Figure 1: Well aligned Silicon nanowires and its visible photoluminescence

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A 026

Photoacoustic spectroscopic and upconversion studies of Er^{3+}/Yb^{3+} co-doped YVO_4 prepared via combustion synthesis method

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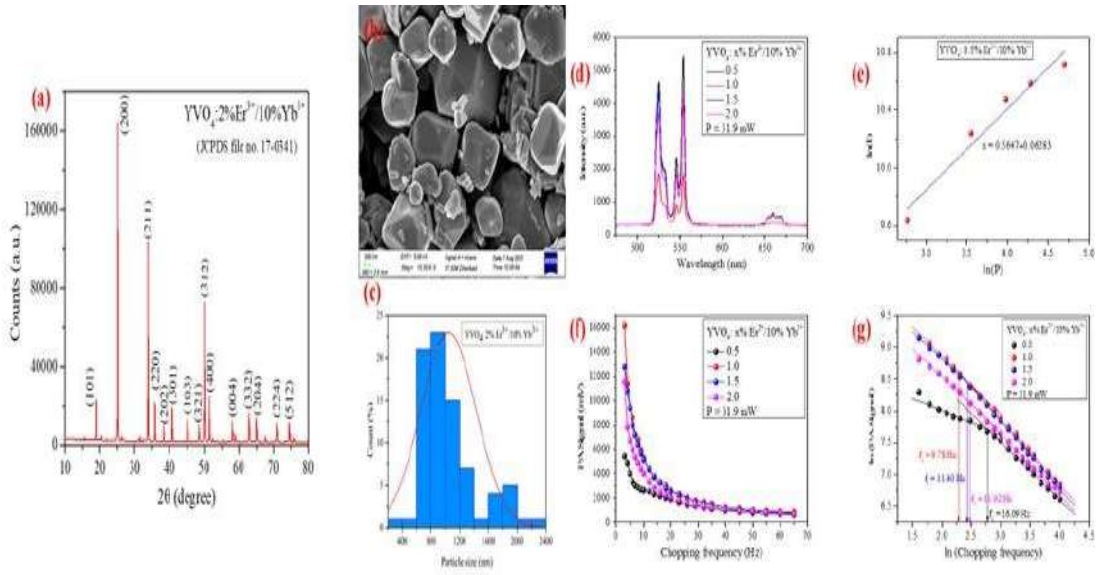
ABSTRACT

Photoacoustic spectroscopy was developed as a result of Graham Bell's discovery of the photoacoustic phenomenon in 1880. In 1975 Allan Rosencwaig and Allen Gersho proposed the theoretical explanation of the photoacoustic effect in solids. This unique technique is very effective for studying the non-radiative transitions in samples while they interact with light. In this work ytterbium (Yb^{3+}) and erbium (Er^{3+}), co-activated yttrium orthovanadate (YVO_4) powder phosphors were synthesized by solution combustion method and were annealed at 800 °C for 2 hours. The X-ray powder diffraction (XRD) patterns confirmed that zircon-type tetragonal structure of YVO_4 with space group I41/and was crystallized. Crystalline (D) size was calculated using the Debye-Scherrer equation and the average size was found to be around 114.25 nm. Scanning electron microscopy (SEM) images showed particles of different shapes having their sizes in the micrometer range. Power-dependent Upconversion (UC) emission and constant wavelength mode photoacoustic (PA) spectroscopic studies of the samples were done using a 980nm laser. The thermal transition frequencies of the samples were also calculated from the Ln(f) – Ln (PAS) plot.



A 027

Impact of Doping on Optical Characteristics of Thin Films of Diketones Derivatives

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ABSTRACT

This research work reports, investigation of the impact of doping on the optical characteristics of thin films of diketones derivative 1-(4'-dodecyl-[1,1'-biphenyl]-4-yl)-3-(4-(nonyloxy) phenyl) Propane-1,3-dione (DK-3) prepared via spin coating method. Specifically, we focus on the newly synthesized diketone derivative DK-3 and its effect on the optical properties of the thin films. The transparent thin films were investigated in the field of photonics applications. UV-Vis spectrophotometer was used to produce absorption spectra for doped DK-3 samples. Through absorption spectra we have quantified important optical parameters such as the refractive index, extinction coefficient, and band gap energies. These parameters were investigated with the effect of doping concentration. Fluorescence spectrophotometers were used to record the emission spectra and described doping effects. FTIR spectra of the thin films were also obtained and compared with pure molecule to detect changes in intensity and peak values. Further we have evaluated the energy band gap theoretically through DFT/TDDFT method B3LYP/6-311(d, p) basis set and compared with experimental results. The results of this study provide appreciating insights into how doping affects the optical properties of thin films of DK-3. The study also highlights the potential use of these samples in photonics application.

A 028

Spectroscopic Characterization of Thin Films of Diketones Derivative for Photonics Applications

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ABSTRACT

In this research paper, we have investigated the optical characteristics and influence of concentration of thin films of diketones derivatives prepared via spin coating method. Specifically, we focused on the newly synthesized diketone derivative 1-(4'-dodecyl-[1,1'-biphenyl]-4-yl)-3-(4-ethoxyphenyl) propane-1,3-dione (DK-2) and its effect on the optical properties of the thin films. Various spectroscopy methods were used to characterize the samples [1]. UV-Vis spectrophotometer was used to produce absorption spectra for DK-2 doped samples. The absorption spectra quantify other important optical parameters such as the refractive index, extinction coefficient, and band gap energies. These parameters were investigated with the effect of doping concentration. Fluorescence spectrophotometers were used to record the emission spectra and described doping effects. FTIR spectra of the thin films were also obtained and compared with pure molecule to detect changes in intensity and peak values. Further, we have evaluated the band gap theoretically calculated by employing DFT/TDDFT method B3LYP/6-311(d, p) basis set and compared with experimental results. The results of this study provide greater insights into how doping affects the optical properties of thin films of DK-2. The study also highlights the potential use of these samples in photonics application [2].

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A 029

Photosalient Responses of Dimethyl Barbituric Acid derivatives

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ABSTRACT

Dynamic exotic molecular crystals under the influence of different stimuli such as light, heat, humidity, vapors etc., have drawn immense attention among researchers due to impressive mechanical motions. Stimuli-induced responsive crystals can be fabricated in developing biomimetics, soft microfluids, smart actuators etc. Innovative dynamic photo salient crystals offer the platform of harnessing light energy into mechanical motions. Hereby we discuss the mechanical motions of two crystals of dimethyl barbituric acid derivatives. Although the crystals are mechanically brittle, they exhibit photomechanical motions due to [2+2] cyclo-addition [1,2] reaction in the solid state. Due to their different packing arrangement along with the topochemical alignment of olefinic bond in the lattice form, crystal **1** bends upon exposure to 532nm LASER irradiation, whereas crystal 2 fragments and jumps off by several centimetres on exposure to 365nm handheld UV LED irradiation. Tuning photo salient motions in crystals [3] is essential in smart actuators, smart optical sensors [4], optical waveguides [5] etc. The study will shed the lights for the development of photo-responsive dynamic barbituric acid derivative crystals.

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A 030

Electrochemical PV Studies of $Zn_{1-x}Co_xSe$ Thin film Electrodes Deposited using a Solution Growth Technique

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ABSTRACT

In the present investigation, $Zn_{1-x}Co_xSe$ ($0 \leq x \leq 0.275$) thin film electrodes were deposited by a chemical method. The effect of Co doping on the electrochemical photovoltaic (EPV) properties of ZnSe thin films were analysed. The electrochemical PV cells fabricated with optimised electrolyte system (NH_4Cl, 0.5 M). The junction ideality factor (n_d) is smaller for a cell formed with a photoelectrode composition of x = 0.075. The n_d values suggest that the effects due to the series resistance and interface states are comparatively lower for x = 0.075. The C-V (vs SCE) measurements revealed maximum flat band potential V_{fb} = -963 for x = 0.075. An EPV cell fabricated with the $Zn_{1-x}Co_xSe$ ($(0 \leq x \leq 0.075)$ photoelectrode showed a maximum efficiency of 1.44%. The improved cell performance at x = 0.075 attributed to the increased photoelectrode absorption, increased flat band potential, decreased series resistance of a cell and improved grain structure of the photoelectrode material.

A 031

Improved Structural, Optical and Electrical Properties of Tin Selenide via Te-Doping for Optoelectronic Application

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ABSTRACT

Tin chalcogenide especially, tin selenide (SnSe) has attracted significant attention due to its excellent optoelectronic properties of its single crystal form. However, the polycrystalline SnSe processes considerably less. In this work, Te-doped strategy is proposed to enhanced the optoelectronic properties of SnSe thin film. Presence of Te atom has been verified by Energy Dispersive X-ray Spectroscopy (EDS) and X-ray Photoelectron Spectroscopy (XPS). X-ray diffraction (XRD) studies confirmed the tellurium incorporation into the SnSe crystal lattice without disturbing the orthorhombic structure. Based on AFM analysis, kurtosis values of 1% Te-doped sample is nearly close to 3, suggesting a more uniform surface. The band gap of Te-doped SnSe has been found to be blue shifted. Hall measurement shows tremendous enhancement in electrical properties due to doping of Te atom in SnSe structure. After detail analysis of structural, morphological and optoelectrical properties of SnSe thin film after doping Te atom, it is confirmed that Te can effectively improve the optoelectrical properties of SnSe thin films, deserving further exploration to improve solar cell performance.

A 032

Self-powered UV Photodetector Based on Solution-Processed CuI/ZnS/ZnO Heterojunction Nanostructures

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ABSTRACT

Wide-bandgap semiconductors plays a crucial role in advancing the field of power electronic devices and various optoelectronic applications, including photodetectors, solar cells, and light-emitting diodes (LEDs) within the realm of semiconductor technology [1,2]. A remarkable class of materials, consisting of copper-based halides like copper iodide (CuI) and copper bromide (CuBr), has lately emergedwithin this group of p-type competitors, exhibiting a wide range of compelling features [3-5]. A straightforward and cost-effective solution process to deposit thin films of γ-CuI, thoroughly investigatingvarious aspects of these films upon annealing, including morphology, crystalline phase, as well as their optical and electrical characteristics. Upon annealing, the CuI films exhibit a hole mobility of 0.53 $cm^2/Vs$and a hole concentration of 8.36 × 10^{18} cm^{-3}. The potential of γ-CuI as a *p*-type material for photodetection by fabricating transparent hybrid ultraviolet (UV) photodetectors using *p*-CuI/*n*-ZnO nanorods and *p*-CuI/*n*-ZnS/ZnO nanostructures is explored. High-resolution transmission electron microscopy (HRTEM)reveals the growth of ZnO nanorods as single crystals along the [001] direction, with smaller CuI particlesattached to their surfaces. A sulfurization process results in the formation of a poly-nanocrystalline ZnS shell layer over the ZnO nanorods. The critical photodetector parameters, including responsivity, external quantum efficiency, and detectivity, are analysed under various illumination intensities and incident wavelengths. Notably, the insertion of the ZnS layer between the ZnO and CuI components enhances these parameters. This study underscores the potential of *p*-type CuI as a transparent, high-performance material for optoelectronic applications.

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A 033

Solution Processable Organic- Inorganic Heterojunction for Photodetectors

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ABSTRACT

Two dimensional organic inorganic heterostructures have recently gained substantial attention for development of high performance and low-cost optoelectronics devices. The inorganic 2D layered semiconductor MoS_2 has been vastly studied and applied for its extraordinary charge transport property, band tunability and absorption over visible to near infrared region. On the other hand, C8BTBT, among organic semiconductors has gained popularity for its solubility and excellent charge transport properties. When combined into a heterojunction both leverages their individual characteristic and offer unique opportunities for enhanced device performance and a photo-detection range from ultraviolet to visible spectrum. Hence, in this work we successfully fabricated solution processed *p-n* heterojunction and studied the charge transport properties as well photoreaction capabilities of interface. We have used micro-Raman spectroscopy to analyze the interaction at the interface and confirm the presence of both the layers. GIXRD implements crystallinity and coherence length. Surface morphology and thickness of overall device is studied through AFM. The study elucidates a low cost, solution processed approach for realizing wide range photodetectors. The finding can be further implemented to fabricate flexible and wearable photovoltaic devices.

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A 034

Engineering Optoelectronic Properties of Graphitic Carbon Nitrate for Advanced Applications

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ABSTRACT

Graphitic carbon nitrate (g-C_3N_4) is an attractive material in optoelectronics, thanks to its unique properties and simple synthesis. In this study, we explore the controlled synthesis and detailed characterization of g-C_3N_4 with finely-tuned optoelectronic properties. The optimization of g-C_3N_4 optoelectronic properties is crucial for its use in various devices like photodetectors, photocatalysts, and LEDs. The low-cost precursor like melamine underwent controlled thermal polymerization to synthesize g-C_3N_4 samples with varying bandgap energies by adjusting reaction parameters. The samples were analyzed using various techniques, including X-ray diffraction, scanning electron microscopy, transmission electron microscopy, and Fourier-transform infrared spectroscopy. These analyses provided valuable information about the crystalline structure, morphology, and chemical composition of the g-C_3N_4 samples. The optoelectronic properties of the g-C_3N_4 materials that were synthesized were evaluated using UV-visible spectroscopy, photoluminescence spectroscopy, and electrical conductivity measurements. The results showed a direct correlation between the synthesis parameters and the optoelectronic properties. This allowed for fine-tuning of the bandgap energy, light absorption, and charge transport characteristics of g-C_3N_4. This research paper showcases how g-C_3N_4 can be developed as a versatile and customizable material for optoelectronic applications. The ability to fine-tune its properties according to specific device requirements opens up a wide range of possibilities for g-C_3N_4 in sustainable energy generation, environmental remediation, and advanced photonic devices. The findings presented in this study enhance our understanding of g-C_3N_4 materials and their potential in various optoelectronic technologies.

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A 035

Synthesis, Characterization and Optical Properties of Tb Substituted Yttrium Molybdate Nanoceramic Prepared by Auto Ignited Combustion Synthesis

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ABSTRACT

Phosphors are the luminescent materials which emit radiations at specific wavelengths under excitation with certain external stimulants in the form of light, electrons or particles. Because of high chemical stability and stable physical properties, rare earth inorganic phosphors are popularly used in solid state lighting, optoelectronic and biomedical applications. In the present work, a series of Tb^{3+} substituted $Y_2Mo_4O_{15}$ is synthesized through the auto ignited combustion method. The prepared nanoceramics are characterized using X-ray diffraction, IR spectroscopy, Raman spectroscopy, UV-visible spectroscopy and photoluminescence spectroscopy. The XRD analysis reveals a single-phase monoclinic structure with space group P21/c. The band gap energy of yttrium molybdate determined from UV-Visible spectrum is 3.58 eV. The highest intensity peak at 545 nm in the emission spectrum excited at 275 nm corresponds to green emission which make the material suitable for application as a green phosphor in light emitting diodes.

Keywords: *Rare earth molybdates, Auto ignited combustion synthesis, Optical properties*

A 036

Intensity-Dependent Optical Non-Linearity of Liquid-Phase Exfoliated Graphene Nanosheets

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ABSTRACT

Graphene, an atomically thin array of Carbon atoms has attracted an enormous worldwide attention due to its spectacular properties. Optoelectronics may make use of graphene's exceptional optical qualities. Understanding the material's underlaying mechanisms is necessary to employ in appropriate applications. Defect-free Graphene is synthesized from Graphite using an Ultrasound assisted Liquid Phase exfoliation in Dimethylformamide. An attempt has been made to boost graphene yield. Properties of the exfoliated Graphene are studied by using various microscopic and spectroscopic tools. Our goal is to investigate the mechanisms underlying graphene's optical and non-linear behavior. As laser usage increases, sensors and human eyes become more vulnerable to the powerful radiations it emits. To construct optical limiters, efforts have been undertaken to improve the optical limiting actions of graphene suspensions. Utilizing an Open-aperture Z-Scan configuration, we investigate the Intensity-Dependent Nonlinear Optical Absorption and Optical Limiting characteristics by stimulating the graphene suspension with a 532 nm pulsed laser.

A 037

Optoelectronic Applications of Europium Ion Doped Lithium Silicate Glasses: W-LED

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ABSTRACT

A novel Europium ion doped Silicate glass system (SiEu1 –SiEu5) is prepared by melt quenching method for Opto-Electronic applications. The density and refractive index values of investigating samples are high and the values showed increasing trend with the increase in Europium ion concentration from 0.2 to 1 mol%. The Hruby's criteria value of the prepared samples is high revealing their high thermal stability and thus suggestible for solar cells as a shield. The physical and optical properties of prepared glass samples are significantly varying as the concentration of the dopant enhances. The Direct energy band gap values are decreasing from 3.13 eV to 2.92 eV and also Indirect energy band gap values are decreasing from 2.92 to 2.63 eV as the concentration Eu^{3+} ion increases and these values unveil the semiconductor characteristics of the material for optoelectronic applications. The Judd-Ofelt parameters Ω_2, Ω_4 and Ω_6 of Europium ion-doped Silicate glasses are computed from the Luminescence spectra. The evaluated radiative parameters from Judd-Ofelt theory such as transition probability (A), radiative branching ratio (β_R) and the stimulated emission cross- section (σ_e) of the emission transitions of the sample SiEu 3 are found interesting amongst the prepared glasses. These parameters are useful in devices for a wide range of applications, including lasers, lighting, sensors, and bio imaging. The CIE plot shows that the glass samples SiEu1 – SiEu 5 emits white light at an excitation wavelength of 377 nm and 609 nm, and thus suitable for white LEDs.

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A 038

Effect of Molybdenum Oxide nanosheet on CVD Graphene

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ABSTRACT

Two – Dimensional (2D) semiconductors have been proven to be excellent for the use in the area of electronics and optoelectronics such as light emitting diode, electrochromic devices, photochromic devices, field effect transistors etc. Since Molybdenum trioxide (MoO_3) is a *n*-type semiconductor which is naturally found in layered form and can be exfoliated into crystalline 2D planes. MoO_3 has been extensively use in the range of electronic, optical, electrochromic, and sensing applications. Since the lower thickness of MoO_3 nanosheets increasing the performance of devices such as sensing response and recovery time in gas sensing devices. We have exfoliated MoO_3 nanosheets by liquid exfoliation, since this technique is easy, facile and non-destructive. Different thicknesses of exfoliated MoO_3 nanosheets characterized by atomic force microscopy and Raman spectroscopy. The effect of MoO_3 nanosheets on electronic properties of CVD grown mono layer graphene was investigated by Raman spectroscopy and resistivity measurement.

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A 039

Influence of Solvents on Non-Linear Optical properties of Ni^{2+} doped ZnO Nanorods

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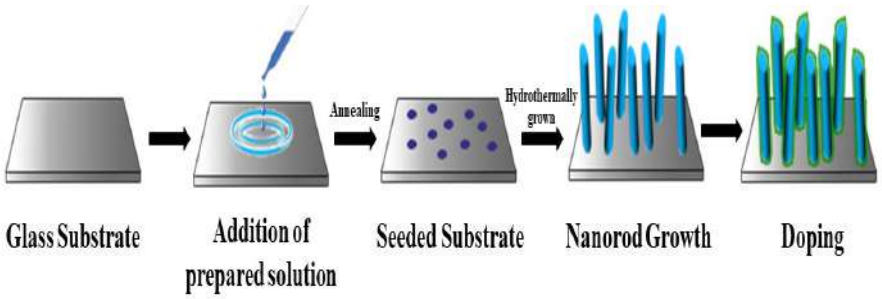
ABSTRACT

We hereby discuss a synthesis Zinc Oxide Nanorods using Zinc Acetate Dihydrate and Monoethanolamine as the common precursors. Solutions were prepared using various solvents (distilled water, methanol, ethanol, isopropanol and 2-methoxy ethanol). Prepared solution is coated on the glass substrate using drop casting method, followed by growth of Nanorods using Hydrothermal method in an aqueous solution of Zinc Nitrate Hexahydrate and Hexamethylenetetramine. The substrates are doped with specified concentrations of Nickel Nitrate Hexahydrate. High Resolution Scanning Electron Microscopy (HRSEM) and X-ray Diffraction (XRD) were studied to understand the morphology and crystal structure which showed a hexagonal wurtzite structure. An average diameter of ~200 nm and a length of ~1 µm were estimated from the HRSEM images. UV-Visible Spectroscopy was studied to determine the optical band gap and linear absorption co-efficient. Photoluminescence Spectroscopy was studied to find its excitation wavelength. We investigate the third-order nonlinearity from the Z-scan studies using a 532 nm pulsed laser which determines their nonlinear refractive index and nonlinear absorption coefficient of the ZnO nanorods. We also analyze the optical limiting properties of ZnO nanoparticles suspension. The direction of the nanorod growth caused by the different solvents, strongly affect the nonlinear optical properties. The results from the non-linear studies shows that the Ni^{2+} dopant can improve nonlinear optical properties of ZnO nanorods. The Zinc oxide nanorods may be a promising candidate for nonlinear optical applications like optical limiting.



A 040

Third Order Optical and Nonlinear Optical Properties of Zinc Vanadates

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ABSTRACT

The zinc vanadate nanoparticles were synthesized by facile hydrothermal method. It contains the mixture of ammonium vanadate and zinc acetate in the presence of CTAB and deionized water, the pH value was adjusted around 8 and yellow precipitate were obtained. The prepared zinc vanadate nanoparticles have been characterized by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS), high resolution TEM (HRTEM) and solid UV–vis diffuse reflectance spectrum. The structure and phase purity of the prepared sample was confirmed by powder X-ray diffraction. The morphology is identified by SEM and TEM. The spinal structured ZnV_2O_4 is made up of face centred cubic structure in which zinc cation occupies tetrahedral holes and vanadium cation occupies octahedral holes. The nonlinear optical properties of zinc vanadate ZnV_2O_4 is studies via open and closed Z- scan technique. The open Z- scan aperture reveals the absorption coefficient of prepared sample and closed Z- scan aperture reveals its third harmonic generation. The Non-linear optical behaviour of Zinc Vanadate nanoparticles have not been reported yet. So, we study the Non-Linear Absorption and its mechanism using a Z-Scan setup using a 532 nm pulsed laser.

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A 041

A Comprehensive Study of the Structural, Optical, Mechanical and Electrical Analysis of Third Order Non-Linear Optical Single Crystals of Imidazolium Perchlorate

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ABSTRACT

Single crystals of imidazolium perchlorate were successfully grown by slow evaporation solution growth technique in constant oil bath at RT. Powder XRD showed very good crystalline quality and confirmed the trigonal crystal system with R3m space group. The UV-Visible spectrophotometer study depicted the band gap value to be 5.1 eV. The FTIR analysis confirmed the presence of $[ClO_4]^-$ group and symmetric stretching of imidazolium cations. A sharp PL peak at 524 nm showed the green band emission. The non-linear absorption and refraction coefficients of the crystal were evaluated using a Z-scan experimental setup to demonstrate its third-order non-linear optical (NLO) response. The mechanical study of the crystal was explored using micro-Vickers hardness technique and demonstrated the crystal to be soft. Imidazolium perchlorate exhibited excellent properties in ferroelectricity and piezoelectricity, making it a promising candidate in sensing applications. The crystal was also employed for monitoring respiration and demonstrated excellent response and recovery characteristics.

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A 042

Investigating the Optoelectronic Properties of Pulsed Laser Deposited CdSSe Thin Films on Different Substrates

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ABSTRACT

Cadmium Sulfoselenide (CdSSe), a member of group II-VI, has gain significant interest in optoelectronics applications due to its excellent properties. The substrate play a crucial role to develop a good thin film in this work we mainly focus on investigating the role of different substrates on microstructural and optical properties of CdSSe thin films. CdSSe thin films are successfully deposited on different substrates via pulsed laser deposition technique. X-ray diffraction (XRD) analysis indicated preferential orientation in the (220) direction. The band gap energy of these films is in the range of 2.28 to 2.64 eV. The energy band gap lies in the range that is suitable for the desired purpose. The results of optical and structural investigation show that these films are suitable for optoelectronics applications.

Keywords: *Pulsed laser deposition (PLD) · thin film · band gap · cadmium sulfoselenide, · optoelectronic application*.

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A 043

A Study on the Optical and Electronic Properties of Nanoparticles Decorated Transition Metal Dichalcogenides

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ABSTRACT

Two-dimensional materials have attracted tremendous research interest recently due to their extraordinarily unique physical and chemical properties, which are helpful for many applications such as electronics, optoelectronics, catalysis, etc. However, their atomically thin layer thickness leads to poor absorptivity, which results in low photo responsivity and quantum yield. Developing effective methods for boosting light-matter interaction is crucial to improving the performance of two-dimensional transition metal dichalcogenides towards next-generation optoelectronic devices. A metal-semiconductor interface like Au-MoS_2 is an outstanding platform for encouraging light-matter interaction and investigating plasmonic-excitonic interactions and charge transfer. Here, we fabricated a hybrid 0D-2D system with Au as a metal nanoparticle and MoS_2 as TMDC. Depending on the doping of Au metal on TMDC, a quenching or enhancement in the photoluminescence spectra of bare and hybrid MoS_2 can be expected, and a shift in the PL spectrum can be arise based on the size of the nanoparticle.

Keywords: 2D materials, Transition metal dichalcogenides, Plasmonic

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A 044

Raman Spectroscopy Study on the Effect of Microwave Irradiation on the Fano Asymmetric Resonance in 2H-MoS_2

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ABSTRACT

This study investigates the influence of microwave irradiation on the vibrational Raman spectra of bulk 2H-molybdenum disulfide (MoS_2) synthesized for different temperatures on preparation with hydrothermal method and its impact on the Fano asymmetric resonance within the material. Raman spectroscopy was employed to explore the changes in the structural and vibrational properties of 2H- MoS_2 nanoflakes under different irradiation time intervals ranging from 10 minutes to two 60 minutes. The results reveal significant alterations in the vibrational modes of 2H-MoS_2 as a result of microwave irradiation. Shifts in vibrational frequencies and changes in intensity ratios between different Raman-active modes indicate induced structural modifications. Notably, the Fano asymmetric resonance in 2H-MoS_2 exhibits sensitivity to microwave irradiation, with changes observed in the asymmetry and linewidth of the resonance as a function of irradiation time. This suggests a coupling between the vibrational modes and electromagnetic fields generated by microwave irradiation. Understanding the structural and vibrational dynamics of 2H-MoS_2 under microwave irradiation is crucial for manipulating its unique properties. This knowledge has implications for applications in nanoelectronics, optoelectronics, and quantum technologies. By elucidating the interplay between the Fano asymmetric resonance and external perturbation, this study contributes to the advancement of 2D transition metal dichalcogenides and their potential use in various technological fields.

Keywords: MoS_2, microwave irradiation, Micro Raman spectroscopy, Fano asymmetric resonance, vibrational modes, structural modifications, 2D materials.

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A 045

Hybrid Quantum Engineering with Photon-Magnon Coupling at Room Temperature for Next Generation Quantum Information Devices.

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ABSTRACT

Photon-magnon coupled (PMC) hybrid systems hold great promise for applications in quantum processing technologies. Specially, controlling the interactions, including various types of anti-crossings, between photon (P) and magnon (M) modes is crucial for the development of information processing devices with desired tunability and scalability. Multimode PM coupling with switching features from level repulsion (LR) to level attractions (LA) is theoretically proposed and demonstrated through numerical simulations for two different hybrid systems i.e., two photon-one magnon mode (2-1 PM) and three photon-one magnon modes (3-1 PM). Although, individual photon modes display dissipative couplings with the magnon mode, when designed as 2-1 PMC system, one photon undergoes a transition to coherent coupling, while the other maintains its dissipative coupling with magnon. On the other hand, in the case of a 3-1 PMC system, their combination results in a shift to coherent coupling for one photon, a transition from dissipative to coherent coupling for the second photon while the third photon retains its dissipative coupling with magnon mode. The numerically calculated LR and LA due to coherent and dissipative coupling in these two PMC systems are presented in Fig. (c-e). Characteristic features of these multi-mode interactions (Fig. g-h) are analysed with the help of our own developed quantum mechanical model just by controlling some parameters at room temperature.

Keywords: photon, magnon, coupling, level attraction, level repulsion

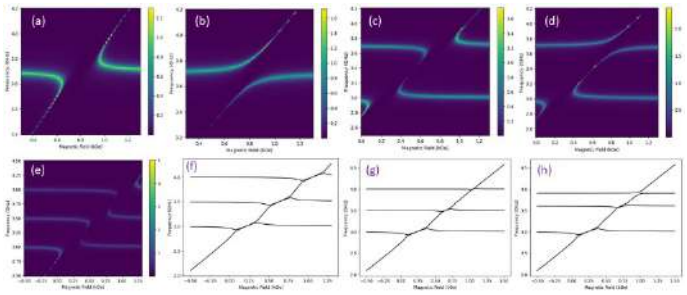

Figure: (a/ b) LA/ LR for 1 magnon and 1photon mode, (c) 1 magnon and 2 photon modes showing LA for individual systems, (d) hybrid of (c) after parameter tuning shows LA+LR (e) 1 magnon 3 photon modes LA for individual systems, (f-h) eigen value curve for (e) after parameter tuning showing transition from LA to LR.

A 046

Synthesis of Hexagonal Boron Nitride by Using Chemical Vapor Deposition Method

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ABSTRACT

Hexagonal boron nitride (h -BN) has newly attracted a lot of attention due to its excellent properties and many applications such as high-temperature stability, high mechanical strength, high thermal conductivity, low Dielectric constant (3-4), and wide band gap (5.9 eV). h-BN is an ideal substrate for graphene because of the low lattice mismatch between them, h-BN as a protective coating, dielectric layer/substrate, transparent membrane, or deep ultraviolet emitter. In this work, we synthesized h-BN deposited on metal foil using two heating Furnace zones with a low-pressure chemical vapor deposition Technique. In this method, we obtained h-BN still challenging of few layers, large-scale as well as high-quality h-BN nanosheets by controlling the surface morphology of metal foil acting as a catalyst. The optical band gap of h-BN was determined to be 5.7 eV. The ammonia boran powder was used as the precursor carried by mixed hydrogen/argon gases, which is easily accessible and more stable under ambient conditions than borazin. It is free of carbon and oxygen-characterization of the h-BN films via Optical microscopy, Raman spectroscopy, XRD, and UV-visible spectroscopy.

Keywords: Hexagonal boron nitride, chemical vapor deposition, ammonia borane, copper foil

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A 047

Vertical *p-n* Diode On (113) Oriented Homoepitaxial Diamond by Utilizing Boron Doped *p* Type Diamond Base

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ABSTRACT

The diamond semiconductor exhibits notable figures of merit within the class of wide band-gap semiconductors, making it particularly suitable for high performance power electronic and quantum optical devices[1,2]. Diamond is the material with the most promising characteristics in terms of breakdown voltage, on-resistance, thermal conductance, or carrier mobility[3,4]. However, it is also the one with the greatest difficulties in carrying out the device technology because of its very high mechanical hardness and smaller size of substrates. Here in this work, we formed pn junction from a boron-doped p-type diamond layer and phosphorus-doped n-type diamond layer grown epitaxially on the {113} surface of a single crystalline diamond. Vertical *p-n* junctions were fabricated on {113} oriented diamond substrates produced from thick heavily BDD (N_A~$5x10^{20}$ cm^{-3}) layers grown on HPHT-grown synthetic Ib diamond crystals using AX510 MWPECVD reactor. The thin lightly doped *p* layer was deposited on the top of the ~200 µm thick P^+-epitaxial layer, oxygen terminated, and covered by phosphorus doped n layer and then evaporated Ti/Au ohmic contacts. The bottom ohmic contact was formed by Ti/Au bi-layer. The I-V and C-V characteristics of the realized *p-n* diodes were measured at temperatures ranging from 25 to 180 °C.

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A 048

Rutile to Anatase Phase Transition in TiO_2 Nanoparticle Doped with Dy^{3+} Ions

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ABSTRACT

Dysprosium-doped titanium dioxide (Dy^{3+}doped TiO_2) is an intriguing material with potential applications in various fields, including catalysis, photocatalysis, and optoelectronics [1]. This study investigates the structural phase transformation of TiO_2 from rutile to anatase phase on doping with dysprosium. The synthesis of Dy^{3+}-TiO_2 was achieved through the Hydrothermal method. X-ray diffraction (XRD) analysis revealed a remarkable phase transition from rutile to anatase. Raman spectroscopy further confirmed this transformation, elucidating the profound influence of dysprosium doping on TiO_2 phase stability [2]. The luminescence properties of Dy^{3+}-TiO_2 were investigated through photoluminescence (PL) spectroscopy. The anatase phase has less electron-hole recombination than rutile TiO_2 [3]. This research provides valuable insights into the structural changes of Dy^{3+}-doped TiO_2 and its luminescence properties, opening avenues for further exploration and utilization of this material in advanced technological applications [4],[5].

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A 049

Spectroscopic Insights into Sm^{3+} doped Strontium Calcium Borate Phosphor

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ABSTRACT

This study seeks to provide a thorough exploration of the spectroscopic characteristics of strontium calcium borate phosphor doped with Sm^{3+}. This phosphor was created using the widely employed solid-state reaction method, a common choice for diverse phosphor types, including borate-based variants. The central objective of our research is to identify highly efficient luminescent materials activated by samarium ions. For elemental composition analysis, we utilized Energy Dispersive X-ray spectroscopy (EDS), which enabled the identification of specific elements through distinct peaks in the EDS spectrum. The absorption spectra exhibited peaks in both the UV-Vis and NIR regions, yielding valuable insights into the energy band gap, determined from the Urbach edge. Band gap values were calculated for both direct (E_g = 5.4 eV) and indirect (E_g = 4.7 eV) transitions. Moreover, the nephelauxetic ratio, derived from the absorption spectrum, suggested a blend of ionic and covalent bonding within the phosphor. Under excitation at 403 nm, the photoluminescence spectrum displayed emission transitions spanning from blue to red, a phenomenon substantiated by the energy level diagram of Sm^{3+} ions. Colorimetric analysis further affirmed the phosphor's capacity to emit white light, positioning it as a valuable contender for White Light Emitting Devices (W-LEDs). The synthesis method resulted in a material with multiple visible wavelength emission channels, making it adaptable to a wide range of technological applications, including LED technology, tunable lasers, optical communication devices, and display technologies. The remarkable spectroscopic attributes of Sm^{3+} doped strontium calcium borate phosphor significantly enhance its suitability for display lighting applications.

A 050

Study of Nonlinear Effect in Magnon Embedded Hybrid Optomechanical System

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ABSTRACT

Recent development in the various phenomena involved in magnons, quanta of collective spin excitations, have attracted extensive attention for several decades because of their potential application in the field of signal processing in the microwave frequency range. Due to high spin density and low dissipation rate ferromagnetic materials, especially the YIG samples, are becoming increasingly popular in the study of the coupling to cavities. We investigate the steady-state dynamic processes of a hybrid quantum system based on magnonics under the influence of a strong control field. The system consists of optomechanical cavity embedded with ferromagnetic-material yttrium iron garnet (YIG) spheres coupled to a cavity mode. The YIG sphere is placed inside a microwave cavity near the maximum magnetic fields. Both quantum information processing and future quantum internet inevitably need efficient quantum information transfers among different physical systems. Hybrid systems based on magnonics may prove to be promising solutions to these challenges.

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A 051

Effect of Yt Doped on PbS Thin Films Produced by the Jet Nebulizer Spray Pyrolysis Method and Construction of p-Yt -PbS/*n*-Si Photodiodes with Luminance Dependence for Photodetector Application

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ABSTRACT

This study describes the preparation of 0, 1%, 3%, and 5% Yt-doped PbS thin films by nebulized spray pyrolysis technique at 300 °C for photosensitive applications. Yt-doped PbS samples exhibit better photodiode performance than pure PbS films. XRD confirm that no new peak is absorbed after adding Yt to PbS and maintaining its hexagonal phase. The FESEM results showed that the samples contained triangular nanostructured PbS thin films and that the morphology could be changed to an amassed form by Yt doping. X-ray photoelectron spectroscopy (XPS) examined the chemical composition and surface binding energy of the Yt doped PbS photosensor, and the XPS spectra confirmed the presence of Pb, S and Yt. The optical characterization reveals that the band gap energy is found 2.5 to 1.75 eV band gap and the red shift in the absorption spectrum indicates that there are no oxygen vacancies on the PbS surface, confirming the reduction in the band gap. Finally, experiments with photosensors show that PbS thin films doped at 5% Yt-doped PbS thin films are promising photodiodes for commercial optoelectronic device applications.

Keywords: *Yt- PbS, photodiode, Responsivity, Photosensitivity and Detectivity*

A 052

Investigation on Microstructural and Optical Properties of Aluminum Doped Vanadium Oxide Films Fabricated by Hydrothermal Method

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ABSTRACT

A standard V_2O_5 nano particle was fabricated by a hydrothermal method. The 0.1M ammonium meta vanadate aqueous solution were used to deposit aluminum doped vanadium oxide films were prepared adding separately 5wt.%, 10wt.% and 15wt.% of aluminum tri chloride. The structural, morphological and optical characteristics of V_2O_5 and Al: V_2O_5 were investigated by FT-IR, XRD and SEM. The morphology of Al: V_2O_5 was observed in quasi-spherical nanoparticles with uniform in size and high crystallinity. The change in crystal structure and surface morphology can induced due to different levels of aluminum doping. The nano V_2O_5 have shown a strong absorption in the visible region and the band gap energy was obtained to be varying from 2.2 to 2.7eV as a function of Al doping. EDAX conforms significant on Al and V_2O_5. Surface morphology and band gap or these powders were modified due to Al impurities incorporated into V_2O_5. The change in crystal structure and surface morphology can induced due to different levels of aluminum doping. Specifically, doping aluminum can introduce extra oxygen vacancies by larger radius (Al^{3+}) which was lower in valance than V^{4+} during the nucleation and growth of V_2O_5 nano particles. It was found that the film growth and gas response were strongly affected by Al impurities were incorporated into V_2O_5 lattice.

A 053

Elucidating the Mechanism of Metal-Catalyst-Free Direct CVD Growth of Few-layer Graphene on SiO_2/Si wafer

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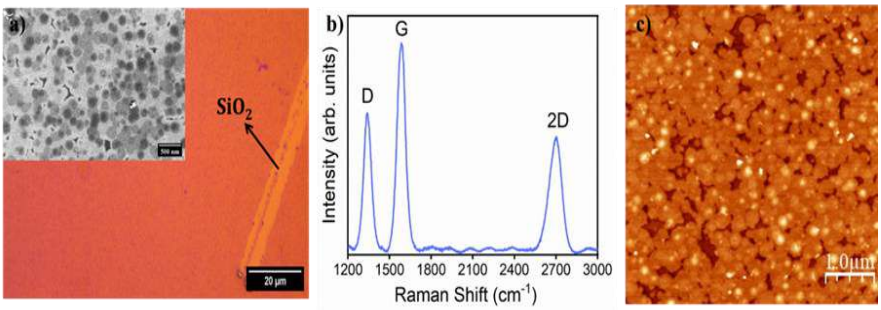
ABSTRACT

The complex transfer process of graphene from dedicated growth substrates to another substrate is prone to induce defects, which has been challenging for graphene-based electronic and optoelectronic applications. A variety of chemical vapor deposition (CVD) techniques have been the focus of various research groups for the catalyst-free direct growth of graphene on dielectric and semiconductor substrates.[1-3] In the present work, transfer free few-layer graphene growth on SiO_2/Si is demonstrated using Atmospheric Pressure Chemical Vapor Deposition (APCVD). A systematic study in the variation of the growth parameters such as total pressure, growth temperature, partial pressure of H_2 and CH_4, and growth time have been carried out. The conventional microscopic visualization of the surface using scanning electron microscopes, and micro-Raman characterization (at a spatial resolution of ~1 μm) indicates the formation of continuous few-layer graphene (FLG), further atomic force microscopy visualization at nanoscale revealed the growth of discontinuous graphene characterized by not fully coalesced domains with grain sizes in the sub-micron (< 500 nm) range. This later fact can account for the strong D peak intensity observed in the graphene Raman spectra. More experimental studies are underway to provide further insights into the defect structure and to understand the mechanism behind the growth.



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A 054

Determination of Self-Assembled Nano Structured Photonic Properties of Peacock Feathers for Turning Nonlinear Optical Properties

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ABSTRACT

Beauty is so important in engineering design that there is whole subject called aesthetics which defines how beauty can be added to man made products. The peacock tail produces different colors. The colors in the peacock feathers are not pigment colors but structural colors which are produce by an optical effect called thin film interference. The eye feather contains remarkable patterns. The eye pattern is made up of rounded shape that has a high resolution. The pupil of the eye is a dark purple cardioids shape and the iris is a blue ellipsoid shape. These shapes are located within a pointed bronze ellipsoid which is surrounded by one or two green fringes. A very important feature of the eye pattern is that it is a digital pattern which is formed by the combined effect of many thousands of individual barbules segments. It is very interest to note that the different colored barbules consisting of various photonic crystals (extracted from eye pattern) were characterized in terms of the bands and other parameters (RI and particle size) identified in the respective spectra. In the present study we made an attempt to find the particle size of the different colors in the feathers eye of the peacock and peahen using powder x ray diffraction for any supporting self-assembled nano structured properties. Results were discussed in details.

A 055

Alkaline Bath Chemical Deposition of Hg - doped Cadmium Sulphide Thin Films

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ABSTRACT

Prime focus of the present letter is to deposit $Cd_{(1-X)}Hg_XS$ thin films via alkaline bath chemical rout and to investigate some of its properties. At optimized condition (Temperature = 600C, Time = 90 min and pH = 10.5) uniformly deposited films are tightly adherent. As-grown thin film samples were then subjected to characterizations like XRD, EDS and SEM for structural, compositional and morphological studies. From XRD analysis hexagonal wurtzite crystal structure was confirmed. An EDS analysis revealed slight non-stoichiometry in deposited samples which depends on the quantity of Hg in reaction bath. Crystallites resembling network of bougenvellia petals were revealed by SEM analysis. Effect of Hg doping can also be observed through the surface features exposed by SEM. The optical measurements in the range of wavelength 300 nm - 800 nm showed direct transition with expected broad absorption edge and high absorption coefficient. Variation in optical band gap is attributed to the merging of donor levels with the incorporation of Hg.

A 056

Comparative Study of Component-Level Reliability Approaches in Power Electronic Components

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ABSTRACT

The increasing acceptance of renewable energies has significantly increased the use of photovoltaic (PV) systems within power grids. In environments heavily dependent on solar power, accurately predicting solar energy output and its lifetime is paramount. There are various factors that impact these predictions and the failure rates. Microinverter is a significant subsystem in a photovoltaic power system. Numerous research has focused on developing new inverter topologies and modifications in commercially available inverters to improve the reliability of photovoltaic systems. Improving the efficiency and reliability of PV inverters is critical for reducing the overall cost of energy produced through photovoltaics. This article analyses diverse reliability techniques, including MIL Handbook 217, RIAC, and FIDES, in-depth to determine the lifetime and reliability of inverter components. Furthermore, all these reliability techniques were compared to determine the most effective approach.

A 057

Two Photon-Induced Optical Limiting Capacity Investigation in $SrWO_4/MoS_2$ Nanocomposites

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ABSTRACT

This work mainly focuses on the hydrothermal synthesis of $SrWO_4/MoS_2$ nanocomposites by exploring linear and non-linear optical properties and their impact on optical limiting capacity. Structural studies through XRD (x-ray diffraction) confirmed the formation of $SrWO_4/MoS_2$ nanocomposites via distinct peaks of both phases of the materials. Morphology and the elemental composition of nanocomposites were examined by a High-Resolution Scanning Electron microscope (HR-SEM) and a High-Resolution Transmission Electron microscope. Linear absorption studies showed the absorption nature of nanocomposites. Open aperture Z-scan experiments using 532 nano-pulsed lasers were employed to investigate the non-linear optical (NLO) behavior of $SrWO_4/MoS_2$ nanocomposites. NLO properties of nanocomposites were extended to the analysis of the optical limiting (OL) behavior with intensity-dependent studies to understand their potential application in OL devices.

Keywords: *Nanocomposites, Optical Limiting, Hydrothermal*

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A 058

Neuromorphic memory devices using Molybdenum oxide and Copper Molybdates deposited using RF Magnetron sputtering.

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ABSTRACT

In past years there were a lot of hurdles to develop an artificial device that mimicked the principles and operations of the biological brain. There was a need for a non-volatile memory that is tightly coupled to signal processing components(brain) so that the emulation of biological synapses could be made easier. The invention of memristive devices paved the way for minimal-size plastic synaptic connections. Two- terminal memristive devices can be used as artificial synapses as they show high scalability, efficiency, and low energy consumption. Transition-metal oxides are promising candidates for artificial synapses due to their CMOS compatibility, scalable processing, and multi-valence states that contribute to the metastable structures. In this work, we report the successful fabrication of molybdates (MoO_X) and copper molybdates ($CuMoO_x$) thin films using RF Magnetron sputtering. Using molybdates and copper molybdates as the intermediate layer, two-terminal memristive devices with configurations FTO/MoO_3/Au and FTO/Cu:MoO_3/Au were fabricated. The structural properties of the films were studied by XRD and the stoichiometry was confirmed through XPS analysis. The synaptic behaviour such as potentiation/depression, Spike Timing Dependent Plasticity (STDP), Spike Number Dependent Plasticity (SNDP), and Paired Pulse Facilitation (PPF) were successfully demonstrated in these synaptic devices. Compared to molybdates, copper molybdates showed enhanced device performance and lesser energy consumption.

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A 059

Neuromorphic Tunnel Junctions for Emulating Highly Reliable Synaptic Functions

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ABSTRACT

Neuromorphic Computing has become an emerging field of research, leading to a paradigm shift from conventional computing architectures for processing massive data like the human brain. Compact nanoscale devices replicating biological synapses are the most significant components for building such brain-inspired computational systems. A wide band of materials systems and device configurations have been proposed for neuromorphic applications. An essential consequence of neuromorphic transitions due to ion migration through a medium is that it causes rapid resistive switching due to the formation of conducting filaments in the dielectric medium. In this work, we show that ultra-thin dielectric Neuromorphic Tunnel Junctions (NTJ) can resolve this issue, where tunnelling restricts the ion migration and filament formation, thereby increasing the reliability of the devices even at a much larger electric field than that required for its intrinsic breakdown. 1-2 nm thick Atomic Layer Deposited (ALD) Al_2O_3 layers deposited on fluorine-doped tin oxide (FTO) with silver electrodes are employed as the Neuromorphic Tunnel Junctions in this work. Compared to thicker dielectric layers, devices with ultra-thin Al_2O_3 layers exhibited reliable, stable performance. They were capable of emulating biological synaptic behaviours such as Paired pulse Facilitation/ Depression (PPF/PPD), Spike Timing-dependent plasticity (STDP), and Spike number dependent plasticity (SNDP). This research lays a path for high-reliable ultrathin layered devices for Neuromorphic applications.

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A 060

Optically Enhanced Memory Using Copper (II) Phthalocyanine-Based Artificial Synapses

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ABSTRACT

Emerging artificial intelligence systems offer advantages over conventional computers in terms of low power consumption, high efficiency, and parallel processing capability. Neuromorphic devices are brain-inspired systems that mimic the functions of biological neurons. The distinguishing feature of human brain is adaptive learning, allowing it to respond more effectively to previously encountered scenarios. A device that replicates this behaviour is termed as neuromorphic device. For a material to be considered optical neuromorphic, it must be sensitive to light. Studies have shown that some devices exhibit increased conductance when exposed to light pulses, forming the foundation for optical neuromorphic devices. Recent studies have identified organic materials as prime candidates for fabricating optical neuromorphic devices. In our study, we used Copper Phthalocyanine (CuPc), which exhibited appreciable optical neuromorphic behaviour when subjected to various LEDs and white light. The Gold-CuPc-Gold (Au-CuPc-Au) surface device features two Schottky barriers due to the high work function of gold. Theoretically, the conductance of this system varies due to ion flow through the interfaces, facilitated by the presence of light. In our research, we observed an enhancement in neuromorphic behaviour when the device was exposed to light. The essential features of a neuromorphic device such as Paired Pulse Facilitation (PPF), Spike Timing Dependent Plasticity (STDP) and Spike Number Dependent Plasticity (SNDP) were realised and were further facilitated under the influence of light. We were able to emulate Pavlov conditioning behaviour upon application and removal of light[1]. The realisation of Pavlov behaviour suggests the potential for optical enhancement of neuromorphic behaviour as a new application domain.

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A 061

Exploring Effective Molecular Charge Transport in Organic Electronics

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ABSTRACT

Conventional electronic technologies have been subject to certain limitations that have become increasingly evident with the downfall of Moore's Law. One major limitation has been the shrinking of discrete devices like transistors, which has been a key driver of performance improvements over the years. However, as the size of transistors approaches atomic levels, it becomes more difficult to reliably manufacture them and prevent leakage of electrical current, leading to decreased performance and increased power consumption. Another limitation is the heat generated by electronic devices, which has become a significant challenge as devices become smaller and more densely packed [1, 2]. These limitations have driven researchers to explore new technologies. The potential of semiconducting polymers/foldamers in electronic applications, such as organic thin film transistors (OTFTs), solar cells, and flexible electronics, has garnered considerable attention. These materials are appealing due to their low-cost processing, flexibility, and unique optoelectronic properties, including high absorption coefficients and low energy bandgaps, biodegradability, and environmental friendliness [3]. The charge transfer properties of organic polymers are heavily influenced by their molecular structure, which has a significant impact on the efficiency of devices such as organic field effect transistors, organic solar cells, and organic light-emitting diodes. Therefore, it is crucial to comprehend and regulate the molecular architecture of these materials to boost device efficiency. This study aimed to comprehend charge transfer in the π-π stacking interactions of a conjugated P1-PEG polymer and its guest-host interactions, as well as understand the π-orientations effect to fabricate potential P1-PEG polymer solution-processed organic thin film transistors and organic photovoltaics.

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A 062

The Influence of In on SnO_2 Thin Films by Jet Nebulizer Spray Coating Method for p-n Diode Application

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ABSTRACT

Indium doped tin oxide thin films are grown at atmospheric pressure using a home-built mist jet nebulizer spray pyrolysis method, which is an environmental-friendly technique with low energy consumption. For obtaining high quality In:Sn films, different concentration (0, 1, 3, 5 wt%) are used to support the film fabrication process. The role of each component in supporting solution is also preliminarily analyzed and studied. In this work, are examined using X-ray diffraction, field emission scanning electron microscopy, UV-visible, DC electrical conductivity. It is found that the film structural analysis of XRD pattern used to obtained crystalline size decreased with increased In concentration. The surface morphology of FESEM were analysis of plate like structure of In doped Tin oxide thin films. The band gap analysis of UV visible spectrum were measured absorption. Absorption spectrum used to analysis of band gap energy decreased with increases of In concentration. The electrical properties of conductivity increased with increase of In concentration corresponding activation energy and resistivity of film decreased. Interestingly, current vs voltage analysis of diode parameters of ideality factor n=3.46 were obtained higher concentration of 5 wt% compared another concentration. Corresponding barrier height increased upto ΦB=894 eV obtained at higher concentration. Our results demonstrate that JNSP is a powerful technique for future application in photodiode for highly efficient optoelectronic devices and photodetector.

Keywords: JNSP, In-SnO_2 thin films, *p-n* diode.

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A 063

Laser-Assisted Tailoring of Semiconductors Properties for Advanced Microelectronics: Unleashing the Possibilities for GeSn Epitaxial Layers

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ABSTRACT

The interaction between laser radiation and the semiconductor materials becomes particularly challenging when the laser intensity falls below the ablation threshold but remains close to it. This interaction can lead to various atomic rearrangements, material recrystallisation, the formation of nanostructures or microstructures, and even to the generation or recombination of intrinsic or extrinsic point defects. This study provides a comprehensive overview of laser-based methods for altering material properties. In particular, we focus on semiconductor materials and apply laser methods to modify epitaxial GeSn layers. Binary GeSn solid solutions present significant potential for mid-infrared Si photonics, due to their ability to achieve a direct band gap at more than 8% Sn content in GeSn and the possibility of forming devices directly on the Si chip. However, growing fully strain-relaxed GeSn epilayers with high Sn content and excellent material quality poses significant challenges for several reasons. These challenges include the high segregation coefficient of Sn in Ge, a substantial lattice mismatch of 14.7% (19.5%) between α-Sn and Ge (Si), and the limited equilibrium solid solubility of Sn in Ge, which is less than 1%. To address these concerns, our study investigates the redistribution of Sn atoms and the strain relaxation of GeSn alloys after employing post-growth laser processing techniques using nano, pico, and femtosecond lasers. Using the reciprocal space mapping (RSM) method, we investigated the impact of laser processing on nature of the strain in GeSn epilayers. Our observations revealed that the laser radiation induced partial compressive strain relaxation, and the extent of relaxation depended on the intensity of the laser. By employing TEM-EDS and X-ray photoelectron spectroscopy (XPS) analysis, we found that nanosecond laser radiation led to an increase in the Sn atomic concentration at the surface layer, reaching up to 14% for initial samples with a 4% Sn content. This increase can be attributed to the thermogradient effect. In contrast, pico- and femtosecond laser radiation had minimal influence on the redistribution of Sn atoms within the GeSn layers.

A 064

Estimation of Switching and Conduction Losses of 10 kW SiC Based T-Type Three-Phase Inverter for V2G And G2V Application

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ABSTRACT

This paper presents the loss analysis of SiC (silicon-carbide) based T-type bidirectional inverter for both G2V (grid-to-vehicle) and V2G (vehicle-to-grid) applications. T-type inverters can lower the amplitude of particular harmonics and produce a uniform output waveform with a lower THD by combining a variety of switching states. The designed structure employs WBG (wide-bandgap) semiconductor devices such as SiC MOSFETs rated at 1200 V and SiC JFETs rated at 1700 V, is operated at a high switching frequency of 100 kHz which improves the parameter performance and power density. The inverter uses SiC freewheeling diodes to overcome the SiC MOSFETs minority charge in their body diodes. Here three main factors are discussed. First, the switching states of T-type inverter are using a 10 kW DC-AC bidirectional inverter. Second, the efficiency of a traction inverter with a Buck and Boost DC-DC converter operation for grid connected electric vehicle applications. Finally, the analysis of overall power losses of inverter is determined. The improved efficiency of the system with SiC traction inverter is achieved up to 98.09%. The peak junction temperature for the devices at various load current is analysed and the SiC JFETs have 28.9ºC, and SiC MOSFETs (T-type) has the 28.3ºC at overall system configuration. Reducing the losses of the inverter demonstrates the overall performance of the application, this consideration is used for future energy storage applications. This T-type inverter lowers the voltage load on specific electronics, improving their dependability and possibly extending their lifespan. The MATLAB environment is used for simulation. Finally, OPAL-RT results are presented to confirm the performance of the designed structure of a T-type three-phase 3L inverter.

A 065

Synthesis and Characterization of TiO_2: ZnO Thin Films for Optoelectronic Applications

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ABSTRACT

TiO_2 doped ZnO thin films were successfully synthesized on FTO coated glass substrate using sol- gel spin coating system. The effect of TiO_2 doping concentration (1at%, 2at% and 2.5at %) on the optical properties of TiO_2: ZnO thin films were investigated using UV-vis spectroscopy, Raman spectroscopy and FTIR spectroscopy. The deposited thin films were annealed at 550 ^{0}C for 4 hours using high temperature furnace in air atmosphere. A sharp absorption band edge has been observed near 300 nm in UV-vis spectrum and the band decreases exponentially with increasing wavelength. The UV-vis spectra analysis reveals that the energy band gap (E_g) of deposited thin films varies from 3.6eV to 3.5eV with increasing TiO_2 doping concentration into ZnO crystalline lattice. Two significant characteristic peaks E_2^{high} mode and E_1^{low} mode identified at 428cm^{-1} and 561cm^{-1} in Raman spectra. FTIR spectroscopy was used to investigate the presence of functional groups in the synthesized thin films. The absorption peak lies at 503 cm^{-1} and 631cm^{-1} in FTIR spectra for 2.5at% are associated with Zn-O and Ti-O characteristic stretching vibrational modes, respectively.

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A 066

Optical Diode Activity in Bilayer Structure Based on PEDOT: PSS

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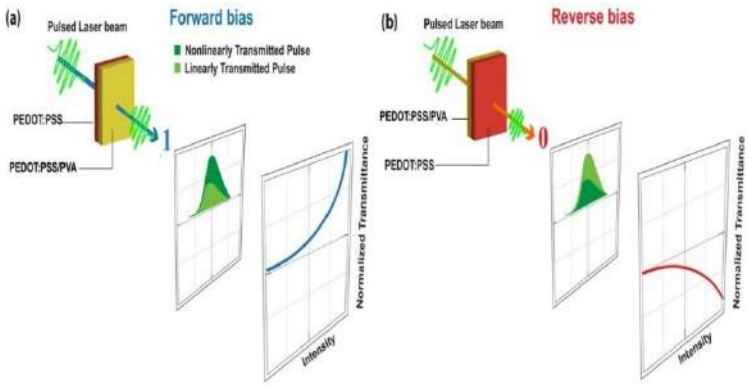
ABSTRACT

Optical diodes facilitating passive nonreciprocal light transmission are fundamental to integrated optical circuits. This work presents an all-polymeric optical diode based on the principle of asymmetric nonlinear absorption in the nonlinear regime[1]. PEDOT: PSS is a conductive polymer that has emerged as a benchmark material in organic electronics. The high density of delocalized π molecular orbital electrons in the PEDOT backbone makes it a promising fast-responding nonlinear material suitable for application in nonlinear optical elements[2]. Here, we report Optical diode activity in bilayer structure based on PEDOT: PSS. This solid-state passive optical diode uses PEDOT: PSS as the saturable absorber and PEDOT: PSS/ Poly (vinyl alcohol) as a reverse saturable absorber. This bilayer optical diode is versatile with high chemical stability, cost-effective, and suitable for large-scale integration. Nonlinear optical characterization was conducted using the z-scan technique, utilizing a Q-switched Nd:YAG laser emitting 7 nanosecond pulses at 532 nm. All-optical diode action in this device is polarisation-independent and has no phase-matching constraints at 532nm. The structure demonstrates a moderate nonreciprocity of approximately 4, making it a promising candidate for the fabrication of compact photonic integrated devices.



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Enhanced Upconversion and Optical Thermometric Performance in $GdVO_4:Er^{3+}/Yb^{3+}$ Phosphor Via incorporation of Li^+ ion

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ABSTRACT

$GdVO_4$ phosphor doped with Er^{3+}/Yb^{3+} and $Er^{3+}/Yb^{3+}/Li^+$ ions was successfully produced by the high temperature solid state reaction approach. The crystal structure of $GdVO_4$ was found to have a tetragonal phase using X-ray diffraction study. The morphological analysis reveals the presence of particles at a micro scale. The upconversion luminescence upon 980 nm laser diode excitation shows the emission bands in green and red regions owing to characteristic emission of Er^{3+}ion. Pump power analysis and energy level diagram were used to explain the observed emissions. Temperature-dependent upconversion spectra were recorded in order to determine the suitability of the produced phosphors as a non-contact temperature sensor. The temperature sensitivity of the phosphors was determined by utilizing the emission bands arising from thermally coupled and non-coupled levels of the Er^{3+}ion. Furthermore, thermal stability, colour coordinate study and anti-counterfeiting application were also explored.

Keyword: Solid-state reaction, Upconversion, Optical thermometry, anti-counterfeiting

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A 068

Design of LO Phase Shifter Based on Quadrature Hybrid Branchline Coupler for IQ Mixer in Synthetic Aperture Radar Applications

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ABSTRACT

Synthetic Aperture Radar (SAR) is a powerful instrument in microwave remote sensing because of its capability for all-weather and day-to-night time operation [1]. SAR has been widely used in many applications, particularly object detection, earth observation, agriculture, and terrain mapping [2]. SAR is constructed by the RF sub-system responsible for managing analog signals, with one of the important components being the IQ Mixer [3]. IQ Mixer mixes the base chirp signal with a carrier signal and increases the bandwidth of the transmitted signal to twice the base chirp signal. It is important because it can reduce the burden on the Field Programmable Gate Array (FPGA) that produces the base chirp signal and simultaneously increase the range resolution of the SAR system that depends on the bandwidth of the transmitted signal [4]. Therefore, to have a good performance of IQ Mixer, a steady supply of components, and demand to reduce cost production, we need to develop it independently. Three sub-parts construct the IQ Mixer: Local Oscillator (LO) Phase Shifter, Matched Mixer, and Power Combiner-Splitter. This paper proposes the design of an LO Phase Shifter based on a Microstrip Quadrature Hybrid Branch-line Coupler as a supporting component for IQ Mixer in Synthetic Aperture Radar Applications [5]. The measurement result from the fabricated coupler shows that all the specification requirement has been fulfilled. S11 has a low reflection of -26.54 dB, S41 has a high isolation of -32.27 dB, S21 and S31 have low attenuation with amplitude unbalance of 0.291 dB and phase unbalance of 2.17 degrees. The requirement bandwidth of 150 MHz at the center frequency of 5.5 GHz was also achieved. Therefore, this coupler can be considered to be used as an LO Phase Shifter.

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A 069

Flash Joules Heating Methods with High Voltage Capacitor for Lab-Scale Graphene

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ABSTRACT

Flash joule heating (FJH) is a process where a material is heated to a very high temperature (3000 °K) in a fraction of a second, turning electricity to heat using a capacitor. This treatment is commonly used to produce some types of carbon allotropes, such as Graphene [1–3]. In this research, the FJH components is consisted of one 450 V 6000 μF capacitor, 450V DC power supply, quartz pipe, copper wool, flash chamber, resistor, switch, cable, and storage tube. Figure 1 shows FJH methods. The resistivity of the material treated by the procedure will be measured, and Raman analysis will be performed. Variables of the process, that is the cable differences in the flash circuit and the types of FJH carbon material will be analyzed to determine the optimal FJH process. From the analysis, we can conclude that the parameters of the experiment are correlated to the FJH, and the process can be optimized.

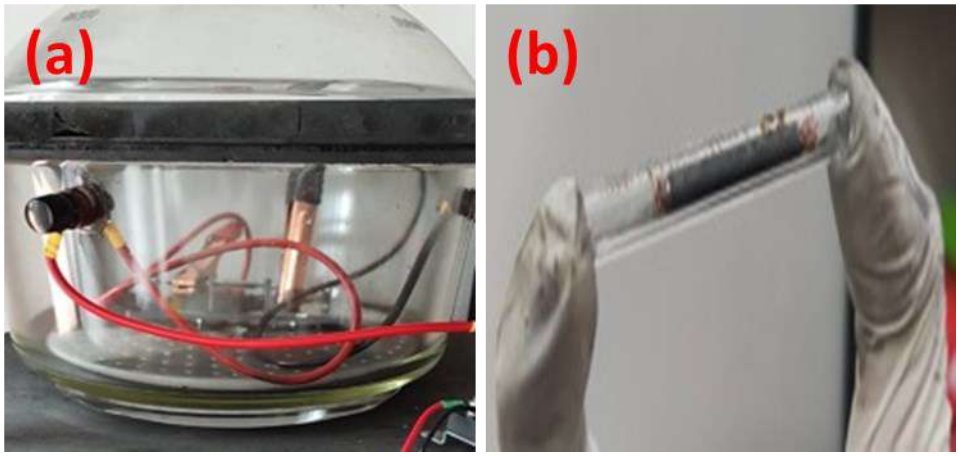

Figure 1. (a) FJH Chamber. (b) Carbon materials.

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A 070

Electro-Optic Effect of Ferroelectric Thin Films: Strain Engineering and Exploration of Emerging Materials

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ABSTRACT

In recent years, novel thin-film-based electro-optic (EO) modulators, which are compact, energy-saving, and high-speed, have attracted a great deal of attention. In such devices, the use of ferroelectric materials, which show large EO coefficients, is preferable compared to that of non-linear polymers from the viewpoint of long-term stability. However, it is widely observed that the EO coefficients of thin, ferroelectric films are often different from those of the bulks, and these origins have not been deeply understood, unlike the ferroelectric and piezoelectric effects. Therefore, the strategy to enhance the EO effect in ferroelectric thin films has not been established yet. In this presentation, we first theoretically and experimentally demonstrate the influence of strain on the EO effect in thin films of classical perovskite ferroelectric (Ba, Sr) TiO_3,[1,2] and discuss the extrinsic contribution, owing to the dynamic domain switching, to the total EO response in classical perovskite Pb (Zr, Ti) O_3 thin films.[3] Then, we explore the EO response in emerging ferroelectric thin films compatible with Si-based CMOS technology. Y-doped HfO_2 thin films showed the evident EO response based on their ferroelectricity,[4,5] and the EO coefficient of Mg-doped ZnO thin films was increased with increasing Mg content and reached 7.6 pm/V, which is over three times larger than the reported values for ZnO-based thin films and over twice larger than that of ZnO single crystals.[6]

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A 071

Amplified Spontaneous Emission through many-body Correlated State in $CsPbBr_3$ Nanocrystals

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ABSTRACT

Electron-hole liquid (EHL), is a collective macroscopic quantum state of matter arising due to the strong correlations among charge carriers, above a critical density and below a temperature, which has recently been found in many semiconducting materials like TMDCs, and halide perovskites [1-4]. The features of EHL as a macroscopic population of nonequilibrium charge carriers may offer its application to high-temperature optoelectronic and photonic devices [5-7]. However, the lasing behavior induced by the EHL state is still unknown. In this paper, we reported that this EHL state is able to produce broadband and sizable optical gain with dual amplified spontaneous emission (ASE) bands. We have observed that Two kinds of the ASE band are successfully observed at 4K: the Biexciton band and EHL band with their respective threshold fluence of 25 μJcm^{-2} and 200 μJcm^{-2}. We have observed no shift in the PL profile at high carrier density, with super-linear dependence behavior, suggesting the transition from the excitonic system to the EHL state. This EHL state produces a large optical gain of ~ 200 meV with a fast radiative decay feature. This EHL-induced ASE behavior is persisted up to 200K. At room temperature, the ASE behavior vanished due to the large contribution of thermal fluctuations and non-radiative recombination. Our work demonstrates a comprehensive and detailed study of the application of many-body correlated states in optoelectronic devices and many other macroscopic quantum phenomena. We believe that the formation of EHL also stimulates other macroscopic quantum phenomena such as super fluorescence.

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A 072

A Visible Light Wide Angle Optical Divider Based on III/Nitride for under Water Application

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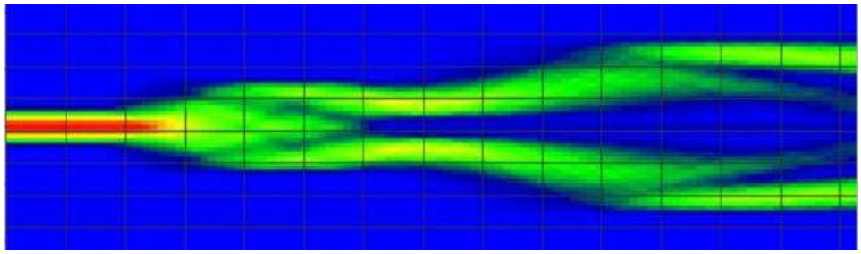
ABSTRACT

In this paper, we propose the design of a wide-angle 1×2 optical power divider using gallium-nitride (GaN) semiconductor on sapphire, suitable for underwater optical wireless communication. The design comprises six rectangular waveguides based on mode coupling phenomena. Numerical experiments reveal that optimal results are achieved with a width of 4 µm for the input and output waveguide ports, and a 15 µm distance between output ports. The design analysis employed the beam propagation method (BPM). Optimization was carried out using the 3D FD-BPM method with an optical signal input at the maritime application wavelength of λ=0.45 µm.The optical signal was injected into the central input waveguide. Results indicate that at a propagation length of 860 µm, the optical power divides into two output beams with an excess loss of 0.75 dB and equalpower output. This proposed design holds promise for further development and application in underwater communication technology.



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A 073

Third-Order Nonlinear Optical Limiting Behavior of Pure, Single, and Co-Doped CuO Nanoparticles

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ABSTRACT

Pure, single (Zn, Bi), and double dopant (Zn/Bi) CuO nanoparticles have been synthesized by the green synthesis method in which *M. oleifera* leaf extract acts as a reducing agent. The powdered XRD pattern confirmed the phase and by the Debye Scherrer equation, the crystallite size was evaluated. The vibration of the molecules was obtained by FT-IR spectra. SEM analysis exhibited different nanostructures and the elemental compositions like Cu, O, Zn & Bi were affirmed by EDAX analysis. The negative charge for pure, Zn-doped CuO, Bi-doped CuO, and Zn/Bi-doped CuO nanoparticles was found to be -34.23 mV, -33.86 mV, -33.16 mV, and -33.9 mV by Zeta potential analyzer. The linear and nonlinear optical studies were studied by UV-Vis spectroscopy and Z-scan technique. Compared with pure and co-dopant materials, single dopant (Zn, Bi-doped CuO) exhibited a high nonlinear absorption coefficient with a low optical limiting threshold value, and therefore it can possible to fabricate laser devices with safety than the more use of powered nanopulse green lasers.

Keywords: copper oxide nanoparticles, Zn, Bi & Zn/Bi-dopants, green synthesis.

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A 074

Indazole-Based Hole-Transport Materials for Advanced Optoelectronic Devices: Synthesis and Characterization

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ABSTRACT

The ever-expanding landscape of optoelectronics demands the exploration of novel materials with superior charge transport properties. The emerging family of indazole-based compounds is highlighted in this abstract as a potential source for hole-transport materials in a range of optoelectronic applications. Because of its distinct chemical structure, indazole offers a fascinating platform for the creation of effective charge carriers. This will present new developments in the production of derivatives of indazoles optimized for the best possible hole transport in organic solar cells, light-emitting diodes, and photodetectors. The impact of molecular design concepts on charge mobility and device performance will be highlighted through an explanation of structural alterations and functionalization procedures. Characterization techniques, such as UV-Visible and Florescence spectroscopies, will be employed to provide a detailed analysis of the electronic properties of indazole-based hole-transport materials. The relationship between molecular structure and optoelectronic performance will be explored, offering valuable insights into the underlying mechanisms governing charge transport in these materials. In conclusion, this abstract aim to showcase the promising role of indazole-based compounds as hole-transport materials in advancing the efficiency and applicability of optoelectronic devices.

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A 075

Structural and Luminescent Properties of $Y_2WO_6:Sm^{3+}$ Nanophosphors for Solid-State Lighting Applications

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ABSTRACT

Rare-Earth doped tungstate phosphors have emerged as promising candidates for diverse applications due to their exceptional optical properties. In this study, a series of $Y_2WO_6:Sm^{3+}$ (1-11 mol %) nanophosphors were synthesized using a solution combustion method. XRD analysis of the prepared nanophosphors confirmed monoclinic phase with P2/c space group. The DR spectra displayed a distinctive peak at ~ 402 nm attributed to the $^6H_{5/2} \rightarrow {}^6P_{3/2}$ transitions of Sm^{3+} ions, accompanied by additional peaks in the inner IR region at ~ 915, 1088, 1241, and 1388 nm corresponding to other transitions of Sm^{3+} ions. Utilizing diffuse reflectance data, the energy gap of the nanophosphors was estimated to be ~3.84-3.9 eV. SEM images revealed a network-like structure with plate-shaped morphology. Photoluminescence (PL) spectra exhibited three intense and sharp peaks at ~570, 603, and 645 nm, corresponding to de-excitation from the $^4G_{5/2}$ state of Sm^{3+} ions to ^6H_J (J = 5/2, 7/2, and 9/2) lower energy multiplets. The PL emission intensity demonstrated an increase up to 3 mol % Sm^{3+} concentration, followed by a declining trend. Notably, the nanophosphor exhibited high color purity (~ 92.5%), with color coordinates in the orange-red region of the CIE diagram. This distinctive orange emission property highlights its potential in solid-state lighting applications.

Keywords: Nanophosphors; Photoluminescence; Solution combustion; Colour purity

A 076

Tailoring the Electrical and Optical Properties of TiO_2 Thin Films on Glass Substrates: Impact of Deposition Temperature, Precursor Molarity, Chelating Agent Molarity and Copper doping for Enhanced Performance in TiO_2 based Memristors

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ABSTRACT

In this work Titanium dioxide thin films were deposited on glass substrates using Spray Pyrolysis technique by varying different deposition parameters. The molarity of TTIP was varied systematically within a small range from 0.09 M, 0.11 M, 0.13 M and 0.15 M to investigate its subtle impact on electrical and optical properties. The deposition temperature was varied from 200 °C, 250 °C, 300 °C, 350 °C and 400 °C and the ratio between TTIP and chelating agent was varied from 1:1, 1:2 and 1:3. Finally, Copper doped TiO_2 film was also synthesized via spray pyrolysis. The thickness of TiO_2 films were found to be in the range of 216 nm to 14.9 µm. Structural analysis conducted by XRD confirmed the formation of anatase TiO_2 thin films. Optical studies were done by UV-Visible spectrophotometer with absorption and optical bandgap analysis. Electrical studies were carried out using National Instruments (NI PX1-1044) workstation with TiO_2 films subjected to voltages from 0.5V, 1V, 2V, 3V, 4V and 5V, pre and post annealing. Impedance studies were carried out using Impedance Analyzer (Solartron SI1260) with input voltages varied from 0.1V, 0.2V, 0.3V, 0.4V, 0.5V, 1V, 2V and 3V for each film pre and post annealing. Nyquist plot and plots for dielectric constant, dielectric loss and conductivity were plotted and comparison studies were carried out. All these results were analysed to optimise the deposition parameters suitable for building a TiO_2 based memristor with enhanced performance.

A 077

Analysis of Performance Degradation in Single-Layer OLEDs Fabricated Using Vacuum-Free Lamination Methods

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ABSTRACT

Since efficient OLEDs were successfully demonstrated in 1987 [1], Organic Light-Emitting Diodes (OLEDs) have attracted significant attention for their promising applications in display [2] and lighting technologies [3]. Among various fabrication methods, solution-based polymers using the lamination method are promising since they offer a much lower cost and enable large-area device fabrication [4,5]. However, using lamination techniques in OLED fabrication has presented challenges in maintaining optimal performance. This study aims to analyze the factors contributing to the decline in the performance of laminated OLEDs. The research employs a comprehensive approach, integrating experimental investigations and theoretical analyses to identify and understand the causes behind the diminished performance. Key factors such as device structure, lamination process parameters, and environmental influences are explored to assess their impact on OLED functionality. Device structure emerges as a critical aspect affecting OLED performance, as improper interactions between layers can lead to reduced fabrication success rate and efficiency and compromised device integrity. The study investigates the effects of double Kapton taping to enhance fabrication success rate, to be used in mitigating performance degradation. Lamination process parameters, including temperature, pressure, and spin coating speed, are scrutinized for their influence on OLED performance. Variations in these parameters can affect the uniformity of layers and alter the overall device characteristics. Furthermore, environmental factors, such as moisture and oxygen ingress during the lamination process, including bias application, are considered potential contributors to performance decline. This analysis draws on a comprehensive review of relevant literature and experimental results, offering valuable insights into the challenges associated with laminated OLEDs.

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A 078

Constructing Metal Oxide @ Carbon Dots Hybrids as Visible-light Photocatalyst for Removal of Toxic Pollutants in Water

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ABSTRACT

The hybrid composite of metal oxide nanoparticles decorated carbon dots hybrids (MO@CDs) were synthesized by the direct hydrothermal method. The synthesized MO@CDs hybrid composite were systematically characterized by several physicochemical techniques including XRD, FTIR, HRSEM with energy-dispersive X-ray diffraction spectroscopy, HRTEM, XPS, UV-visible and fluorescence spectroscopy. The influence of heterogeneous structure and homogeneous arrangement of MO@CDs hybrid composite is responsible for the various photo responsive applications. Moreover, the economic natural bio-source or bio-waste was employed for the synthesis of CDs which was used for MO@CDs hybrid composite preparation and displays an excellent photocatalytic degradation under UV-light irradiation which is an alternate for other carbon-based metal oxides. For photocatalytic energy conversion applications, composite, or hybrid nanostructures derived from the carbon-based quantum dots may represent a more promising platform, and significant advances in high-yield CO_2 photo-conversion and water-splitting may be expected. In addition, the resulting bare CDs were employed as a fluorescent-ink and security information studies, owing to their remarkable properties such as bright fluorescence with high quantum yield, and excellent water solubility. The CDs displays a multi-colour fluorescence based on their changing of excitation wavelength and these properties could be applicable for real biological system in the near future.

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A 079

Decoration of the Sb_2Se_3 Nanowires with $CsPbBr_3$ Nanocrystals and Study the Nonlinear Optical Response

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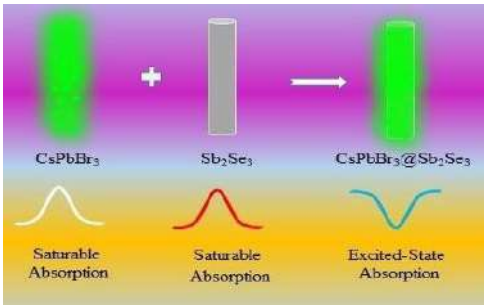
ABSTRACT

The incorporation of lead halide perovskite nanocrystals with low dimensional materials shows anenormous tendency in optoelectronic devices as in solar cells and photocatalysts processes [1-4], while a comprehensive study of the nonlinear optical (NLO) properties is yet to be established in these co-operatives systems because a robust nonlinear response is of essential for optical limitingand switching applications [5]. In this study, we decorated the $CsPbBr_3$ nanocrystals on the Sb_2Se_3nanowires and studied the nonlinear optical behavior of the decorated system $CsPbBr_3@Sb_2Se_3$ using the Z-scan technique. Our findings reveal a remarkably strong excited-state absorption (ESA) phenomenon in $CsPbBr_3@Sb_2Se_3$, starkly contrasting to the pristine materials ($CsPbBr_3$ nanocrystals and Sb_2Se_3 nanowires) with 532 nm excitation wavelength in the nanosecond regime.We attribute this observed ESA to the efficient charge transfer processes, which occurs between the $CsPbBr_3$ nanocrystals and Sb_2Se_3 nanowires. Further, quenching in the photoluminescence (PL) intensity of $CsPbBr_3$ nanocrystals in the presence of Sb_2Se_3 nanowires corroborates our idea. Moreover, we also demonstrate our device's optical limiting and switching performance. Overall,our results provide a valuable degree of freedom to engineer nonlinear optical responses for hybridsystem-based photonic devices.



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A 080

ESIPT Inspired Solid-State Emitters for Picric Acid Turn-On-Off on Detection with Acidofluorchromism, Anticounterfeiting, and Latent Fingerprinting

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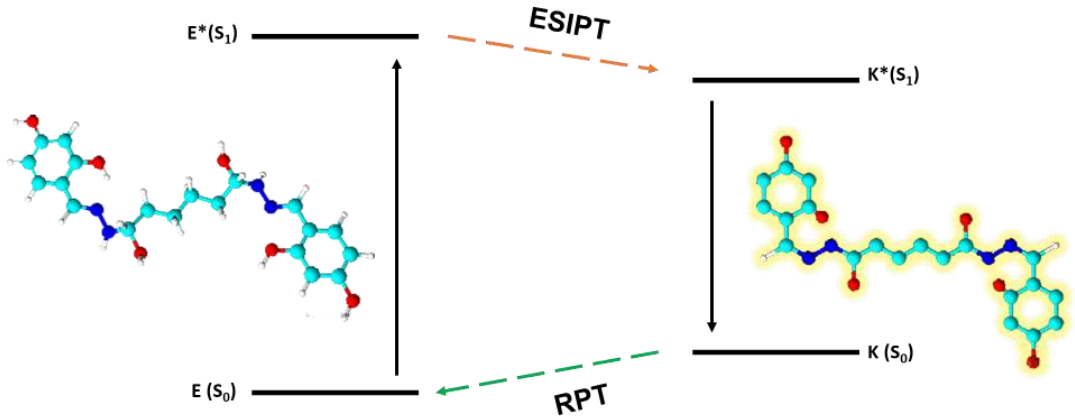
ABSTRACT

The stimulus-responsive multicolor solid-state photoluminescence based on single fluorescent compounds has potential applications in biomolecule identification and anti-counterfeiting. In this study we have developed an ESIPT active fluorescent probe, Generally, such systems generate fluorescence response through excited-state intramolecular proton transfer (ESIPT), or a combination of fluorescence mechanisms (AIE/ESIPT, PET/ESIPT, or FRET/ESIPT) supporting sensing chemistry. Reversible fluorescence switching depending on the order in which acid and base are added is also found. This work demonstrates both excited state intramolecular proton transfer (ESIPT) and aggregation-induced emission (AIE), leading to multilayer and extremely secure anti-counterfeiting capabilities. Because of keto-enol tautomerism, the fluorophore exhibits fluorescence in both the solution and solid states. This property makes it useful for anti-counterfeiting, LFP applications as well as for the detection of biomolecules in the solution state. We also developed PVA-probe blue-emitting composite films utilising solid-state fluorescence, and we utilized them to investigate the pH-responsive behaviour.



A 081

Charge Transfer Mediated Third-Order Nonlinear Optical Response in $CsPbBr_3$-Single-Wall-Cabon Nanotube Hybrid

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ABSTRACT

The realization of the large optical nonlinearities at low fluence holds great promise in fundamental studies and photonic applications. In this letter, we experimentally demonstrate large reverse saturable absorption (RSA) and self-focusing in the $CsPbBr_3$-single-wall carbon nanotube (SWCNT) hybrid. Strikingly, we perceive that a higher excited state absorption cross-section exceeds the ground state absorption cross-section, which suggests that they can be employed as passive optical limiters. The observed RSA coefficient and nonlinear refraction are discussed in the framework of an efficient charge transfer between the $CsPbBr_3$ nanocrystal (NCs) and SWCNT. Further, steady-state photoluminescence (PL), time-resolved PL, and transient absorption measurements corroborate our idea of charge transfer from $CSPbBr_3$ to SWCNT. Moreover, we also demonstrate a liquid cell-based optical limiter device with performance parameters such as onset threshold (F_{ON}) of 0.01 GW/cm^2, and optical limiting threshold (F_{OL}) of 0.03 GW/cm^2, which are on par with several other benchmark optical limiters.

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A 082

Effect of Capping Ligand on the Emission of Inorganic Perovskite Mixed Phase Nanocrystals

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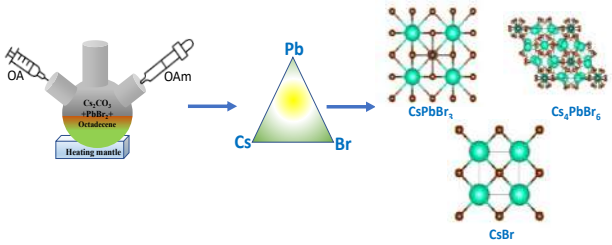
ABSTRACT

Colloidal perovskite nanocrystals are widely studied these days because they exhibit alluring optoelectronic properties compared to their bulk counterparts, such as high photoluminescence quantum yield (PLQY ~ 50-70%), low full width at half maximum (fwhm< 30 nm) [1], defect tolerance and luminous efficiencies making them suitable contenders for application in LEDs, displays, solar cells, lasers, etc. Moreover, inorganic perovskites are solution processable. The traditional quantum dots require precise control over the size needed to achieve narrow FWHM, whereas perovskite nanocrystals are excellent emitters even in weak confinement regimes [2].

In this work, we report the study of emission characteristics of Inorganic lead bromide perovskite mixed-phase nanocrystals. The variation in the acid-to-amine ratio is known to have a visible effect on the formation of inorganic perovskite nanocrystals [3]. Cs, Pb, and Br constitute the ternary compound's three ends and can coexist. We have used a bottom-up chemical route-based hot injection method and varied the quantity of oleyl amine to study the effect of capping ligands on the absorption, emission, and growth of phases of the nanocrystals. The impact of change in oleyl amine, the capping ligand, is visible in the emission spectra, showing growth and suppression of multiple peaks in the 400 - 600 nm wavelength region. The nanocrystals are highly luminescent and form at a low temperature (140 ˚C) in a few seconds. Their luminescence properties make them suitable as active layer in nanocrystal-based light-emitting diodes (nano-LED).



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A 083

Observation of Rapid Decay and Optical Properties of Micro-Pyramidically Grown Molybdenum Diselenide $MoSe_2$ Crystal

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ABSTRACT

In two-dimensional transition metal dichalcogenides (2D-TMDs), the existence of excitons and trions promises their fascinating optical properties for applications in nanophotonic. The more exotic the nanostructure geometry, the less explored its optical responses. The chemical vapor deposition (CVD) technique enables the synthesis of nanostructures with different geometries ranging from monolayers to pyramids driven by a screw-dislocation mechanism. Here we report the CVD synthesis of micro-pyramids with a curious optical response exotic geometry like pyramid. The photoluminescence of as-grown micro-pyramids is significantly diminished compared to their flat-layered structures. In contrast, nanostructured micro-pyramids exhibit a large number of higher-order phononic resonances when excited resonantly by the Raman signal, allowing a more detailed exploration of exciton dynamics. The spectral peak position, intensity, and ratio of the spectral peak reveal local variations in the atomic arrangement of the center and sides of the micro-pyramid. We have investigated the optical response of $MoSe_2$ micro-pyramids and correlated them with their growth-induced nano geometry. In this study, we have taken into account the first step towards producing tunable nanophotonic devices with applications ranging from optoelectronics to nonlinear optics.

Keywords: Transition metal dichalcogenides, vacancy defects, screw-dislocation, photoluminescence, time-resolved photoluminescence, exciton dynamics.

A 084

Collective Degradation of a Mixture of Textile Dyes and Industrial Effluents by Nanorods of Cesium Titanium Bromide ($CsTiBr_3$) Perovskite

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ABSTRACT

Textile effluent is severely adulterated with contaminants like dyes, toxic metals, suspended solids, and dissolved solids. The wastewater expelled from the dying unit comprises a muddle of dyes. Here we address the challenge of using a single catalyst for the collective photocatalytic degradation of a mixture of six textile dyes and two samples of textile effluents collected from a dying unit. The all-inorganic halide perovskites (IHP)especially titanium-based are excellent photocatalysts owing to outstanding optoelectronic properties[1] [2][3][4]. The lead-free perovskite of $CsTiBr_3$ nanorods prepared via the solvothermal process is effective in the collective degradation of dye mixture containing toxic dyes like congo red, crystal violet, malachite green, methylene blue, rhodamine, and methyl orange without causing secondary pollution. The presence of electron scavenger $AgNO_3$ augmented the individual degradation of each dye. The removal of electrons by the scavenger and the enhancement of the degradation rate indicate that electrons do not play any roles in the photocatalytic degradation process. The six-dye mixture turned colorless within three hours of direct sunlight exposure. The individual degradation percentage of each dye is different, but the dye mixture exhibits a uniform pattern for the degradation of respective dyes in the mixture. The collective degradation of six dyes in the mixture is achieved through the synergistic effect due to the presence of multiple dyes [5]. The collective photocatalytic degradation ability of $CsTiBr_3$ nanorods is fruitfully exploited for the degradation of the textile effluents. Deep blue colour textile effluent showed fast degradation and within 90 minutes 97% of the dye degraded. But the degradation of dark maroon-coloured textile effluent was slow, it took nearly 200 minutes for 96% percentage degradation of the dye. The chemical oxygen demand (COD) analysis guarantees the degradation of dye into non-toxic components [6].

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A 085

A Comprehensive Insight into the Optical Characteristics of Co Incorporated ZnO Nanostructures

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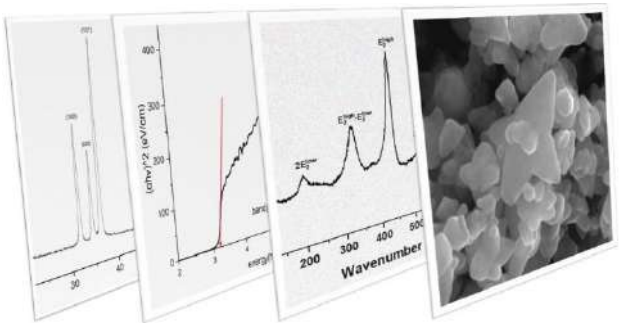
ABSTRACT

Doped ZnO materials are known for tuning their properties, making them suitable for a range of applications in optics, magnetism, electronics, and biology. Cobalt (Co) doped ZnO, belonging to the class of DMS (Diluted Magnetic Semiconductors) has been studied extensively to probe into its magnetic behaviour [1]. Moreover, the antibacterial and photocatalytic properties have also been examined by different groups [2]. However, a detailed optical investigation of Co:ZnO is scarce in the literature. To utilize materials for optical applications, it is essential to have information regarding their optical constants and the factors influencing them. Here, we prepared Co doped ZnO nanoparticles by co-precipitation method and studied the structural and optical properties with changing concentrations of cobalt. HRSEM images show flower like structures with triangular shaped clustered petals, which is not the expected structures as per the scientific reports available. The structural and morphological attributes analysed from XRD, HRSEM etc are correlated to the findings obtained from the optical studies viz., UV-Visible spectroscopy, FTIR, Raman analysis and Photoluminescence spectroscopy. A comprehensive evaluation of the optical constants has been done using Kramers-Kronig model [1]. The observations suggest the capability of the prepared samples to function as optical materials by tuning their structural defects that assist in tailoring the excitonic states and hence the optical traits.



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A 086

Enhancing Structural, Morphological Optical and Photocatalytic Activities of CdO Nanoparticles Under UV And Visible Light Illumination by Solution Combustion Process

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ABSTRACT

Present work, we focused on the physico-chemical properties of CdO nanoparticles annealed at 350, 450 and 550 ◦C, prepared by solution combustion method. The crystalline structure, morphological, compositional, optical properties of CdO samples were comparatively investigated by the XRD, FT-IR, TEM-EDX, UV-Visible and PL analysis. Form XRD patterns, all the diffraction peaks indicates cubic phase of CdO samples. No additional peaks were detected due to impurities. The spherical-like morphology with uniform distribution of CdO host matrix was observed. From TEM studies, the grain-size of CdO samples was found to be 55, 32 and 19 nm, respectively. The higher bandgap energies of prepared samples were obtained in the visible region and it's indicating a blue-shift compared to bulk CdO due to smaller particle size. The photocatalytic degradation of prepared samples was comparatively investigated using methylene blue under UV and visible light illumination. It is the most effective towards these potential applications, despite increase in the optical bandgap energies. It is useful for optoelectronic and photo thermal applications. This work demonstrates the CdO samples contributing main factors like increase in electron degeneracy and improved crystallinity for enhanced performances under various annealing temperature.

Keywords: CdO; Annealed; Solution combustion method; Optical; Photocatalytic

A 087

Resistive Switching studies of Plasma Treated TiO_2 Nanorods Synthesised by Hydrothermal method

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ABSTRACT

Memristors are brain-inspired electronic components. They can revolutionise computing by providing parallel computing and efficient data processing like neurons. Memristor-based neural networks may overcome von Neumann's inability to replicate the human brain, making them significant to the future of artificial intelligence.[1] Transition metal oxides (TMO) are commonly utilised to make memristor devices. As a TMO, Titanium dioxide has good physical and chemical qualities, environmental compatibility, and low production cost. Also, the first actual memristor device was developed from TiO_2 thin film.[2] In this work, we report the synthesis of TiO2 nanorods using the hydrothermal method followed by a plasma treatment. The as synthesised and plasma processed TiO_2 nanorods were characterised using scanning electron microscopy (SEM), X-ray diffraction (XRD), and Raman spectroscopy. These TiO_2 nanorods were then used to fabricate memristor devices. The memristor parameters of the device were studied. The results of this study demonstrate the application potential of plasma treated hydrothermally grown TiO_2 nanorods as a promising material for memristor devices.

Keywords: Memristor, TiO_2, Hydrothermal, TMO, Neuromorphic memory.

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A 088

A Machine Learning Approach for The Identification and Characterization of 2D Materials Using Raman Spectroscopy

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ABSTRACT

Raman spectroscopy is a powerful analytical tool for the identification and characterization of various materials and their structural nature. This paper introduces a novel machine learning (ML) framework designed for the precise identification and characterization of two-dimensional (2D) materials through Raman spectroscopy. As the exploration of 2D materials expands in nanoscience and materials engineering, the need for efficient and accurate characterization techniques becomes paramount. Raman spectroscopy, with its capability to probe vibrational modes and structural nuances, offers a valuable tool for the analysis of 2D materials. The proposed ML approach integrates advanced algorithms to decipher complex Raman spectra, enabling automated identification of diverse 2D materials such as graphene, and other emerging 2D materials. The model is trained on a comprehensive dataset encompassing various material compositions and environmental conditions, ensuring robust performance across a spectrum of scenarios. The effectiveness of the ML approach is demonstrated on graphene and its various types, like monolayer graphene, bi-layer graphene, tri-layer and highly oriented pyrolytic graphite (HOPG). The program/software has the ability to identify the number of atomic layers in samples, detect stress and strain, and analyze other defects by examining data through peak detection, measuring FWHM (full width at half maximum), fitting peaks with Gaussian and Lorentzian theoretical curve models, analyzing various peak ratios such as G and G' peaks for graphene, conducting quantitative analysis, and performing calculations. The ML program process final pdf format report for the users with analysis details. This ML program will certainly be helpful even for layman who has limited or no knowledge of Raman spectroscopy.

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Nanoscrolled Monolayer MoS_2 with Enhanced Photoluminescence Quantum Yield and Improved FET Device Performances

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ABSTRACT

In the realm of two-dimensional materials, monolayer molybdenum disulfide (1L-MoS_2) stands out as a remarkable semiconductor with intriguing properties. Sporting a direct optical gap of approximately 1.84 eV, coupled with a high exciton binding energy and robust optical absorption, this material exhibits strong photoluminescence (PL) emission even at room temperature. Recent investigations have delved into understanding the nuanced relationship between PL quantum yield (QY) and local temperature. Notably, our studies have uncovered that larger-area flakes, spanning around 6000 μm^2, showcase a superior PL QY compared to their smaller-area counterparts (~30 μm^2), owing to their enhanced heat dissipation capabilities. However, the existing results fall short of meeting the demands for fabricating compact and miniaturized devices, necessitating innovative approaches. In response to this challenge, we embarked on a journey to engineer a solution that harnesses the advantageous properties of large-area 1L-MoS_2 while circumventing the limitations posed by heat dissipation. Our strategy led us to fabricate nanoscrolled 1L-MoS_2 structures, which exhibit superior optoelectronic characteristics. These nanoscrolls, despite their morphological resemblance to multilayers, retain the electronic properties of monolayer MoS_2. Remarkably, they boast a direct optical gap and exhibit enhanced PL QY, attributed to the weakened interlayer coupling among constituent layers. This assertion finds support from low-frequency Raman measurements and Kelvin probe force microscopy observations. Moreover, our investigations using conducting atomic force microscopy have unveiled a notable increase in photocurrent within the nanoscrolled 1L-MoS_2 compared to its pristine counterpart. This enhancement underscores the potential of nanoscrolled structures in facilitating efficient charge transport. Furthermore, our efforts in fabricating field-effect transistor devices using nanoscrolled MoS_2 have yielded promising results. We proudly report achieving the highest recorded mobility value of 2400 $cm^2V^{-1}s^{-1}$ in any form of 1L-MoS_2 to date. Such exceptional mobility values hold immense significance for the development of compact and high-performance optoelectronic and electronic devices. In conclusion, the advent of nanoscrolled 1L-MoS_2 introduces a paradigm shift in the realm of two-dimensional materials, offering a pathway towards realizing compact and high-performance devices that can meet the demands of modern electronics and photonics applications.

A 090

Interface State Characteristics of TiO_2-Based MIS Devices Developed by Reactive Sputtering

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ABSTRACT

Defects at the interface of high-k/semiconductor have a significant role on the reliability of metal-insulator-semiconductor (MIS) devices. Titanium oxide (TiO_2) layers are promising high-k dielectric layers developed by different physical and chemical methods. Despite the wide use of atomic layer deposition (ALD) to develop TiO_2 layers [1], Ti/O content in the layer requires change in precursors, and control of the interfacial layer becomes critical [2]. The TiO_2 layers were developed by reactive sputtering on p-Si substrates at room-temperature and annealed at different annealing temperatures in the range, 400-900 °C under Ar ambient. The interfacial characteristics of TiO_2/Si were studied using capacitance-voltage and current-voltage measurements by evaluating flat-band voltage (V_{FB}), interface defect density (D_{it}), fixed charge density (Q_{eff}), etc. The D_{it} at the interface of TiO_2/Si was found to be $2.8x10^{12}$ $eV^{-1}cm^{-2}$ for room temperature (RT) deposited films, which reduced nearly by one order ($4.6x10^{11}$ $eV^{-1}cm^{-2}$) at annealing temperature of 700 °C. Flat-band voltage (V_{FB}) values changed from 0.6 V to 2.1 V when the annealing temperature varied from RT to 700 °C, revealing the presence of negative fixed charges in the layers. The leakage current density was found to be as low as $8.4x10^{-7}$ A/cm^2. The defect levels were also evaluated using deep-level transient spectroscopy and the traps are found to be majority carrier type. The layers have shown strong photoluminescence at the wavelengths of 574 nm and 675 nm above the annealing temperatures of 600 °C, and intensity of which enhanced remarkably at the higher annealing temperatures, indicating the reduction of non-radiative transitions. The interface of TiO2/Si has been found to be smooth and conformal with nominal thickness of SiO_2 layer. The XPS and UPS measurements were performed to know the oxidation states and band-offset. The conduction band offset was found to be 0.61 eV as evaluated from the UPS analysis [3]. The study demonstrated the importance of processing conditions in developing the devices with minimum interface defects and conformal high-quality interface of the TiO_2/Si based MIS device structures developed at room-temperature.

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A 091

Enhanced Optical Nonlinearity in Bi^{3+} Doped $CePO_4$ Nanostructures for Optical Limiting Applications

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ABSTRACT

Pure and Bi^{3+} doped $CePO_4$ were synthesized by simple co-precipitation method. Successful dopant incorporation in the host lattice of orthophosphate without altering the crystalline structure was confirmed by structure analysis, X-Ray diffraction and Raman characterization. Morphological investigation were done using HR-SEM which portrays the co-existence of nanospheres and nanorods in doped $CePO_4$ and only nanospheres in pure $CePO_4$. The absorption band in the range 200-300 nm accounts for 4f-5d electronic transition and a red shift in the band edge owes to increase in band gap with addition of dopant. Photoluminescence emission spectra shows broad blue-green emission owing to transition of Ce^{3+} from excited state to ground state and also due to oxygen vacancy. The nonlinear optical absorption and optical limiting behavior of Bi^{3+} doped Cerium orthophosphate ($CePO_4$) were investigated using an open aperture Z-scan technique under excitation source of 532 nm nano pulsed lasers. The recorded open aperture transmittance curve reveals a transition from saturable absorption to reverse saturable absorption in pure $CePO_4$ at 2.46 GW/m^2 whereas, all the doped samples exhibit RSA attributed to 2PA. Increase in nonlinear absorption coefficient with on-axis intensity and the availability of near resonant energy state due to Bi^{3+} dopant ensures sequential 2PA (1PA+ ESA) phenomenon. Comparing the NLA coefficient of pure $CePO_4$, doped nanostructures shows improved nonlinear absorption coefficient due to the availability of defect state and oxygen vacancies in Bi^{3+} doped $CePO_4$. Interestingly, lower optical limiting threshold of 0.14 x 10^{-13} W/m^2 is observed in 0.3% Bi^{3+} doped $CePO_4$. The lower optical limiting threshold value of Bi^{3+} doped $CePO_4$ ensures its potential candidature for optical limiting applications in protecting optical sensors and human eyes.

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A 092

Effect of Volume Compensation on Photoluminescence Behaviour of Li^+ Co-doped $Y_4Al_2O_9:Eu^{3+}$ Phosphors for Solid State Lighting Applications

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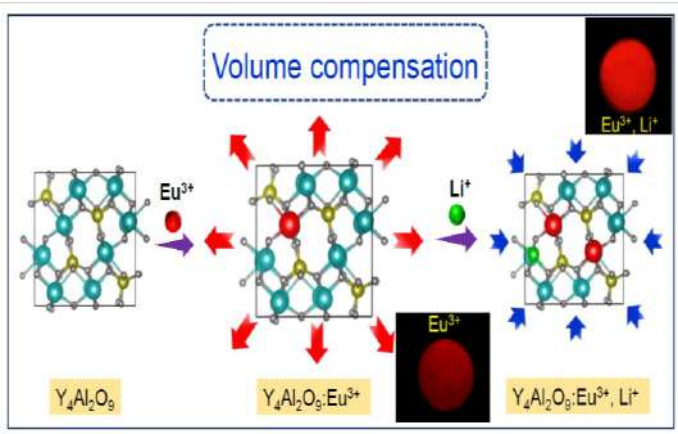
ABSTRACT

Rare-earth activated red phosphors are now an essential part of phosphor-converted white light emitting diodes (PC WLEDs), that produce warm white light. Since Eu^{3+} doped Yttrium-based hosts are thought to be the most promising red phosphors, they have been the subject of extensive research in recent years. However, the mismatch in the size of Eu^{3+} and Y^{3+} restricts their PL enhancement below the desired limit. Herein, Li^+ co-activated $Y_4Al_2O_9:Eu^{3+}$ phosphors have been synthesized via facile solvothermal technique. All the phosphors exhibit characteristic $^5D0 \rightarrow {}^7Fj$ (j=1-4) transitions of Eu^{3+} and introduction of Li^+ co-activator results in more than 2-fold enhancement of PL intensity as compared to pristine Y4Al2O9:Eu^{3+} phosphor. In addition, both the excited state lifetime and thermal stability of the phosphor are remarkably improved upon Li^+ co-doping. The enhancement in PL efficiency has been elucidated in light of volume compensation induced lattice relaxation mechanism. Strong red emission was achieved from the red LED fabricated by employing Li^+ co-activated $Y_4Al_2O_9$: Eu^{3+} phosphors under 3.5 Volt driving potential. The demonstrated volume compensation technique possesses great promise to play the pivotal role in designing highly luminescent phosphors for LED applications.



A 093

Comparative Study of Bulk and Thin Films of 2-Methylbenzimidazole and 4-Aminobenzoic Acid: Structural, Optical, and Electrical Analyses for Optoelectronic Device Applications

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ABSTRACT

The research presents a comprehensive comparative analysis between bulk and thin film forms of 2-methylbenzimidazole (2-MI) and 4-aminobenzoic acid (4-ABA) [1,2]. The thin films were deposited by using the spin-coating method, the bulk crystals were grown by the slow evaporation method, and their structural, optical and electrical properties were systematically investigated. The deposition process resulted in uniform and adherent thin films with controlled thickness in the nanometer range. X-ray diffraction analysis confirmed the crystalline nature of the films and bulk materials. SEM analyses were employed to assess the surface morphology, indicating a smooth and compact film structure. Optical characterization, including UV-Vis spectroscopy, unveiled variations in the absorption spectra, suggesting differences in band gap and transparency of the materials. FTIR spectroscopy revealed distinctive vibrational modes, enabling a precise identification of molecular functionalities and potential variations including by the dimensionality shift. The FTIR analysis sheds light on structural changes in both bulk and thin film phases. Photoluminescence studies were conducted to explore the optical properties of the materials. The thin films exhibited unique photoluminescent characteristics compared to their bulk counterparts, showcasing differences in emission spectra and quantum yields. These findings elucidate the influence of dimensionality on the optical behaviour of 2-MI and 4-ABA. The electrical conductivity of the materials was recorded in the frequency range of 50Hz to 5MHz. Furthermore, nonlinear optical properties were investigated to evaluate the potential of these materials for nonlinear optical applications. The experimental results demonstrate that the thin films exhibit reverse saturable absorption and positive nonlinearity at specific wavelengths, indicating their potential for optical limiting applications. Additionally, the optical and structural quality of thin films is crucial for their potential applications, including sensors and other devices [3].

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A 094

Distributed Acoustic Sensing Signal Model Under Static Fiber Conditions

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ABSTRACT

This research presents a statistical model for distributed acoustic sensor interrogation units, which utilize laser pulses transmitted into fiber optics. The interactions within the fiber lead to localized acoustic energy, resulting in backscatter – the reflection of light. Explicit equations are employed to calculate the backscattered signal's amplitude and phase. The proposed model accurately predicts the amplitude signal spectrum and autocorrelation, aligning well with experimental observations. The research also explores phase signal characteristics relevant to Optical Time Domain Reflectometry (OTDR) system sensing applications, demonstrating consistency with experimental results. The experiments were conducted using Python coding, enabling the analysis of individual components of the Distributed Acoustic Sensing (DAS) system. Assumptions of the model include the static condition of the fiber, implying the absence of external forces or vibrations. Consequently, no external acoustic disturbances are considered. The backscattered signal is identified as comprising a random noise component resulting from intrinsic fiber imperfections and a coherent component arising from the interplay between the laser pulse and the fiber.

Keywords: *Distributed Acoustic Sensing, Fiber Optics, Optical Time Domain Reflectometry, Rayleigh scattering.*

A 095

Design and Implementation of Fault Tolerant LZW for Reliable Data Compression Using Verilog HDL

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ABSTRACT

Data Compression plays a vital role in various domains, where efficient data storage and transmission are essential. Due to the vast amount of data that needs to be processed and transmitted in real-time, compression techniques are crucial in order to optimize the bandwidth and storage resources. The basic idea here is to develop a fault-tolerant implementation of the Lempel-Ziv-Welch algorithm using Verilog HDL. LZW is one such typical compression technique known for its effectiveness in reducing data size without significant data loss. However, many systems, for example Avionic systems demand higher levels of reliability and fault tolerance due to the critical nature of operations. Hence, to address this issue, the idea considered will incorporate fault tolerant mechanisms into LZW scheme. Effective replication of the LZW module can develop the fault tolerant system for the same which is a reliable, effective, and efficient data compression solution for an application. Integration of LZW with the fault-tolerant mechanisms ensures the system's resilience to failures and faults, thereby enhancing the safety of the system. This fault tolerance can thus be ensured by techniques such as Clock gating, Isolation Cells and Level Shifters which make sure of reliable data compression at the module level.

A 096

Characterizing the Structural, Electronic, Optical, and Photocatalytic Performance of Lead-Free Ba_2FeVO_6 Double Perovskite for Methylene Blue Dye Removal

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ABSTRACT

Exceeding the capabilities of single perovskites, lead-free double perovskites (DPs) emerge as promising materials for photocatalytic and related applications, offering enhanced stability, excellent catalytic efficiency, and minimal toxicity. This study delves into the synthesis of vanadium-based double perovskite Ba_2FeVO_6, employing a straightforward solid-state reaction method and subsequent sintering at 750 ºC for 4 hours. Analysis of the X-ray diffraction (XRD) pattern confirms the tetragonal crystalline structure of Ba_2FeVO_6. Surface characteristics are revealed through SEM, with EDX analysis validating the chemical composition and purity of the compound. The average particle size is determined via analysis of the particle size distribution curve. Further insights into the compound's composition are gained through FTIR spectroscopy, confirming the presence of functional groups and chemical bonding. Raman spectroscopy is employed to scrutinize the vibrational modes of the sample. Optical properties are explored using ultraviolet-visible (UV–vis) absorption spectroscopy, with the energy band gap determined through the Tauc plot. Photoluminescence responses across the UV–Visible spectrum are observed by illuminating the sample with excitation wavelengths around 370 nm, and the characteristic band gap of crystalline Ba_2FeVO_6 is identified through photoluminescence analysis. Our findings collectively highlight the compound's suitability as a visible light active photocatalyst due to its narrow band-gap, as substantiated by UV-visible spectroscopy. Significantly, the compound demonstrates effective degradation of Methylene Blue (MB) under visible light conditions, achieving an impressive degradation efficiency of up to 80% within a span of 40 minutes.

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A 097

Unveiling Astonishing Electrical Conductance in Non-Conductive Polymers through Vibrational Strong Coupling

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ABSTRACT

Creating innovative techniques for altering the charge transport characteristics of materials through external stimuli like light, magnetic fields, and electric fields show significant prospects in the realms of molecular electronics and spintronics[1]. Vibrational strong coupling (VSC) is increasingly recognized as a versatile tool for manipulating the physicochemical attributes of molecules and materials[2]. In this investigation, we utilized vibrational strong coupling (VSC) to modify the electrical properties of non-conducting polymers (Fig.1).

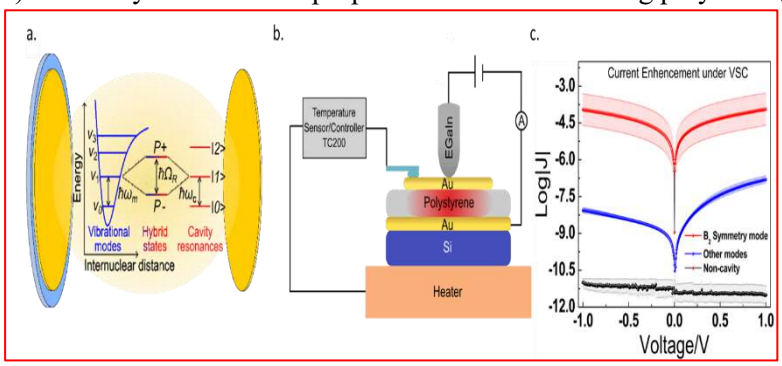

***Figure 1**: (a) Schematic illustration of vibrational strong coupling in a Fabri Parrot cavity configuration. (b) Schematic of Electrical measurement setup used to measure the conductivity of polymer under VSC. (c) Electrical conductance measurements of polystyrene cavities, strongly coupled B2 symmetry mode of the polymer under cavity VSC (red curve), other modes (blue curve), and non-cavity polymer (black curve.*

Our results show a remarkable increase in electrical conductance by at least six orders of magnitude[2] when the cavity resonances are coupled to the out-of-plane bending mode of the polymer (polystyrene) (Fig.1). Our research also emphasizes the crucial role of delocalized hybrid light-matter states formed through the VSC of out of plane bending mode of polymers (Ar. C-H bond) in driving electrical transport. The enhancement in conductance is thermally activated at the onset of strong coupling and becoming temperature and cavity path length independent at the highest coupling strengths, giving rise to the extraordinary electrical conductance in polystyrene. We conducted experiments on different polymers, including PS, PBMA, PMMA, and d-PS, and used the EGaIn junction technique to measure their electronic behavior and transport properties[3]. These results were obtained without light excitation, underscoring the vital role of electromagnetic vacuum fluctuations in controlling electron transport in molecular materials.

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A 098

Investigation on the Thermoelectric Properties of PANI Composited Ag_2Se for Waste Heat Recovery

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ABSTRACT

Silver selenide (Ag_2Se) emerges as a highly promising thermoelectric (TE) material, showcasing remarkable performance within the temperature range of 300-400 K. Employing a sonochemical-assisted hydrothermal method followed by hot-press densification, we synthesized Ag_2Se and its composites with Polyaniline (PANI). The reduction in carrier concentration contributes to lower electrical conductivity while concurrently elevating the Seebeck coefficient, resulting in a notable enhancement of the power factor. At 393 K, Ag_2Se with 0.3 wt % PANI achieves a peak thermoelectric figure of merit (zT) of ~ 0.64. Our findings underscore the significant potential of Ag_2Se as a promising material for thermoelectric applications near room temperature[1].

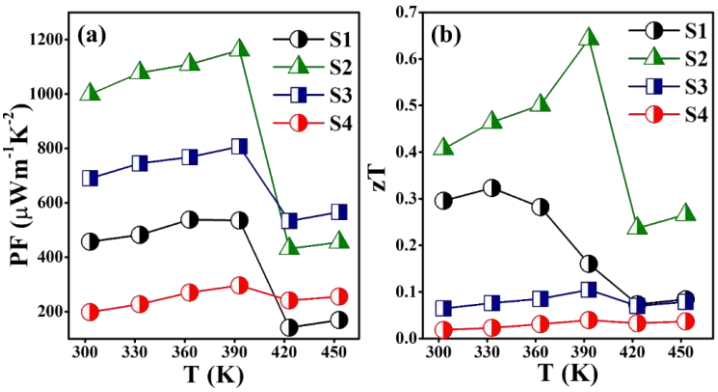

Fig 1. Temperature-dependent, (a) Power factor (PF) and (b) Figure of merit (zT) forS1, S2, S3 and S4 samples.

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A 099

Comparing Different Mobility Models for TCAD Simulation of Amorphous Si-Zn-Sn-O Thin Film Transistor

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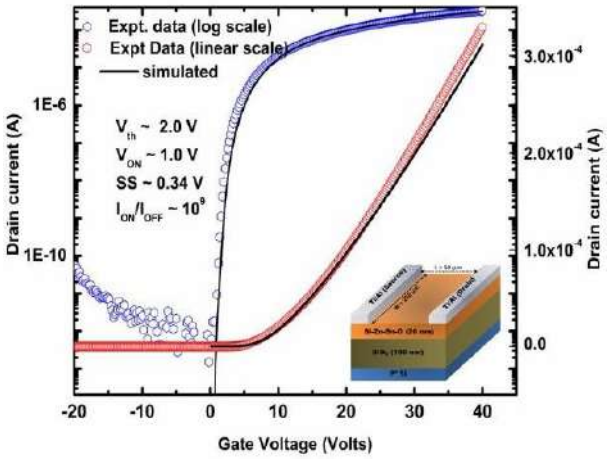
ABSTRACT

A 2D numerical simulation of amorphous Si-Zn-Sn-O Thin Film Transistor (TFT) has been carriedout using physics based TCAD simulations. The simulated data is found to be in good agreementwith the experimental current-voltage characteristics. In the simulation process, disordered amorphous oxide density of states (DOS) has been used, which consists of conduction band (N_{TA})and valence band (N_{TD}) tails states, Gaussian donor states N_{GD} (peak energy at E_{GD} ~ 3.5 eV) andGaussian acceptor states N_{GA} (peak energy at E_{GA} ~ 1.2 eV) [1]. To model the field effect mobilityof TFTs, percolation and constant field effect mobility models have been compared. The critical carrier concentration value is found to be ~ $6.3x10^{19}$ cm-3 in the percolation model, which is closeto the reported value of amorphous IGZO based TFTs [2]. The value of N_{TA}, N_{TD}, N_{GD} and N_{GA} are compared by using these two mobility models. The simulated results provide detailed insights into the defect states, current conduction mechanism, induced carrier density, current density, potential distribution, Quasi-Fermi level position of the TFT.



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A 100

Impedance Study of Green Synthesized Silver Sulfide Nanoparticles

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ABSTRACT

A facile, convenient, environment friendly green synthesis methods have been used to synthesized Ag_2S nanoparticles using Jara lemon extract. The different characterizations such as XRD, FESEM, FTIR and UV-Vis absorption spectrum confirm the good quality of synthesized Ag_2S NPs. The XRD pattern confirms the well crystallinity of the sample and there are no impurity peaks. The FESEM images confirm the spherical shape of synthesized Ag_2S NPS and the EDX results of Ag_2S sample clearly indicates that there are no impurity elements. Also, the average grain sizes of sample were calculated, which agrees with the XRD results. The UV-Vis spectrum and corresponding Tauc plot clearly indicates that particles are very small compared to bulk materials due to quantum confinement effect. The Nyquist plot of the sample gives two semi-circular arches, which suggests both the grain and grain boundary effect in the Ag_2S NPs. These grain resistance (R_g), as well as grain boundary resistance (R_{gb}) decreases with increasing temperature, which suggests the negative temperature coefficient of resistance (NTCR) behaviour like a semiconductor.

Keywords: *Silver sulfide, Green synthesis, Nyquist plot, FESEM, Negative temperature coefficient of resistance (NTCR)*

A 101

MOF Derived Cobalt Nickel sulfide as Supercapacitor Material

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ABSTRACT

Supercapacitors are an emerging energy storage technology, that has promising energy density and power density that have an important role to play in powering electronic devices (Deka et al., 2017) In this work supercapacitor electrode material using MOF derived Cobalt Nickel Sulfide was synthesized. $CoNi_2S_4$ is reported to have a high specific capacitance of 1890 F/g(Wang et al., 2017) when synthesized as a hollow nanocage structure. In our work we have synthesized the Cobalt MOF initially and then used Cobalt MOF as a template for the sulfaration reaction by refluxing the solution. Also the effect of reflux temperature on the material's performance was studied. There was an increasing trend in specific capacitance observed while increasing the reflux time by a factor of 2. It was noted that the surface area of the MOF has changed upon refluxing and that might be the contributing factor to the increasing trend in specific capacitance, A noteworthy finding was the alteration in the surface area of the MOF following the refluxing process. This observation prompted an in-depth investigation into the relationship between changes in surface characteristics and the consequential enhancement in specific capacitance this is the main aspect that is being explored through this work.as we aim to elucidate the underlying mechanisms driving the changes in the material's electrochemical performance. The findings from this study contribute valuable insights into the synthesis and optimization of MOF-derived electrode materials for supercapacitors, paving the way for enhanced energy storage solutions in electronic devices.

A 102

RF-Sputtered TiO_2-Based Memristive Devices for Resistive Memory and Artificial Synaptic Applications

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ABSTRACT

A paradigm shift in computing and memory technologies is required for applications like big-data processing and artificial intelligence. The intrinsic inefficiencies of conventional Von-Neumamm architecture along with the high latency of current memory technologies leads to slow computation and energy in-efficiency. These inefficiencies can be overcome by realizing brain-inspired in-memory computing with artificial synapses. Among different technologies utilized for simulating synaptic behavior, memristive devices achieved great attention due to their non-volatile resistive switching nature, high switching speed, high scalability, and low energy consumption[1]. A memristor, a contraction of a memory resistor, stores information in the form of resistance. It generally has a structure of the top electrode, resistive switching layer, and bottom electrode, which is similar to the pre-synaptic neuron, synaptic cleft, and post-synaptic neuron of a biological brain[2,3]. This study consists of the fabrication of TiO_2-based memristors which emulates various synaptic behaviors. The TiO_2-based memristors were fabricated by reactive sputtering of TiO_2 on ITO-coated glass and depositing Al or Ag as the top electrode. These devices show bipolar resistive switching due to the formation or rupturing of the conductive filament (CF). The devices with an Ag top electrode exhibit electrochemical metallization memory (ECM) type resistive switching, as the CF formed is due to the Ag ions migrating from the top electrode. Al top electrode devices show valance change mechanism (VCM) type resistive switching, where migration of oxygen vacancies through the switching layer is responsible for CF. Various synaptic behaviors like potentiation, depression, spike rate-dependent plasticity (SRTP), and paired-pulse facilitation (PPF) were also manifested in TiO_2-based memristive devices.

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A 103

Ultraviolet Pulse-Driven Neuromorphic Device for Pattern Recognition

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ABSTRACT

In the quest for improved efficiency in neuromorphic computing, the integration of memristor-based optoelectronic artificial synapses has emerged as a promising avenue [1]. The current challenge is to advance these synapses to better meet the requirements of the upcoming era in neuromorphic computing and neuromorphic visual systems [2]. Optoelectronic artificial synapses, capable of operating beyond the confines of visible light, hold great potential for enhancing neuromorphic visual systems, allowing them to closely replicate essential human visual functions. This study presents an enhanced optoelectronic artificial synapse (ITO/ZnO/Ag) exhibiting numerous fundamental bio-synaptic characteristics. The fabricated devices demonstrate excellent paired-pulse facilitation with both electrical and optical input stimuli. A transition from short-term memory to long-term memory was observed with frequent and high numbers of input stimuli, resembling bio-synaptic behavior. Essential Hebbian learning protocol (spike-timing-dependent plasticity), and spike-rate-dependent plasticity were successfully emulated in this artificial synapse. Additionally, it features light-tunable synaptic plasticity, enabling real-time neuromorphic visual pre-processing for the realization of advanced neuromorphic visual systems. We also demonstrated that optoelectronic synaptic behavior could be employed in a neural network for handwritten digit recognition. The handwritten image recognition was done by simulating a neural network by implementing the synaptic activation function derived from the device properties.

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A 104

Effects of PMMA/TiO_2 on Mechanical and Optical Property

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ABSTRACT

Polymer films are gaining increasing recognition as an innovative material with a wide range of applications. Due to their excellent thermal stability, environmental resistance, optical characteristics, chemical properties, and mechanical qualities, polymeric materials serve as suitable matrices for nanocomposites. This study focuses on investigating how the introduction of titanium influences the optical and mechanical characteristics of transparent hybrid thin films. Nanoindentation experiments were conducted on a PMMA/TiO_2 thin film using a Berkovich indenter to analyze the material's response under a constant load, considering variations in unloading position, holding duration, and loading times of 5, 10, 20, and 50 seconds. The study explores the impact of the activation volume of titanium dioxide (TiO_2) on the properties of a thin film composed of polymethyl methacrylate (PMMA). Additionally, during the optical characterization process, several parameters, including absorption, transmission, optical band gaps, refractive index, and extinction coefficient, were determined based on experimental data. Notably, the optical band gap consistently decreases with the increasing weight fraction of TiO_2 in the PMMA nanocomposite.

A 105

Probing the Defect Levels in Pure and Cobalt-doped Zinc Oxide Nanoparticles for Optoelectronic Applications

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ABSTRACT

Zinc Oxide (ZnO) is a direct band gap multifunctional semiconductor. The exciton binding energy of ZnO is 60 meV at room temperature, making it suitable for optoelectronic applications. The Synthesis methods and conditions affect the defect formation in Zinc oxide. The foresight of defects opens a path for defect engineering, where we can modulate the optical and electronic properties by tuning the defects. Hence these native defects widely influence the optical and electrical properties. This talk describes the temperature-dependent conductance characteristics of low-temperature synthesized Zinc oxide nanoparticles and cobalt-doped ZnO (Co-doped ZnO) nanoparticles. In this work, we report the synthesis of ZnO and Co-doped ZnO nanoparticles with different particle sizes by solution processing. X-ray diffraction (XRD) studies on these nanoparticles show that the particles are highly crystalline, which was further proved with transmission electron microscopy. From XRD peaks, Hall-Williamson plots were constructed, from which it was understood that the micro-strain in the particles linearly reduces with increasing deposition temperature. The defects in the ZnO nanoparticles also reduce with doping with cobalt as seen from Photoluminescence measurements and X-ray photoelectron spectroscopy analyses. The DC Conductivity measurements of ZnO and nanoparticles were measured by constructing FTO/ZnO/FTO devices. From Arrhenius plots, the activation energies of the defects were estimated. The temperature-dependent conductivity of ZnO and Co-doped ZnO nanoparticles was explained with the help of these above-mentioned measurements.

A 106

Hydrothermal Growth of ZnO Nanoflowers on Stainless Steel Mesh for Photodetector Application

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ABSTRACT

Due to the rapidly increasing population and energy demands in recent years, energy-efficient viable optoelectronic devices have become a major source of worry. Because of their broad applications in a variety of fields, such as molecular sensing, aerospace, health, pollution monitoring, water purification, and biomedical imaging, photodetectors which convert optical impulses to electrical signals are receiving a lot of attention. Exploring the progress in nanoscience and nanotechnology has led to the examination of various materials for their photodetection capabilities. While Silicon and GaN-based photodetectors were initially investigated, they faced challenges such as low efficiency and elevated material costs. As a result, semiconductors such as CuO, ZnO, ZnS, CdS, etc., were subsequently introduced as replacements. Specifically, ZnO is renowned for its photodetection capabilities, attributed to its wide band gap (3.3 eV), significant exciton binding energy (60 meV), ease of preparation, and stability. Nevertheless, in order to fulfill the demands of broad-spectrum photodetectors, the optoelectrical properties of ZnO need to be adjusted through modification. Therefore, in this work, we try to grow the ZnO nanoflowers on the stainless-steel mesh via the hydrothermal method and observe the morphological characterizations of the nanoflowers. Further to analyze the detection properties of the prepared samples through the IPCE measurements.

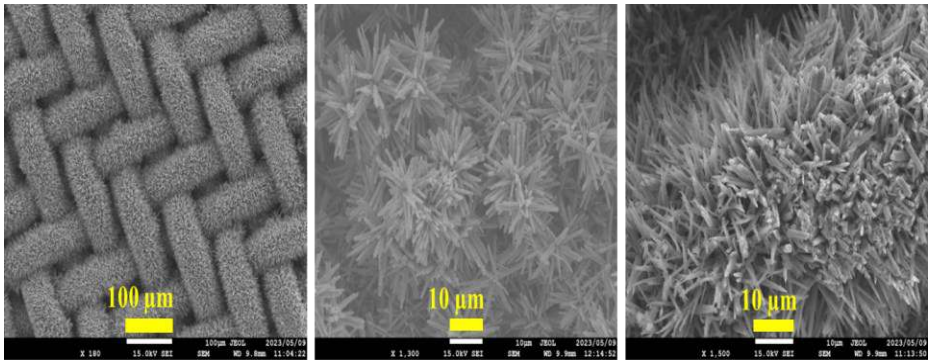

Fig.1 Morphological Analysis for Pure ZnO nanoflowers

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A 107

Synthesis and Characterization of Tin Diselenide ($SnSe_2$) Nanoparticles for Photodetector Applications

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ABSTRACT

The unique layer dependent structural and electronic properties of single and few layered metal dichalcogenide materials like WS_2, MoS_2, $MoSe_2$, $MoTe_2$, and TaS_2, have led to extensive exploration in the development of various electronic devices, including energy storage, humidity sensors, transistors, photodetectors, and photocatalysis due to high surface to volume ratio, surface states, and tunable electronic properties [1]. TMDCs are widely used for photodetector applications due to the absorption in the 200–850nm range from the ultraviolet region to the near-infrared region. Tin diselenide ($SnSe_2$) is a binary compound semiconductor used in a wide range of opto-electronic applications [2,3]. $SnSe_2$ has an optical bandgap of ~1 eV in its bulk state and the bandgap can be tuned depending on the layer thickness. Photodetectors with 2D $SnSe_2$ nanoparticles have showed superior performance, such as high on/off ratio, high responsivity, good stability, and a fast response time of 5 µs which was almost shorter than those of reported photodetectors based on other 2D materials [2,3]. Herein, we synthesized tin diselenide ($SnSe_2$) nanoparticles by varying the concentration of the precursors by using the hydrothermal method. The morphology of the as-synthesized $SnSe_2$ nanoflakes were characterized using a field-emission scanning electron microscope (FE-SEM). The nanoflake-like structure indicates the anisotropic nucleation growth kinetics in the hydrothermal process. UV-Vis spectroscopic studies were performed to probe the optical characteristics of the active layers of $SnSe_2$. The $SnSe_2$ bandgap values were obtained in the range of 1.0–2.04 eV. This variation is due to the particle size, defects, presence of phases and nature of crystallinity etc. which originates from the different synthesis techniques in various environments.

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A 108

Design of Low Power SPI Protocol using Clock Gating Techniques

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ABSTRACT

Serial Peripheral Interface (SPI) is a synchronous serial communication protocol employed for exchanging data between electronic devices. It facilitates full-duplex communication, allowing simultaneous transmission of data in both directions at high speeds. The protocol establishes a master-slave relationship, where the master device controls the slave device. The master issues instructions, and the slave device follows those instructions. The integration of clock gating techniques will enhance the performance of the Serial Peripheral Interface (SPI) protocol commonly used in embedded systems. This approach involves selectively disabling the clock signal during idle states of the blocks, resulting in significant reductions in power consumption while maintaining high-speed and reliable data transfer. Through extensive simulations and experimental validations, our study demonstrates the efficiency of the proposed clock gating strategy in achieving a balance between power consumption and communication speed. Clock Gating not only benefits SPI applications but also serves as a model for optimizing other communication protocols. The results presented in this paper offer valuable insights into implementation challenges and considerations associated with integrating clock gating into the SPI protocol, paving the way for further advancements in power-aware design methodologies.

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A 109

Synthesis, Growth, Structural and Characterization of Non-Linear Optical Materials for Optoelectronics Device Applications

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ABSTRACT

A novel nonlinear optical single-crystal of manganese bis(15-Crown-5-ether) barium tetra - thiocyanate) [MGBCBA] was synthesized by slow evaporation technique in a room temperature. The title crystal, which measured 8×5×2 mm3, was gathered over a period of 10 to 15 days [1]. By using the single crystal X-ray diffraction techniques, the unit cell parameter, crystal symmetry, and structure were examined. The powder x-ray diffraction method was used to index the distinct facets of different crystal planes. The result reveals that the title compound is Tetragonal, with space group of (I41/a) centrosymmetric structure. The spectroscopic properties of FT-IR, Micro-Raman, UV-optical were observed the cut-off wavelength (~348nm) and optical band gap (~3.28 eV) was studied. The reverse growth rate, surface shape, and presence of synthesized components were confirmed by etching studies [2,3]. The thermal stability, mechanical stability was calculated by TG-DTA, Vickers hardness tester. The dielectric constant(ε_r), dielectric loss (tan δ) with low frequency was studied. The linear and nonlinear coefficient such as, nonlinear refractive index (n_2), nonlinear absorption coefficient (β), third order susceptibility (χ^3) then hyper polarizability (γ) were measured by Z-Scan studies.

Keywords: *Slow Evaporation Techniques; Single crystal XRD, Thermal and Surface properties; Dielectric and Z-Scan analysis.*

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A 110

Synergistic Enhancements in Dysprosium Oxide-Polyvinylpyrrolidone Nanocomposites: Unveiling Optoelectronic and Dosimetric Applications

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ABSTRACT

Dysprosium oxide (Dy_2O_3) stands as a pivotal rare-earth material with multifarious applications spanning metal halide lamps, magneto-optical memory materials, glasses, and neodymium iron boron permanent magnet additives. This study employs a low-temperature solution combustion technique utilizing urea as a fuel to synthesize Dy_2O_3, ensuring the formation of a pure cubic phase as confirmed by powder X-ray diffraction (PXRD). Subsequently, the pristine cubic Dy_2O_3 sample undergoes coating with Polyvinylpyrrolidone (PVP), paving the way for comprehensive structural and optical analyses. The investigation delves into the determination of energy band gaps for Dy_2O_3 and PVP-coated Dy_2O_3 (at 9 mol%) utilizing both Tauc and Wood plot method, yielding values of 4.43 eV and 5.21 eV, respectively. Fourier transform infrared spectroscopic (FTIR) studies further validate the formation and purity of cubic Dy_2O_3, revealing a prominent absorption peak at approximately 573 cm^{-1} attributed to the Dy-O bond vibration, alongside absorption peaks within the 1300-1500 cm^{-1} range indicative of CO_3^{-2} anion groups. This research unveils promising prospects for the application of Dy_2O_3coated with PVP in thermoluminescent dosimeters (TLD) and optoelectronic devices. By combining the unique properties of $Dy_2O_3$with the advantageous characteristics imparted by PVP coating, such as enhanced optical properties and stability, the resulting composite material holds considerable potential for advancement in radiation dosimetry and optoelectronic technologies.The structural and optical properties of Dy_2O_3 coated with PVP not only contributes to the fundamental understanding of rare-earth materials but also underscores the practical implications for emerging applications in TLD and optoelectronics.

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A 111

Spectral and third order nonlinear optical properties of Cobalt doped $LaWO_4$ nanostructures for optoelectronics application

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ABSTRACT

The growing need for advanced materials that can control light intensity in a non-linear way, known as nonlinear optical materials. These are crucial for building better photonic devices. Luckily, researchers have found transition metal tungstates to be promising candidates thanks to their unique optical and light-emitting properties. In short, these materials are shining stars in the world of next-generation optoelectronics. In this study, we present findings on the nonlinear optical behaviour of nanostructures composed of Lanthanum tungstate (LaWO4) doped with Cobalt ions (Co^{3+}), which were synthesized using a co-precipitation method. Analysis through X-ray diffraction and Raman spectroscopy affirms the development of $LaWO_4$ nanostructures exhibiting a monoclinic structure with the C2/c space group. The high-resolution scanning electron microscopy (HRSEM) images of the pristine LaWO4 reveal the nano-sized grain like structures. Furthermore, the introduction of cobalt doping induces a reduction in particle size, attributed to lattice contraction-ray photoelectron spectroscopy was employed to verify the chemical state of the elements within Co^{3+} -doped LaWO4. The optical characteristics of the samples were investigated using UV-Vis Spectroscopy, revealing an increased bandgap upon Co^{3+} doping. The nonlinear optical (NLO) response was assessed through the open aperture z-scan technique, utilizing a Nd: YAG pulsed laser (532 nm, 7 ns, 10 Hz). The results demonstrated a reverse saturable absorption attributed to a two-photon absorption (2PA) process. The observed enhancement in the 2PA coefficient, coupled with a simultaneous reduction in the onset of the optical limiting threshold, underscores the promising potential of Cobalt-doped LaWO4 nanoparticles for effective optical limiting applications.

Keywords: *Optical limiting, lanthanum tungstate, cobalt, Z-Scan*

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A 112

Alcohol-Titanium (IV) alkoxides mixtures for TiO_2 thin film formation

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ABSTRACT

Titanium dioxide (TiO_2) is one of the most studied materials around all over the world because of its abundance, chemical stability, semiconducting properties, and environmental friendliness like properties. Therefore, this material has wide range of application and by now a plenty of research articles have been published on synthesis, characterization, and application of TiO_2 and TiO_2 based derivatives. Among them TiO_2 thin films coating have gain the attraction due to wide range potential applications such as, electronics, solar cells, UV-protection, water and air purification, sensors etc. It has been reported number different techniques used for synthesis of crack free thin and controllable TiO_2 thin films. Each of these methods have advantages as well as disadvantageous that are dependent on applications and requirements. Among them, hydrothermal synthesis and Sol-Gel Processing are popular among other techniques. Overall simple, inexpensive, efficient, environmentally friendly, and fast techniques are most useful. In this study, the possibility of usage of titanium alkoxide alcohol mixtures for synthesizing TiO_2 thin films were investigated using five different alcohols (ethanol, 1-propanol, 1-butanol, 2-propanol and 2methyl 2-propanol) and two titanium alkoxides (titanium-tetra-isopropoxide (TTIP), titanium-tetrabutoxide (TTBu)) under different experimental conditions. Unlike sol-gel based synthesis techniques, instead of acidification, in this technique reaction was controlled by content of water vapor and temperature around the reaction environment. Experiments were done under different water vapor content, different concentrations of titanium alkoxide and under different spin coating/dip coating conditions. formation of TiO_2 thin films were confirmed by Raman spectroscopy and Energy Dispersive X-ray (EDX) analysis. Morphology of thin film was analyzed by scanning electron microscope and laser microscope. The chemical structure estimation was done by nuclear magnetic resonance spectroscopy and

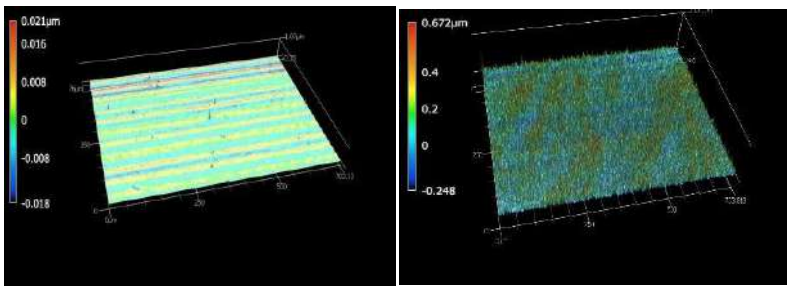

Figure 1 Surface analysis of TiO2 coating by laser Microscope mass spectroscopy. Overall, it was observed that lower hydrolysis rate of titanium alkoxide in alcohols facilitate formation of smooth thin TiO_2 coatings.

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A 113

Design of a Multiband Mimo Antenna For 5g Application

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ABSTRACT

As the world embraces the advent of 5G technology, there's a growing need for advanced wireless communication systems that can support the diverse and demanding applications of this new era. One key technology enabling 5G is Multiple Input Multiple Output (MIMO) antenna systems which enhance data rates, coverage and reliability by utilizing the multiple antennas at the both transmitter and receiver ends. MIMO systems come in various configurations such as 2x2, 4x4, 8x8, etc., representing the number of transmitting and receiving antennas. These configurations impact system performance, capacity and complexity. The objective is to create an antenna solution capable of operating across multiple frequency bands including. The design of multi-band MIMO antennas for 5G applications involves antenna design, simulation, prototyping and real-world testing to optimize performance metrics such as gain, efficiency and radiation patterns. Advanced electromagnetic simulation tools such as the HFSS (High Frequency structure Simulator) will be used to model and simulate the antenna system's performance. ANSYS HFSS is 3D full-wave electromagnetic field solver designed for higher frequencies and high-speed electronic component designs.

A 114

In-situ Growth of Cu-doped ZnO Nanoflowers via Mist CVD for Photodetector Application

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ABSTRACT

In recent years, energy efficient feasible optoelectronic devices are of much concern owing to the rapid growing population and energy demands. Photodetectors convert optical signals to electrical signals are of immense attention because of its wide applicability in various sectors that include, space communication, pollution monitoring, water sterilization, health, biomedical imaging, aerospace, and molecular sensing. With the advancements in nanoscience and nanotechnology, several materials were studied for photodetection properties. Initially, Silicon and GaN based photodetectors were studied however, they suffer poor efficiency and high material cost. Therefore, later it was replaced with semiconductors (CuO, ZnO, ZnS, CdS, etc). Particularly, ZnO is well known for its photodetection attributed by its wide band gap (3.3 eV), large exciton binding energy (60 meV), ease of preparation and stability. However, to meet the requirements of broad band photodetectors, the optoelectrical properties of ZnO has to be tuned via doping. Therefore, in this work we fabricated ZnO nanoflowers and Cu-modified ZnO via facile mist CVD. Cu-doping has altered the morphological characteristics of the nanoflowers. Further, the PL analysis confirmed the defects influenced by 6at% of Cu-doping. The prepared ZnO and Cu-ZnO showed selectivity towards wide spectra extending from UV (340 nm) to visible (600 nm). The 6at% Cu-ZnO nanoflowers found to possess higher IPCE value of about 98% among other samples attributed by Cu- induced deep acceptor levels. Further, the detectivity (Dt) of 245.9 x 10^{8} for pure ZnO and 34.4 x 10^{11} for Cu-ZnO nanoflowers ensured the feasible candidature of prepared Cu-ZnO nanoflowers for UV Visible detection.

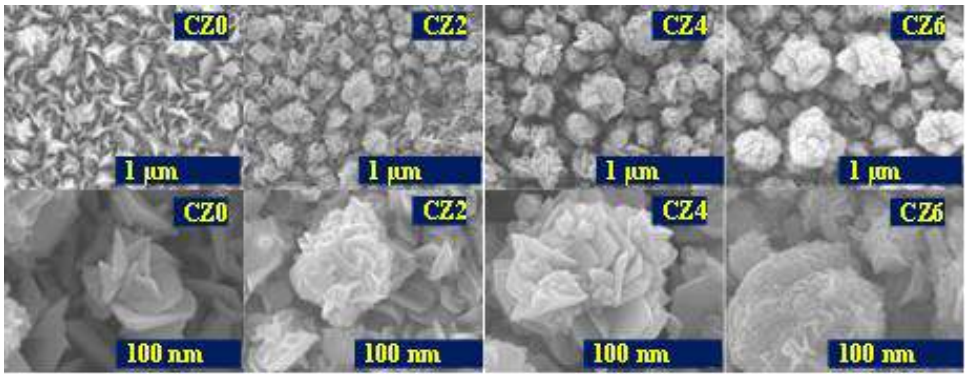

Fig.1: Morphological analysis

A 115

Enhancing Employability and Skill Sharing through a Mern-Stack web chat with AI Powered Query Forum

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ABSTRACT

Success in education depends on collaboration and communication. Particularly for freshmen, face-to-face contact and collaboration might be difficult. In order for students to improve their relevant skills under the direction of teachers or mentors, there is a need for a digital platform that may enable efficient communication and collaboration between them. The goal is to build and create a student chat application that will let students communicate in real time with each other and with lecturers that have competence in the student's interested skill so that the student will get guidance on which skill will have a better scope for job opportunities. The objective is to- Create a chat application for students to use to connect with one another by looking for other students or instructors with the interested skill or expertise. It offers a user-friendly user interface so that students can pose questions in a chatbot with artificial intelligence (GPT-3) that can answer them, as well as any other users who have registered to the app. Ascertain the app's security and respect for users' privacy. To safeguard user privacy and data, encryption using the bcrypt hashing algorithm is utilized.

Keywords: *Encryption, hashing algorithm, body-parser, Web Socket, React Hooks, React Context API,API.*

A 116

Physical Modification of $CdCl_2$ doped with Polyvinyl Alcoholic films

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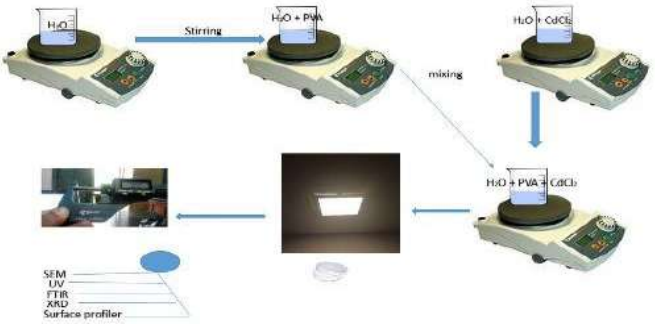
ABSTRACT

The structural features of Cadmium Chloride ($CdCl_2$) doped polyvinyl alcohol (PVA) blend films are correlated with their optical and electrical properties. The phenomenon of doping polymers with inorganicsalts like $CdCl_2$ can result in modifications in microstructure of the polymeric material. It also affects optical, electrical and thermal properties of the material. The SEM images show the Nano-crystals changein shape from spherical to rod-shaped structures, and with further increase in doping level flower shaped crystalline features are observed evidencing increasing in particle size. In this work doping percentage of $CdCl_2$ is varied from 5% to 30%. The PVA doped $CdCl_2$ films are prepared using solution cast technique with slow evaporation. The optical property was examined using UV-Vis Spectroscopy. Studies reveals film has large transparent region and absorbance of materials increases with doped percentages up to 95%. FTIR analysis validates that PVA sample is sensitive to IR spectrum region also evidences the presence of Carbon, Hydrogen and Oxygen group. SEM morphology shows increase in doped concentration and good distribution of Cd ion over the surface. Surface profilometry supports surface morphology and eventuality of film. XRD evidences the semi crystalline nature and structure. This enhancement in energy band gap, semi crystalline nature, and surface morphology helps in the bettermentof optical application.

Keywords: *PVA, Surface Profiler, SEM, UV-NIR Spectroscopy, XRD,FTIR*



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A 117

Enhancing the Performance of Phenoxazine – Oxadiazole based TADF Molecule Through di-CF_3 Substitution in OLEDs

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ABSTRACT

The chemical tailoring of thermally activated delayed fluorescence (TADF) active molecules is beneficial in improving the efficiency as well as color purity of organic light emitting diodes (OLEDs). In this perspective, the role of substituting an electron withdrawing segment i.e., bis-Trifluoromethyl (di-CF_3) in 10-(4-(5-Phenyl-1,3,4-oxadiazol-2-yl) phenyl)-10H-phenoxazine (PXZ-OXD) molecule have been studied in detail. The above-mentioned substitution in PXZOXD increased the overall acceptor strength of the molecule together with an enhancement in photoluminescence quantum yield. The thin film of the di-CF_3 added PXZOXD in PMMA matrix revealed a notable increment in prompt lifetime. The detailed Density functional (DFT) and time dependent density (TDDFT) functional theories analyses the possible variation occurred hole/electron reorganization energies along with the changes occurred in singlet-triplet splitting energies (ΔE_{ST}). The OLED devices fabricated with 3, 5' diCF_3-PXZOXD as emissive layer show enhanced maximum external quantum efficiency of 14.5 % in comparison to PXZOXD (13.2%).

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A 118

Enhancement of Terrestrial Images vision using Dashboard Camera lens models

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ABSTRACT

High-grade cameras serve as essential sensors in aided and autonomous driving. Specifically, advanced front-facing cameras with a long range can offer crucial data regarding the upcoming road conditions. This includes the ability to recognise and identify objects as well as provide early warnings for potential hazards. These vehicle cameras are designed to dependably capture high-resolution images even under harsh operating circumstances of the car, ensuring reliable performance. This research seeks to present the design of fixed-focus lenses that are passively athermalized for vehicle cameras in the next generation. Dash cameras will initiate filming upon driving, documenting all of your on-road (and occasionally off-road) escapades. Drive data will be continuously saved to the internal storage of the dash cam in a cyclical manner. Additionally, if the dash cam model is equipped with its own software, it may also immediately record to an application.An image sensor records the incoming light from the lens to create a digital image. Increasing the size of the image sensor results in a higher pixel count, leading to enhanced light absorption and improved image quality with less noise. Dashcams typically have a field of view ranging from 130 to 160 degrees, which is the most commonly seen range. In our proposed model, the Dashboard camera when evaluated with lens parameters like modulation Transfer function (MTF), spot diagram, point spread function (PSF) shows better performance over other existing models. The MTF value ranges from 0.9 in field 1 with 0 degrees to 0.58 in Field 4 with -20 mm, -7.5 degrees. The spot diagram exhibits the value of 0.061682 for field position 1 with relative field height of 1, 1, 20 with-15 degrees to -0.061824 for field position 4with relative field height of -1, 1,-20 with 15 degrees. The Ray Aberration curve plot shows the value of 0.064296 to -0.064296 for relative field height of -1.00, 0.49,-20.0°, -7.5°. The dashboard camera is able to capture the images effectively with various levels of view.

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A 119

Women's Defense System with Electric Shock, Image Capturing and Fingerprint Timer

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ABSTRACT

In recent years, concerns surrounding women's safetyhave escalated, highlighting the pressing need for innovative solutions to address this issue. This paper presents a comprehensive project aimed at enhancing women's safety through the development of a wearable band with multiple integrated features. The proposed wearable band incorporates a Shock Effect Mechanism, image capturing capabilities, and a Fingerprint-Based Timer, collectively designed to empower women to protect themselves in various situations. The Shock Effect Mechanism serves as a primary defense mechanism by delivering a non-lethal electric shock to potential assailants when activated. This feature provides an immediate and effective deterrent to potential attackers, giving the wearer valuable seconds to escape or seek help. The shock intensity is carefully calibrated to ensure the safety of the wearer while incapacitating the attacker temporarily. The image capturing functionality of the wearable band allows users to discreetly captured image evidence in situations where they feel threatenedor unsafe and the image goes to telegram BOT. This feature canbe valuable in documenting incidents and providing evidence for legal proceedings, thus increasing the accountability of wrongdoers. Furthermore, the Fingerprint-Based Timer adds an extra layer of security and peace of mind. Users can set a predetermined timer using their fingerprint authentication, ensuring that they can alert emergency contacts or authorities automatically if they do not deactivate the timer within the specified period. This feature is particularly useful in caseswhere the wearer may be unable to use their device actively, such as during a potential abduction. The combination of these features in a single wearable device offers women a powerful toolfor personal safety, allowing them to proactively protect themselves and take control of their security. This project represents a significant step towards addressing the growing concerns surrounding women's safety, providing an innovative and technologically advanced solution to empower women and create safer communities.

B 001

Numerical Investigation on Anodic Corrosion of Aluminium Metal Air Batteries

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ABSTRACT

Our global energy demand is increasing day by day because of the rapid development of technological growth in every field and it fully depends on fossil fuels which creates carbon footprints leads to acute problems in the environment such as Global warming, Climatic change, Air pollution, and Respiratory issues. To overcome such issues a novel approach is to produce higher capacity batteries that can be incorporated into electrical energy storage applications to reduce the dependence of fossil fuels. Hence, the best alternative way is to utilize electrochemical energy storage system for the replacement of conventional internal combustion engines to produce an energy for electric vehicles. In this context, Metal air batteries will be a most futuristic promising electrochemical energy storage systems. Aluminium air battery is the attractive candidate because of higher theoretical energy density, theoretical voltage, inexpensive, lightweight, abundance in earth crust and safety. Recently many research works are focusing on the performance improvisation of aluminium air batteries that restricts the commercial development. The problem in aluminium air batteries is corrosion on anode surface and hydrogen gas evolution during the discharge period. In this research work, COMSOL Multiphysics simulation software were utilized to do numerical analysis of aluminium metal air batteries to predict the anodic corrosion behaviour through different kind of plots such as cyclic voltammetry, Nyquist plot, Bode plot and Tafel plot.

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B 002

Studies Of Phase Transition of Some Superionic Solids

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ABSTRACT

Investigation and Confirmation of phase transition of Some Superionic Conductors are presented through magnetic susceptibility (χ_M) and dielectric Constant (K) Studies. Uncommon to other ionic solid, Superionic Conductor Show great anomaly in their behavior in certain temperature range in the χ_M V_s T plots of each solid. The distinctively sharp peak is observed at this temperature in the $\frac{dK}{dT}$ V_s T plot which yields phase transition temperature. Phase transition temperature of some superionic solids have been already evaluated from electrical conductivity and thermoelectric power experiments and also examined & verified by magnetic susceptibility and dielectric constant studies. The dielectric loss of the superionic solids have been also measured and calculated from electrical conductivity data. The experimental and calculated value of dielectric loss from electrical conductivity data are nearly same.

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B 003

2D ZrS_2 /Graphene Nanocomposite by Solvo and Hydrothermal Synthesis and Characterization for Supercapacitor Applications

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ABSTRACT

The graphene-based nanocomposites are promising candidates for energy storage applications due to its high surface area, outstanding electrical conductivity, excellent chemical stability and mechanical property. In this work, pure ZrS_2 nanosheet, GO and 2D ZrS_2/G nanocomposite were synthesized with the help of chemical bath deposition (CBD) method, modified Hummers method and Solvo and hydro thermal methods. The 2D ZrS_2/G nanocomposites are synthesized by two different methods. The first method is the glycol based solvothermal method with a ratio of 70:30 and second method is the water based hydrothermal method with a ratio of 80:20. Further, the 2D ZrS_2/G nanocomposites are characterized using XRD, Raman spectra and HRSEM. The electrochemical studies namely the CV, GCD and EIS are also inferred. The objective is to study the effect of the graphene on the 2D ZrS_2 and the structural modification in the nanocomposites due to the different synthesis of thermal routes. The 2D ZrS_2/G nanocomposites have the potential to be the viable candidate for energy storage applications.

Keywords: *2D ZrS_2, ZrS_2 Supercapacitors, Solvo/Hydrothermal method.*

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B 004

Investigation of Different Ratio Ce doped MnO Nanostructures for Energy Storage Applications

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ABSTRACT

Pure Manganese oxide (MnO) and Cerium doped manganese oxide $MnO_{1-x}Ce_x$ (X=1, 1.5, 2) at different ratios are successfully synthesized using solvothermal method. The utilization of XRD, FTIR and HRSEM involves distinct characteristics when employed to analyze crystallinity, functional group and morphology. The diffraction peaks indicates the presence of MnO and as the concentration of dopant (Ce) increases, the peak shifts to the higher angle side. It is also found that the crystalline size also decreases with the increase in Ce concentration. The morphology of the MnO nanoparticles shows the spherical structure and they are almost in an agglomerated state. For Ce doped MnO, there is a combination of nanorods and nanospheres which implies that the doping attributes the change in morphology. As the concentration of the dopant (Ce) increases, the morphology of the MnO changes from sphere to rods and platelets i.e., the surface area of the particles increases with porosity. This leads to the increase in the capacitance of the electrode materials and hence it is observed that Ce- doped manganese oxide can be used in an effective way for supercapacitor applications.

Keywords: *Ce doped MnO, Solvothermal, Nanostructures, Supercapacitor*

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B 005

Investigation of Chemical Network, Electronic Environments and Electrochemical Performance of FeZn-rGO Nanocomposites

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ABSTRACT

Reduced graphene oxide-reinforced iron and zinc oxide (Fe_3O_4/ZnO/rGO) nanocomposites with varying ZnO content were synthesized using chemical reduction and investigated for energy storage application. The size of composites varied between 8.00 and 17.09 µm on surface of graphene sheet. Crystalline wurtzite hexagonal phase structure of ZnO was confirmed with (101) and (102) peaks at 36.42 and 47.03° respectively. From W-H plot, crystallite size and lattice strain varied from 14.18 to 19.37 nm and 0.0018 to 0.0093 respectively. The Fe content varied from 21.5 to 24.48 at.% and that of Zn content from 37.93 to 40.65 at.%. Carbon network study shows C-Zn, C-Fe, C-O-/C=O functional groups. Dominance of s-orbital in valence band is observed in all nanocomposites and *p*-orbital is dominant in valence band of pure rGO. Structural defect study shows that I_D/I_G varied from 0.44 to 0.62, indicating decrease in defects. Specific capacitances are 550 and 645 Fg^{-1} respectively at 5 mVs^{-1} scan rate, indicating increase in specific capacitance.

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B 006

PEO/PVDF Based Solid Polymer Electrolyte Films for Developing All Solid-State Li-S Cells

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ABSTRACT

Increasing energy demands in large-scale and grid applications have intensified research into developing new cost-effective materials for efficient energy storage applications. Lithium-sulfur cell chemistry is considered as one of the most promising ways for developing next-generation energy storage devices. Sulfur cathode has a high theoretical capacity of 1675 mAh/g. But low electrical conductivity of sulfur and the polysulfide shuttling effect limit practical applications. To overcome these limitations, several effective approaches have been adopted. The capacity and cyclability of Li-S cells can be increased through the creation of sulfur composites with carbonaceous and polymeric materials, as well as electrolyte optimization. The replacement of the typical liquid organic electrolytes with solid polymer electrolytes has been shown to be one of the most effective and promising electrolyte changes. In the present work, lithium enriched, PEO/PVdF based solid polymer electrolyte (SPE) film serving as both solid electrolyte and separator has been investigated to develop all solid state Li-S cells. The limitation of low ionic conductivity in the crystalline phase of PEO is handled by blending PEO with PVdF. The structural and morphological characterizations of the developed SPE film and modified sulfur cathode were done using XRD and FE-SEM techniques. Electrochemical characterizations were carried out by assembling stainless steel Swagelok cells. The SPE membrane is expected to function as a physical barrier to prevent the sulfide anion's shuttling between the electrodes. The assembled all solid-state Li-S cells are found to exhibit enhanced specific capacity with impressive cycling stability.

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B 007

Supercapacitive Performance of CTAB Modified Ammonium Zinc Phosphate Nanoflowers

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ABSTRACT

Herein, we demonstrate CTAB modified ammonium Zinc Phosphate (AZP) nanoflowers by using a simple, facile, cost-effective hydrothermally assisted thermal annealing process for supercapacitor application. The crystal nucleation and growth of ammonium zinc phosphate into distinct morphology are controlled by the addition of CTAB. The AZP nanoflowers have uniform morphology of ~ 50 nm and high surface area of 31 m^2/g. The CTAB modified AZP exhibits a high specific capacitance of 412 F/g at current density of 1 mA/cm^2 and superior cycling stability after 5000 cycles. Moreover, the AZP//Activated carbon hybrid supercapacitor device achieves a high specific capacitance of 93 F/g at 1 mA/cm^2 and an energy density of 22.68 Wh/kg at a power density of 212 W/kg. The effects of the CTAB concentration on the electrochemical performance of AZP were also examined. AZP with this remarkable electrochemical performance may be considered a prospective candidate for high performance supercapacitor applications.

B 008

Papaya stem modified Molybdenum Disulfide as Counter Electrode Catalyst for Bifacial type Dye-Sensitized Solar Cells

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ABSTRACT

The development of low-cost, high-performing cells is the primary goal of current research on dye-sensitized solar cells [1,2]. In this study, Molybdenum disulfide embedded biomass-derived carbon from papaya stems (MoS_2@PS) was synthesized using the hydrothermal approach which was subsequently subjected to various temperatures of annealing. The maximum photovoltaic conversion efficiency was over 7% for the DSSCs based on MoS_2@PS counter electrode (CE) which shows a promising potential for Pt free CE. Cyclic Voltammetry and Tafel Polarization studies further confirms the high electrocatalytic activity towards reduction of triiodide ions (I_3^-) for MoS_2@PS (CE). Transmittance studies were done to confirm the bifacial nature of DSSCs. Electrochemical Impedance spectroscopy (EIS) shows that the as made MoS_2@PS CE based DSSCs shows the fast charge transfer at electrode/electrolyte interface. The optimum conversion efficiency, high transmittance, simple preparation and fast charge-transfer and low cost show the potential application of MoS_2@PS CE in for DSSC applications.

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B 009

Synthesis and Electrocatalytic Activity of Au@Pd Core-Shell Nanooctahedron for Ethanol Oxidation

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ABSTRACT

The development of efficient and cost-effective electrocatalysts for the oxidation of ethanol has garnered significant attention due to its critical relevance in fuel cells and direct ethanol fuel cells (DEFCs). Ethanol is considered a promising alternative energy source because of its renewable nature and high energy density. In this context, the design and synthesis of advanced nanomaterials with enhanced electrocatalytic properties have become a focal point of research in the field of electrochemistry. The synthesis of Au@Pd core-shell nanooctahedra typically involves seed-mediated growth synthesis. These methods enable precise control over the size, composition, and morphology of the nanooctahedra, which is crucial for optimizing their electrocatalytic activity. The resulting nanocrystals exhibit a high surface area, abundant active sites, and favorable crystal facets for catalyzing the ethanol oxidation reaction.

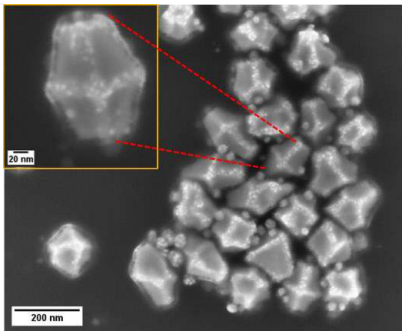

Figure 1. SEM images of Au@Pd Core-Shell Nanooctahedron with high magnification.

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B 010

Advancements in Low-Temperature Solid Oxide Fuel Cells: A Novel Heterostructure Composite Approach

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ABSTRACT

Solid oxide fuel cells (SOFCs) have long been recognized as a clean and efficient energy conversion technology, but their widespread commercialization has faced various challenges, including high operating temperatures and material limitations [1,2]. This abstract highlight recent breakthroughs in the field of low-temperature solid oxide fuel cells (LT-SOFCs), introducing a novel approach to address these challenges [1]. A key strategy involves the structural design and doping of electrolyte materials to enhance oxygen ionic conductivity, which is crucial for the efficient operation of SOFCs. However, despite these efforts, hurdles remain in the path to SOFC commercialization. Recent progress has emerged through the development of semiconductor ionic materials, opening new avenues for LTSOFC design [3,4]. A notable achievement in this regard is the creation of a heterostructure composite material comprising $La_{0.6}Sr_{0.4}Fe_{0.8}Cu_{0.2}O_{3-\delta}$ (LSFC) and $Sm_{0.2}Ce_{0.8}O_{2-\delta}$ (SDC). This composite serves as an advanced electrolyte for LT-SOFCs. The LSFC-SDC composite demonstrates exceptional performance, with ionic conductivity exceeding 0.1 S/cm at 600 °C. This high conductivity facilitates efficient ion transport within the fuel cell. Furthermore, symmetrical NCAL ($Ni_{0.8}Co_{0.15}Al_{0.05}LiO_{2-\delta}$) coated electrodes are employed, optimizing electrochemical reactions within the cell. In practical terms, LT-SOFCs utilizing the SDC-LSFC electrolyte exhibit a significant improvement in open-circuit voltage (OCV) and power output compared to conventional SDC electrolytes at 600°C. This work represents a paradigm shift in LT-SOFC technology, departing from conventional approaches. It showcases a promising route for the development and commercialization of low-temperature solid oxide fuel cells. These advancements address critical challenges and offer a greener and more efficient energy conversion solution, bringing LT-SOFCs closer to practical implementation in various clean energy applications.

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B 011

Advancements in $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$ Composite Cathodes for Enhanced Performance in Intermediate-Temperature Solid Oxide Fuel Cells

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ABSTRACT

A perovskite oxide-based $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$-$Gd_{0.}Ce_{0.9}O_{2-\delta}$ has been investigated as a novel cathode for intermediate-temperature solid oxide fuel cells (IT-SOFCs). $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$ was synthesized by solid-state reaction method, by varying x from 0 to 0.15. The phase purity of as prepared $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$ powders was evaluated by powder X-ray diffraction with Cu-Kα radiation. No additional phases and peak shifts were detected, which confirms the phase purity of the prepared $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$. The calculated lattice parameter *a* and cell volume *V* are found to vary from 0.3946 *nm* to 0.3965 *nm* and 61.4 $Å^3$ to 62.3$Å^3$ respectively. The reliability factors 2 to 4 indicate that the refinement results are reasonable and all the $Bi_{0.5}Sr_{0.5}Fe_{1-x}Nb_xO_{3-\delta}$ oxides show the cubic structure with space group $Pm\bar{3}m$. Scanning electron microscopy (SEM) was performed to analyse surface morphology. Electrochemical Impedance spectra (EIS) from room temperature (RT) to 600°C confirm the enhancement of the electrochemical performance of BSFNbO cathode materials. The detailed investigation results will be presented at the conference.

B 012

Electrochemical Performance of $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$ - $Gd_{0.1}Ce_{0.9}O_{2-\delta}$ Composite Cathodes for Intermediate Solid Oxide Fuel Cells

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ABSTRACT

The suitability of $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$ (x=0.05, 0.10, 0.15, 0.20) as an efficient cathode material for low and intermediate temperature solid oxide fuel cell (LT-SOFCs) operating from 200 ^{0}C -600 ^{0}C was investigated. The $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$material is prepared through solid state route and exhibited a singular cubic perovskite structure. Incorporating Sb through doping enhanced the structural stability of pristine $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$. Porous microstructure was investigated by the scanning electron microscope. The electrochemical characteristics of both porous cathodes $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$ and the composite cathodes $Bi_{0.5}Sr_{0.5}Fe_{1-x}Sb_{0.x}O_{3-\delta}$- $Gd_{0.1}Ce_{0.9}O_{2-\delta}$ based on were thoroughly assessed with in the intermediate temperature range 200 ^{0}C -600 ^{0}C. A comprehensive exploration was conducted to understand the intricate connection between electrochemical properties, microstructural features and Sb content. Specially, a $Bi_{0.5}Sr_{0.5}Fe_{0.9}Sb_{0.1}O_{3-\delta}$- $Gd_{0.1}Ce_{0.9}O_{2-\delta}$ composite with an optimized composition was selected as the cathode material for constructing high-performance anode supported solid oxide fuel cell (SOFCs).

B 013

Synthesis and Characterization Studies of Biomass-Derived Calcium and Magnesium Self-Doped Porous Carbon for Eco-friendly Symmetric Supercapacitor

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ABSTRACT

Supercapacitors are emerging energy storage devices with much higher energy density than traditional capacitors, very high-power density than batteries and are environmentally friendly. These features of supercapacitors have attracted focus on research interest in academics and industries. Carbon-based materials such as graphene, carbon nanotube and activated carbon are popular choices for supercapacitor electrodes because of their high surface area and porous structure. Carbon from biomass waste materials is an excellent choice as recycling waste materials is becoming more and more difficult because of the increasing human population. This work presents the synthesis and analysis of device characteristics of supercapacitors made of biomass-derived electrodes. Curcuma longa plant waste is collected and cleaned, powdered and carbonized at 700 ^{0}C for 3 hours. Electrochemical characterization is done to find the specific capacitance of the supercapacitor prototype. The physicochemical characterization of the carbon obtained from the Curcuma Longa plant is done by X-ray diffraction (XRD) analysis, Fourier Transform Infrared Spectroscopic (FTIR) analysis, Raman spectroscopy, Scanning Electron Microscopy (SEM) and Electron Diffraction Spectroscopy (EDS). From the physicochemical characterization, the carbon is found to have an amorphous nature with high porosity. The presence of Calcium and Magnesium from EDS indicates the presence of porogens naturally in the biomass which enhances the capacitance of the device.

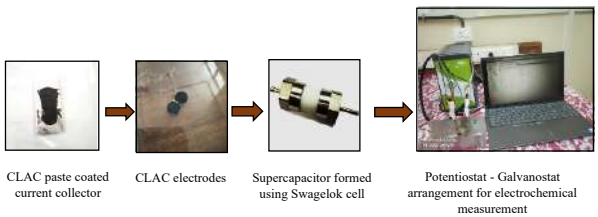

Fig. 2. Schematic illustration of the process of synthesis of supercapacitor and electrochemical measurement

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B 014

Fabrication and evaluation of $Ca_2Fe_2O_5$ –$Ce_{1-x}Sm_xO_{2-\delta}$ composite cathodes for Intermediate Temperature Solid Oxide Fuel Cells

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ABSTRACT

Solid oxide fuel cells (SOFCs) are electrochemical energy conversion devices with high working efficiency [1]. Recently, brownmillerite oxides have been drawing attention due to mixed ionic and electronic conductivity at low and intermediate operating temperatures. A cobalt-free composite $Ca_2Fe_2O_5$-$Ce_{0.9}Sm_{0.1}O_{1.90}$ and $Ca_2Fe_2O_5$ - $Ce_{0.8}Sm_{0.2}O_{1.90}$ with different wt% were synthesized and investigated as a cathode material for intermediate-temperature solid oxide fuel cells. The pristine $CaFe_2O_5$, $Ce_{1-x}Sm_xO_{2-\delta}$ and composite cathodes were prepared by solid state synthesis route. X-ray diffraction and Rietveld refinement of the samples confirms the Brownmillerite and Fluorite structure of $CaFe_2O_5$ and $Ce_{1-x}Sm_xO_{2-\delta}$ respectively. The electrical conductivity behaviour of the prepared cathode was studied through electrochemical impedance spectroscopy in controlled atmospheres, operating within temperatures (40 ºC–500 °C), in the frequency range of 20 Hz to 2 MHz. The activation energies of $CaFe_2O_5$, $Ce_{0.9}Sm_{0.1}O_{2-\delta}$ and $Ce_{0.8}\ Sm_{0.2}\ O_{2-\delta}$ were evaluated to be 0.55 eV, 0.78 and 0.71 eV. The synthesized composite cathodes were used to develop half cells and details of the results will be presented.

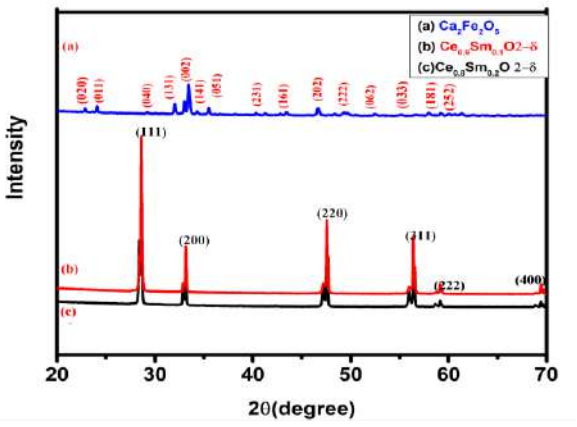

Figure. 1 X-ray diffractograms of (a) $CaFe_2O_5$, (b) $Ce_{0.9}Sm_{0.2}O_{2-\delta}$ and (c) $Ce_{0.8}Sm_{0.1}O_{2-\delta}$ powders prepared by solid state synthesis route.

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B 015

Interfacial Modification of Bimetallic LDH/MXene Heterostructure Electrode for Flexible Hybrid Supercapacitor

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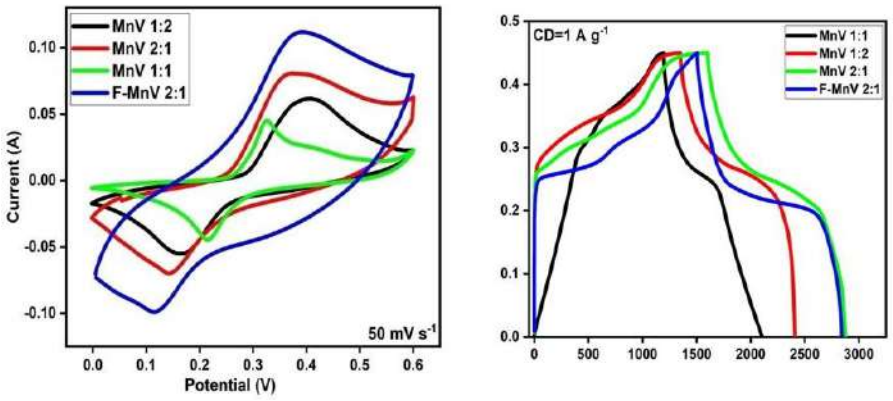
ABSTRACT

Layered double hydroxides (LDHs) have been attracting a lot of focus in energy storage applications due to their exchangeable anions, excellent charge storage, low internal resistance and variable interlayer spacing. In addition to the significant volume fluctuations and reduced accessible active sites attributed to poor electrical conductivity and flakes aggregation, rate performance and cycle stability are compromised. To address these critical issues, in this work, the Bimetallic-LDH/MXenes nanosheet composites with strong contact b/w MXenes nanosheets. However, MXene sheets that are negatively charged will offer lots of heterogeneous nucleation sites for Bimetallic-LDH during the in-situ crystallization process, and the surface functional groups can enhance the chemical bond between MXene and Bimetallic-LDH compared with Composite of MXene and Bimetallic-LDH. Therefore, this bimetallic LDH/ MXenes electrode shows a good specific capacitance of 1853 Fg^{-1} at 1 Ag^{-1} with capacitance retention 86% retention of capacitance after 10,000 cycles. This planar supercapacitor device is a new strategy to fabricate the stretchable micro-supercapacitor devices for wearable electronic applications.



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B 016

Mesoporous, Anti-Corrosive RuO_2 thin films prepared by Ultrasonic Spray Pyrolysis for Supercapacitor Application

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ABSTRACT

Ultrasonic spray pyrolysis technique used for preparation of RuO_2 thin films on stainless steel substrate for different decomposition temperatures (K). $RuCl_3.nH_2O$ (0.003M) as a precursor, dissolved in propanol medium. All deposited samples exhibit amorphous nature as indorses by XRD analysis. Pristine RuO_2 phase formation was confirmed by Raman spectrum. Surface morphological evaluations like SEM and HRTEM elucidates the formation of uniform, meso porous, nano flex like morphology. The morphological outcomes reveals that the interconnected porous nano flex morphology offers large surface area for electrochemical activities as compared to dense, flat, bulky morphology. Wettability glimpses exhibit hydrophilic nature of the deposit. BET analysis shows mesoporous architecture. Pristine RuO_2 phase formation confirms by XPS spectrum. Electrochemical studies of RuO_2 were carried out in 0.5 M H_2SO_4 electrolyte for all electrodes. Optimized RT_4 electrode shows 1889 F/g SC at 2 mV/s scan rate. Achieved highest specific energy, power and columbic efficiency (h) obtained by charge-discharge methods were 65.27 Wh/Kg, 99.66 KW/Kg and 86.42% respectively. The observed very less rate of corrosion is~ 0.1005 (mm/year).

Keywords: *Mesoporous (RuO_2), Ultrasonic spray; HRTEM; XPS; Supercapacitor; Anticorrosive, Energy and power.*

B 017

The $CuFeP_2O_7$ Composites for High-Performance Supercapacitor Applications

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ABSTRACT

Recently transition metal pyrophosphates have gained wide attention for supercapacitors and catalyst applications owing to their highly stable structure, and excellent capacitance. The effects of different precursor concentrations on the microstructure and the electrochemical properties of the hydrothermally deposited $CuFeP_2O_7$ electrodes were investigated. With the increase in Cu, Fe, and P concentrations morphology of the electrodes altered from unevenly shaped structures to circular granules. The optimum $CuFe(P_2O_7)$ electrode reveals an encouraging capacitance of 1609 mF g^{-2} (192.84 Fg^{-1}) at 3 mA cm^{-2} and a wonderful rate capability. The optimized $CuFe(P_2O_7)$ electrode delivers high energy and power densities with 70% stability over 5000 cycles. The encouraging electrochemical activity of $CuFeP_2O_7$ can be correlated to the low impedance and high ECSA. This simple economic approach can offer a viable tactic for transition metal pyrophosphates for high-performance multifunctional applications.

B 018

Reduction of Graphene Oxide Through Microwave Assisted Hydrothermal Method

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ABSTRACT

The ever-growing need in the production of graphene and graphene-based systems demands a much shorter and briefer synthesis technique. Herein we adopt microwave assisted hydrothermal method for the reduction of graphene oxide (GO) rather than time-consuming reduction procedures. An improved Hummer's method is used for the synthesis of GO eliminating the usage of toxic $NaNO_3$. From the prepared GO, reduced graphene oxide (rGO) was obtained via microwave assisted hydrothermal method. The as prepared synthesis procedure is much more transient than other traditional procedures. Different characterization techniques such as XRD, Raman spectroscopy and UV-Vis spectroscopy were carried out to elucidate the structure of rGO. There electrochemical analysis was also carried out. In comparison to other existing techniques like chemical and thermal treatments, microwave assisted hydrothermal synthesis method is found to be facile and efficient.

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B 019

Enhancing Bifunctional Strontium Ferrite ($SrFe_2O_4$) for Energy Storage Applications

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ABSTRACT

Bifunctional materials have gained significant attention in recent years due to their versatile applications in energy storage and conversion [1-3]. Strontium ferrite nanoparticles (NPs) have outstanding magnetic and electrochemical characteristics due to their exceptional physical and chemical properties [4-5]. In this study, the development of low-cost and highly efficient electrode materials for electrochemical energy storage applications. Magnetic and chemically stable catalysts of $SrFe_2O_4$ ferrite NPs were prepared by the simple co-precipitation method. The prepared $SrFe_2O_4$ ferrite NPs were characterized by powder X-ray diffraction (XRD), energy-dispersive spectroscopy (EDS), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy and vibrating the sample magnetometer (VSM). The $SrFe_2O_4$ electrode exhibits a specific capacitance of 363.1 F/g, and excellent capacitance retention was found to be 87.5% after 3000 cycles. The columbic efficiency remained at 95.2% after 3000cycles, which agrees that the $SrFe_2O_4$ electrode has superior electrochemical performances.

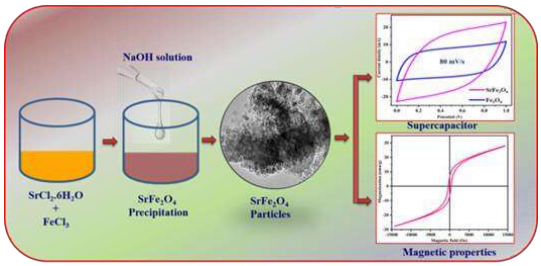

Figure: Schematic diagram of $SrFe_2O_4$ ferrite NPs preparation

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B 020

Scalable Microbial Fuel Cells: Carbon Veil and SS Mesh as Electrodes

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ABSTRACT

Scalability of microbial fuel cells (MFCs) on a large scale depends on the cost of electrodes. To address this challenge, the potential of stainless steel (SS) mesh and carbon veil (CV) as electrodes for MFCs due to their affordability was investigated here. The study aimed to assess the suitability of both materials as anode and cathode viz Carbon Veil-Carbon Veil, Carbon Veil-Activated Carbon Modified Carbon Veil, Carbon Veil-SS mesh, and Carbon Veil-Activated carbon modified SS mesh, with a focus on optimizing the anodic area (5,10 and 20-times cathodic area), which was found to significantly impact system performance. Electrochemical characterization of these electrodes in glucose medium revealed highest anodic peak current for CV (1.2 A/m^2), indicating its suitability as anode material. Performance studies showed that the Carbon Veil-Activated carbon modified SS mesh system gave the highest current and power density with values 0.7 W/m^3 and 0.06 A/m^2, respectively. Furthermore, an increase in anodic area enhanced MFC performance, with the maximum power density observed at an anode/cathode area of 20, corresponding to 1.2 W/m^3. When the MFC system was fed with real-time kitchen wastewater (KWW), a maximum power density of 0.83 W/m^3 was achieved, confirming its suitability for real-time wastewater treatment. The COD removal efficiency of system in different cycles of run were 89.4±6.6 %. Overall, this study highlights the potential of utilizing low-cost electrodes, such as SS mesh and carbon veil, to enhance the scalability and practicality of MFCs for real-time application.

Keywords: microbial fuel cell, anode, carbon veil, scalability, power density.

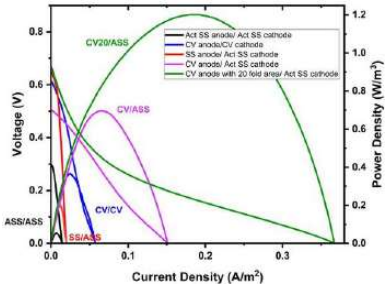

Figure Comparison of MFC performance for various electrode combinations

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B 021

Vanadium-Substituted Phosphomolybdic and Tungstic Acids Combined with Polypyrrole Using Pyridinium and Ammonium Linkers for Electrochemical Electrodes

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ABSTRACT

High-performance energy storage devices have emerged as a favored choice owing to their remarkable efficiency, sustainability, and environmental friendliness. Nowadays, polyoxometalate-based supercapacitor electrode materials have gained much attention. Here, we have reported a few new POMs combined with ionic liquids were incorporated in conducting polymer electrode materials to get enhanced high-energy, long-life electrochemical storage devices. The $H_6[PV_3Mo_9O_{40}].34H_2O$ (PV_3Mo_9) and $H_6[PV_3W_9O_{40}].34H_2O$ (PV_3W_9) POMs were treated with tetrabutylammonium chloride (TBA) and 1-Butyl-4-methyl pyridinium chloride (BMP) and finally combined with polypyrrole for the supercapacitor studies. An extensive array of analytical techniques was employed to delve into the interplay between the constituents within the composite materials, such as FTIR, PXRD, TGA, NMR (^1H and ^{13}C), FESEM, EDS, XPS, and BET. The electrode material PV_3W_9-BMP-PPy shows a specific capacitance of 294.79 Fg^{-1} and an energy density of 28.89 $Whkg^{-1}$ at 1 current density in 0.25 M H_2SO_4 medium followed by an excellent cycle life of 78.6% after 10000 gcd cycles. The fabricated supercapacitor device is performed to light up the bulbs of red, yellow, and green LEDs for 50, 30, and 28 seconds, respectively.

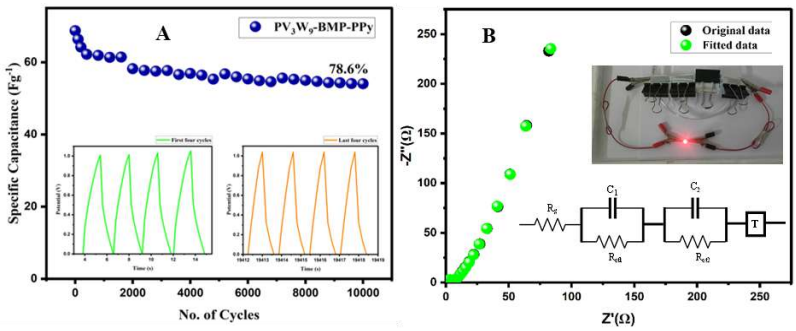

Fig. 1: (A) Cycle stability of PV_3W_9-BMP-PPy (B) Nyquist plot with the circuit diagram of PV_3W_9-BMP-PPy and the fabricated cell for lighting bulb.

B 022

A Heterostructured VS_2/Sb_2S_3 Material as Anode for Lithium Ion Battery

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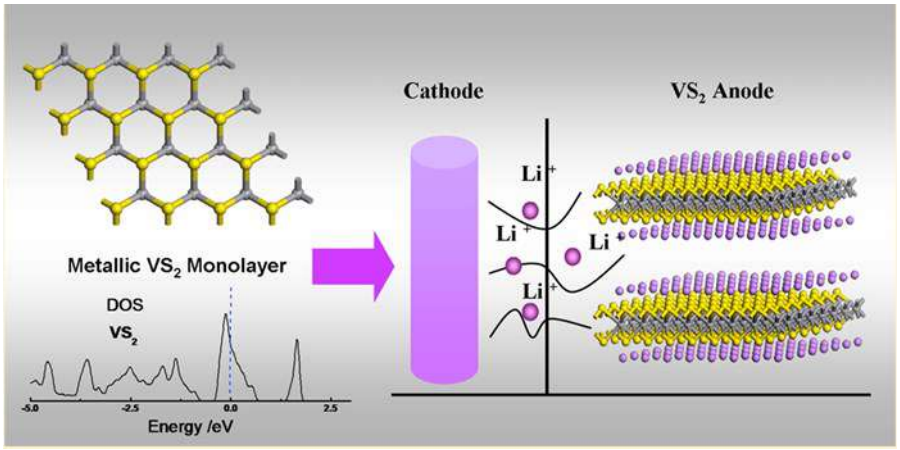
ABSTRACT

Lithium-ion batteries (LIBs) have revolutionized rechargeable mobile electronic technology, such as electric vehicles, laptops, and mobiles. However, there are issues with efficiency, stability, and high-power delivery, which require further research. The "Rocking Chair" mechanism, which involves intercalation-deintercalation, affects the stability of electrodes during charge-discharge. Transition metal dichalcogenides (TMDs) are two-dimensional (2D) materials are known for their stability and electrical properties with 6-7 stacked layers, where each layer is hexagonally packed by transition metal atoms and surrounded by chalcogens bounded by weak Van Der Waal's forces. In this work, VS_2 was chosen as the TMD due to its excellent cyclic stability, large interlayer spacing (0.69 Å) for Li^+ ion intercalation and higher capacity as compared to other counterparts. However, achieving few-layered VS_2 nanostructures without a support substrate is difficult due to self-restacking and monolayer degradation. To overcome these limitations, VS_2/Sb_2S_3 heterostructure material was synthesized and tested as an anode material. The material was characterized and fabricated in coin cells using the testing material as an anode.



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B 023

Synergistic Effects of Manganese Molybdates Incorporated Graphitic Carbon Nitride as Electrode Material for a Solid-State Symmetric Supercapacitor

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ABSTRACT

In this study, the hydrothermal method was used to manufacture homogeneous $MnMoO_4$ rhombohedral-shaped nanoparticles covered by g-C_3N_4 nanosheets[1,2]. The electrochemical characteristics of pristine $MnMoO_4.H_2O$, $MnMoO_4$, g-C_3N_4, and $MnMoO_4.H_2O$/g-C_3N_4, $MnMoO_4$/g-C_3N_4 composite materials were analyzed. Fundamental characterizations such as X-ray diffraction, Fourier transform infrared (FTIR) spectrometry, and Raman spectroscopy were employed to confirm the physical and chemical properties of the materials. Field-emission scanning electron microscope (FE-SEM) revealed a well-grain boundary $MnMoO_4$ with a rhombohedral structure and the composite was covered by g-C_3N_4 nanosheets[3]. The as prepared $MnMoO_4.H_2O$, $MnMoO_4$, and $MnMoO_4.H_2O$/g-C_3N_4, $MnMoO_4$/g-C_3N_4 composite materials showed specific capacitance of 282.7 F/g, 590.23 F/g, 1072.98 F/g, and 1441.4 F/g at 1 A/g, respectively. Based on our findings, $MnMoO_4$/g-C_3N_4 can be considered as a potential electrode material for supercapacitor applications. Furthermore, two identical electrodes of $MnMoO_4$/g-C_3N_4 sandwiched between the polymeric gel electrolyte (PVA-KOH) were used to construct the solid-state symmetric supercapacitors (SSCs).

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B 024

Influence of Acid Strength on the Supercapacitive Properties of Hydrothermally Synthesized α-MoO_3

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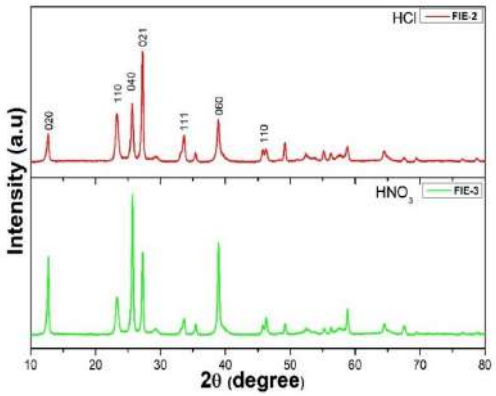
ABSTRACT

α-MoO_3 was successfully synthesized by hydrothermal method using ammonium hepta molybdate and different mineral acids as the starting materials. Conc. HNO_3 and Conc. HCl with different acid strengths were used for the synthesis. In all cases, formation of orthorhombic α-MoO_3 phase with different morphology was observed. Other polymorphs such as h-MoO_3 and β-MoO_3 were not observed. The obtained products were characterised using a variety of techniques such as PXRD, IR, SEM, TEM and BET. The supercapacitor performance was investigated using Cyclic Voltametry (CV), Galvanostatic Charge Discharge (GCD) and Electrochemical Impedance Spectroscopy (EIS) techniques in three electrode configurations. Specific capacitance varied with nature and strength of the acid used. High specific capacitance of 1235 F/g was obtained at a current density of 1 A/g under optimum conditions.



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B 025

Correlating the Properties of Li_2O Doped Barium Vanadate Glasses for Li-Ion Battery Application

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ABSTRACT

Novel glass system of composition $60V_2O_5$- (40-x) BaO-xLi_2O with x=10, 15, 20, 25(mol%) were prepared using conventional melt-quench technique. The glass transition temperature (T_g) exhibited a continuous decrease in T_g with an increase in Li_2O concentration. The thermal activation energy (E_g) calculated using the Kissinger equation[1,2] was related to the fragility parameter F. Investigation of the thermal and physical properties elucidated an increase in the number of non-bridging oxygen (NBO). The interpretation of obtained IR spectra using Fourier Transform Infrared Spectroscopy[3] gave an insight into the structural units present in these glasses. IR study also confirmed the increase in these NBO with increasing Li_2O. The conductivity studies done using Jonscher's power law[4,5] showed an increase in conductivity with increasing Li_2O. The cyclic voltammograms of best glass showed good reversibility with anodic peak intensities higher than the cathodic peaks. This study helps in understanding the vital role that Li_2O plays in the structural network of glass and in determining its properties. This kind of study is useful in further understanding the application of these glasses as electrodes for Li-ion batteries.

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B 026

Hierarchical Self-Assembly of CoFeOOH Nanoparticles on Nickel Foam: Highly Active and Ultra-Stable Electrocatalysts for Overall Water Splitting

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ABSTRACT

The green hydrogen production faces the challenge of developing efficient, low-cost electrocatalysts to meet society's current energy needs. The two essential approaches for improving their catalytic activity are increasing the number of active sites by modifying their shape and structure and increasing the reactivity of active sites by including additional components. In the present work, by merging these two approaches, a unique three-dimensional hierarchical self-assembled cobalt iron oxyhydroxide layer on the nickel foam (CoFeOOH@NF) was successfully prepared by a one-step alcohothermal method and served as a working electrode. The CoFeOOH@NF electrode delivers a prominent performance that requires an overpotential of 250 and 135 mV at 10 mA/cm^2 for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in 1M KOH, respectively. Tafel and electrochemical impedance spectroscopy further reveal favourable kinetics during electrolysis. The CoFeOOH@NF//CoFeOOH@NF electrodes used in the water electrolyzer need 1.62 V at 10 mA cm^{-2}. Moreover, the strategy and synergistic effect of the iron can also be used to prepare other bifunctional and cost-efficient electrocatalysts for various applications.

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B 027

Surface Modification of One Step Facile Synthesis Ni_3S_2/MoS_2/rGO Direct Grown on Ni-Foam as Binder Free Electrode for Ultra-High Supercapacitor with Better Cyclic Performance

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ABSTRACT

Supercapacitor used to achieve sustainable very high-capacity production because of composition and microstructure for enhancing the specific capacity, rate capability and cycle stability of electrode materials in energy storage applications. Herein direct growth of surface modified hierarchical Ni_3S_2/MoS_2/rGO hybrid nanomaterial on Ni foam was successfully synthesized by a one-step hydrothermal technique. Furthermore the structural, morphological, elemental composition and electrochemical properties of as synthesized electrode materials were analyzed. The as synthesized Ni_3S_2/MoS_2/rGO composite electrode delivers a very high specific capacity 2580F/g at 1A/g and excellent cycling stability 100% capacitance retention after 10000 charge-discharge cycles with specific capacitance 600F/g at current density 20A/g. In addition, the assembled two electrode symmetric system showed high specific capacity 100.26 F/g @1A/g and superior energy density of 112.79 Wh/kg with corresponding power density of 2699.82 W/kg @ 1A/g. The results provided that the surface modification of Ni_3S_2/MoS_2/rGO direct grown on Ni foam without added any external nickel sources and binding polymer were an ideal candidate for supercapacitor applications.

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B 028

Incorporation of f–MWCNTs with ZnCo2O4 Nanoparticles as an Effective Counter Electrode For Dye-Sensitized Solar Cell (DSSC) Application

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ABSTRACT

Dye-Sensitized Solar Cells (DSSCs), consisting of a photoanode, dye molecules, an electrolyte, and a counter electrode (cathode), have traditionally played a significant role in third-generation solar cell technology. One of the key components of DSSCs is the counter electrode, with Platinum (Pt) being the most commonly used material due to its outstanding catalytic activity, excellent electrical conductivity, and stability. However, the high cost, limited availability, and susceptibility to photo-corrosion of Platinum make it imperative to seek alternatives. In recent times, bi-metallic oxide materials have emerged as promising candidates, exhibiting remarkable electrocatalytic activity and electrical conductivity. Among the various materials, the $ZnCo_2O_4$ is selected due to its excellent electrocatalytic activity and stability. Another crucial criterion for the selection of materials in DSSCs is their electrical conductivity. Therefore, it is essential to identify a suitable material that can augment the electrical conductivity of the $ZnCo_2O_4$ compound. Due to its expansive specific surface area, excellent electron conduction properties, and remarkable flexibility, carbon-based materials 1D Multi-Walled Carbon Nanotubes (MWCNTs), characterized by their high electron mobility and large surface area, present a superior option for incorporation into the $ZnCo_2O_4$ network. However, it's important to note that untreated MWCNTs, in their pristine state, exhibit insolubility, which can potentially impede device performance. To address this, an acid treatment process is employed on the MWCNTs. The synthesis of both $ZnCo_2O_4$ and $ZnCo_2O_4$/f-MWCNTs nanocomposite is accomplished through a straightforward hydrothermal method, followed by a comprehensive investigation of their properties and performance.

B 029

Enhancing the Performance of MA-Based Perovskite Solar Cells via Polymer Additive

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ABSTRACT

The efficiency of $MAPbI_3$ perovskite films is often attributed to their strong crystallinity and controlled morphology. However, the susceptibility of these films to environmental changes can potentially affect both their performance and marketability. A polymer additive approach has been used in perovskite precursors via the one-step spin coating method. The polymer-added perovskite film shows an improved morphology, high crystallinity and fewer defects compared to the pristine film. These properties generate more charge carriers and suppress the recombination rate, enabling the perovskite film quality. The fabricated hole-transport-free carbon-based perovskite solar cells show higher power conversion efficiency (~11 %) than the pristine devices. Moreover, these films show higher open-circuit voltage than the pristine device. The perovskite films that have been enhanced with polymers exhibit remarkable resistance to moisture, and they also maintain around 85% of their original device performance even after 10 days, which is comparable to the performance of devices without any enhancements. Hence, the additive approach method provides a way to open the door for the commercialization of the perovskite PV market.

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B 030

Advancement in Electrocatalytic Water Splitting Performance: Hybrid Core-Shell Heterointerface

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ABSTRACT

Recently, electrocatalytic water splitting has paved a great interest in fostering green energy production. The state-of-art for the first time we have synthesized different hybrid core-shell architectures for the electrolyzer application. Compositional analysis endorses the formation of core-shell heterointerface with targeted elements. Herein, core-shell CuAlS@MnCo-LDH architecture delivers excellent HER and OER performance with a low overpotential of -199 mV, and 133 mV respectively to produce a current density of 10 mA cm^{-2}. The obtained HER, and OER overpotentials are comparable or even superior than the recently reported core-shell materials. The exceptional electrocatalytic performance can be credited to “honeycomb-like structures-on-spherical crystallites” which allows easy and fast diffusion of electrolyte ions and electron transport promotes gaseous product releasing, and results in improvements in EC activity. Further, the core-shell CuAlS@MnCo-LDH-based electrolyzer works on very low potential (1.553 V) with outstanding long-term stability (only 1% decay) after 50 h at a current density of 10 mA cm^{-2}. Thus, such a facile synthesis strategy for the growth of hierarchical core-shell nano architectures displays reduced overpotentials and remarkable stability toward both OER and HER in an alkaline medium, consequently operating as a versatile electrode for efficient overall water splitting.

B 031

Incorporating Carbonaceous materials (G,GO,rGO) for enhanced color modulating Supercapacitor

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ABSTRACT

The demand for energy storage electrochromic indicator is increasing due to its ability to address the current societal environmental pollution and energy problems. A certain type of materials called as electrochromic[1] active material has the capacity to change its color or optical characteristics when a slight bias is applied. Additionally, these active materials have the capacity to hold charge on their own. The ability to store charge along with electrochromic property make it suitable for multiple functions. Various active materials such as polymers[2] (poly(3-hexyl thiophene), polypyrrole, etc), metal oxides[3] (tungsten oxide, cobalt oxide, etc) shows significant optical change along with supercapacitive property. Nickel oxide (NiO) is one such material which shows electrochromic property along with supercapacitive nature[4]. In this article, NiO is used as active material, synthesised by simple spin coating method whose performance has been improved further by doping it with three different carbonaceous substances: graphene, graphene oxide, and reduced graphene oxide having nano flakes dimensionality as confirmed by SEM micrographs. Further, symmetric solid state electrochromic indicative supercapacitive device has been fabricated, which shows the suitability for real life application. Overall, the doping of carbonaceous materials in electrochromic indicative supercapacitive device enhances its performance.

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B 032

Rapid Reflux Synthesis of Manganese Dioxide Nano crystallites for Supercapacitor Application

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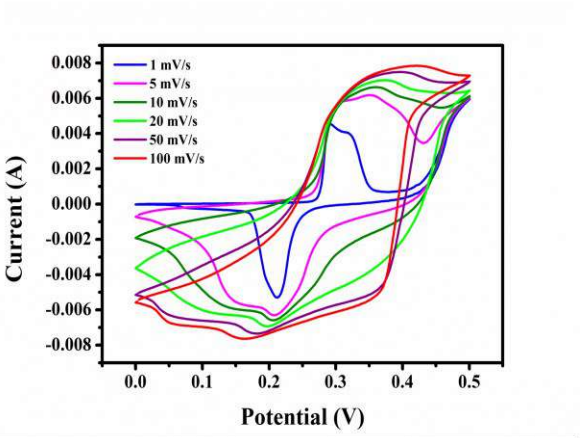
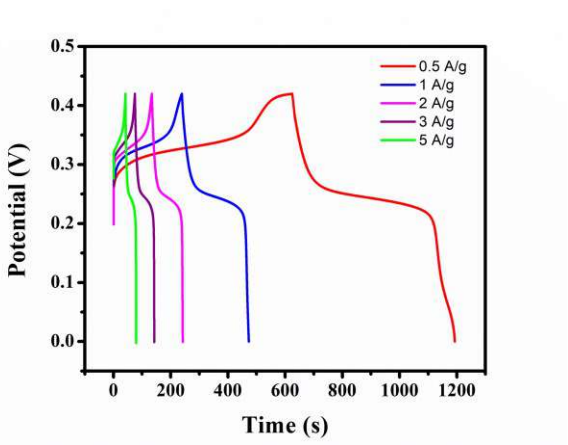
ABSTRACT

A growing attention has been paid to nanostructured manganese oxides as emergent energy materials because of their natural abundance, low cost and environmental friendliness. Herein, we synthesized nanoscale MnO_2 crystallites by a simple and rapid reflux method. The structural and morphological properties of the synthesized material were characterized via XRD, FT-IR, FE-SEM and BET measurements. The MnO_2 coated nickel foam was fabricated in a three-electrode configuration and the electrochemical properties were examined via CV, GCD and EIS methods. The prepared MnO_2 nanocrystallites exhibited a high gravimetric capacitance of ~675 Fg^{-1} at a current density of 0.5 Ag^{-1} in 3M KOH aqueous electrolyte and showed negligible decline in the capacitance after 5000 GCD cycles.





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B 033

Nickel-Doped Cobalt Spinel Ferrite-Based Nanomaterial with Activated Carbon for Energy Storage Devices

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ABSTRACT

$Ni_xCO_{1-x}Fe_2O_4$ was synthesized using double distilled water (x= 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 1) through the Sol-Gel Auto Combustion method. Different techniques were employed to investigate the effect of Nickel-Cobalt ferrite [1]. Using VSM, magnetic properties such as Coercivity, Magnetic remanence, Saturation Magnetization, etc. were studied. The crystallite size was calculated from the Debye Scherrer equation [2], varies from 22 to 32 nm. The XRD pattern confirms single-phase cubic with crystalline planes 220, 311, 222, 400, 422, 511, 440. The morphological observation was conducted through SEM (x=0.3). The FTIR technique was utilized to analyze the presence of functional groups, stretching, and vibrational modes [3]. The energy band gap was calculated from absorbance spectra using Tauc's relation [4]. The electrochemical properties were investigated by cyclic voltammetry, galvanostatic charge-discharge, electrochemical impedance spectroscopy in an aqueous electrolyte-1M Na_2SO_4 [5]. The results suggest that Nickel-Cobalt ferrite with activated carbon enhances specific capacitance. Notably, $Ni_{0.3}CO_{1-0.3}Fe_2O_4$ showed a remarkable specific capacitance of 564 Fg^{-1} at current density 1 Ag^{-1}. The cycling tests operated at potential window of -0.1 to 0.8 V suggesting that electrode had excellent cycling performance.

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B 034

Exploring the Utilization of Morton Fractals in Micro-Supercapacitor Design: A Simulation Study

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ABSTRACT

Micro-supercapacitors (MSC) have garnered widespread attention for their exceptional attributes, including high specific capacity, formidable power density, extended cycle life, economic efficiency, environmental compatibility, heightened safety, and rapid charge/discharge capabilities. Serving as robust reservoirs of electrical energy, supercapacitors demonstrate precise and swift power release, positioning them as versatile solutions seamlessly integrated into a diverse spectrum of applications. Concerted efforts have been dedicated to the meticulous design of flexible and scalable supercapacitors, aiming for seamless integration into a diverse array of applications, encompassing wearable electronics, energy storage systems, and electric vehicles. Recent scientific inquiries have systematically explored an innovative architectural approach known as fractal electrode design. This sophisticated technique strategically augments the effective surface area of the electrode-electrolyte interface with the primary objective of optimizing capacitance—a focused and nuanced advancement in the field. This research delves into the profound influence of device architecture on the energy storage capacity of Morton Fractal-based electrodes. Simulations employing COMSOL Multiphysics are conducted, and the subsequent analysis, including cyclic voltammetry, galvanic charge-discharge techniques, and electric field distribution, elucidates performance metrics. The outcomes reveal superior power and energy densities compared to traditional non-fractal supercapacitors and elevated specific capacitance figures. These findings underscore the potential for enhanced supercapacitor performance by strategically incorporating Morton Fractal-based electrode architectures.

Keywords: *Micro-supercapacitors, COMSOL, Morton fractal, electrode-electrolyte*

B 035

Electrocatalytic Synthesis of Ammonia using Reduced Graphene Oxide (rGO)/ Nickel Foam (NF) Heterostructures

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ABSTRACT

Frequent global energy demand and dwindling fossil fuel resources are the major causes of concern for sustained economic prosperity. In this regard, water splitting is considered a novel platform for the production of hydrogen as a green and clean fuel owing to net-zero CO2 and carbon emissions thus making it a more sustainable and greener alternative fuel of the future. Besides this, hydrogen storage system is also a complex problem. Hence, the smart swift of electrocatalytic (EC) nitrogen reduction reaction (NRR) appears to be a game-changer in the futuristic alternative energy career approach and the ample scope for the development of electrocatalysts for large-scale implementation of this technology. In the quest for suitable catalyst materials, we have integrated reduced graphene oxide (rGO) on nickel foam as an efficient electrocatalyst that is rich in active sites, minimizes the energy barrier at the limiting reaction step (N→NH*), and enhances the binding affinity of N2. Nickel foam is an ideal electrocatalyst for NRR due to its multifaceted properties as a three-dimensional interconnected conductive matrix and easy electrolyte permeation. Besides, the energy conversion efficiency can be increased further by depositing co-catalyst material. Typically, platinum, ruthenium, iridium and other noble metals are extensively used as co-catalysts. However, the noble metal electrodes have significantly hindered their commercial viability due to high cost and limited availability. In that context, to improve the characteristics of the nickel foam catalyst, we anchored rGO on the nickel matrix as an efficient co-catalyst. The selectivity, stability and reproducibility of electrocatalysts were carried out for long-term chronoamperometry analysis. Further, the ammonia yield and Faradaic efficiency and its electrochemical properties will be presented in detail.

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B 036

Transition Metal Nanomaterials Dispersed Nickel Oxides Nanostructures for Enhanced Oxygen Reduction Reaction

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ABSTRACT

Highly efficient oxygen reduction reaction (ORR) electrode materials are vital for energy technologies and the significance of ORR in developing fuel cells and batteries. Despite the significant developments in finding effective catalysts, the reasons for the higher activity rate in alkaline conditions remain undefined [1]. Over the last several decades, substantial research efforts have been addressed to enhance ORR activity by improving various transition metal nanomaterials [2]. In the present work, the uniform dispersion of gold nanostructures on nickel oxide nanomaterials is developed using a galvanic replacement reaction (GRR) for the oxygen reduction process under an alkaline electrolyte. The bimetallic and core-shell nanostructures with low quantity of precious metal concentrations may also be applied in ORR. The electrocatalytic activities of the as-prepared electrodes are tested towards ORR using several electrochemical techniques such as cyclic voltammetry, linear sweep voltammetry, chronopotentiometry, etc.

Keywords: *Oxygen reduction reaction, Transition metals, Nickel oxide, Electroless deposition, Fuel Cells.*

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B 037

Solvent-Mediated Spray Pyrolysis of 2D Vanadium Oxide Nanostructures for High-Performance Energy Storage Applications

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ABSTRACT

Solvent-mediated spray pyrolysis (SMSP) is a versatile technique for synthesizing a wide range of nanomaterials, including 2D vanadium oxide nanostructures. In SMSP, a precursor solution is sprayed onto a heated substrate, where the solvent evaporates and the precursor decomposes to form the desired nanomaterial. The use of a solvent in SMSP offers several advantages, including improved control over the morphology and size of the nanostructures, as well as the ability to synthesize nanomaterials on a variety of substrates. In this study, SMSP was used to synthesize 2D vanadium oxide nanostructures for high-performance energy storage applications. The precursor solution was prepared by dissolving 0.05M ammonium metavanadate (NH_4VO_3) in 50 ml of different solvents like methanol, ethanol and propanol. The precursor solution was then sprayed onto a heated (at 673K) stainless steel (SS 304) substrate using an automatic spray nozzle with compressed air as a carrier gas at a flow rate of 10 L/min. The solution spray rate was constantly maintained at 10 ml/min, and the nozzle-to-substrate distance was optimized to be 30 cm. The synthesized 2D vanadium oxide nanostructures were characterized using a variety of techniques, including physical and electrochemical techniques. The XRD results confirmed the formation of a tetragonal crystalline structure of 2D vanadium oxide nanostructures. The SEM images revealed that the nanostructures were sheet-like in morphology with a thickness of a few nanometers. The electrochemical properties of the 2D vanadium oxide nanostructures were evaluated using a standard three-electrode system at 1 M Na_2SO_3 electrolyte. The nanostructures synthesized using methanol solvent exhibit a high specific capacitance of 721.28 F/g at a scan rate of 5 mV/s as compared to the others. The nanostructures also exhibited good long-term cycle stability, retaining over 90% of their initial capacitance after 3000 cycles. The high specific capacitance and good capacitance retention after a large number of cycles feature the 2D vanadium oxide nanostructures as promising electrode materials for high-performance energy storage devices.

Keywords: Solvent-mediated spray pyrolysis, 2D vanadium oxide, high-performance energy storage.

B 038

Synthesis and Electrochemical Characterizations of RGO-Decorated MnO_2 Nanorods Electrodes for New Generation Wearable Symmetric Supercapacitor Devices

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ABSTRACT

Flexible RGO-decorated MnO_2 nanorod electrodes were synthesized using two step method on a carbon cloth substrate. Initially, the MnO_2 electrode material was deposited onto the CC substrate using the hydrothermal method. Then, RGO was deposited on the surface of the MnO_2 using a simple ex-situ method. The influence of different GO concentrations on the structural, morphological and electrochemical properties of MnO_2 electrodes has been systematically investigated by using various physical and electrochemical characterization techniques. The RGO-decorated MnO_2 electrode with 20 mg/100ml concentration of GO exhibited the maximum specific capacitance of 1072.28 F/g at a scan rate of 5 mV/sec in 1M Na_2SO_4 electrolyte. The electrode also exhibits good long-term cycle stability, with retaining over 87% of initial capacitance after 2000 cycles. For practical application purposes, a symmetric prototype supercapacitor device has been fabricated using symmetric electrodes and an aqueous electrolyte. The symmetric device shows promising electrochemical properties. These outstanding structural, morphological and electrochemical properties of RGO-decorated MnO_2 nanorod grown on the CC substrate make them superior electrode materials for the next generation of wearable energy storage applications.

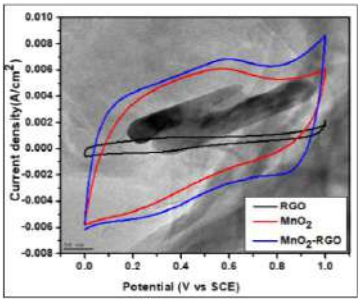

Fig.: Graphical abstract illustrating TEM image of RGO-decorated MnO_2 and combined CVs of RGO, MnO_2 and RGO-decorated MnO_2 electrodes at a scan rate of 5 mV/sec.

B 039

Improving HER Catalytic Activity of Triangulene GQD through P-Block Dopant: Insights from a DFT Study

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ABSTRACT

The hydrogen evolution reaction (HER) is a crucial electrochemical process for sustainable energy applications[1]. Triangulene Graphene Quantum Dots (T-GQDs) is known for its unique electronic and structural properties [2][3] making it an intriguing candidate for catalytic applications. We investigate the HER activity of pristine T-GQD and with dopants[4] like B, N, Si, P, and S using Density functional theory (DFT) simulations. All positive frequencies of obtained IR spectra, indicate the stability of pristine and doped T-GQD. The study of binding energy, structural alterations, Mulliken charge transfer, and changes in the PDOS reveals the interaction between an adsorbed hydrogen (H) atom and the T-GQD. The volcano plots represent the exchange current density as a function of Gibbs' free energy (G_H). For Volmer reaction, the ΔG_H are essential during the primary H-atom adsorption preferable to be near to Zero. However, during secondary H adsorption, the evolution of H_2 molecules is observed via the Volmer-Tafel (VT) reaction or Volmer-Heyrovsky (VH) reaction. Pristine Triangulene is not an ideal candidate for HER, given the high ΔG_H (-1.35 eV) and strong adsorption energy (-1.59 eV). However, the Volmer Gibbs free energy is lowered with considered dopants. We observed the evolution of H_2 molecules dominantly with VH mechanism for B, S, and Si-doped T-GQD, with ΔG_{HV} values of 0.21 eV, -0.46 eV, and -0.06 eV, respectively. On the other hand, N and P-doped T-GQD display -0.11 eV and -0.15 eV ΔG_{HV}. These results imply that the HER activity of T-GQD increases upon doping.

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B 040

Tunable Organic Dye with Binary Metal oxides for Dye Sensitized Solar Cells (DSSCs)

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ABSTRACT

A photo anode and the binary metal oxides carried by the tunable semiconductor that typically affect DSSC technology. The Dye act as a photoanode, semiconducting was carried by UV-Visible spectroscopy. The photo anode band energy gap is 2.08 eV long electron diffusion length is needed for DSSCs. The film morphology and enhanced charge-carrier transport were achieved in FESEM. The Cyclic Voltammetry carried by HOMO and LUMO energy and the band energy gap is 2.1 eV . The I- V characterized by Open – circuit voltage (Voc), and the Short- circuit current (Isc), Maximum voltage, Maximum Current, fill factor (FF), efficiency are calculated electronic device, the DSSC was able to achieve a cell efficiency of 2.9% using graphene, a photo anode, a counter electrode, and conducting material. Additionally, DSSCs with flexible counter electrodes and photo anodes made of novel materials were created to the efficiency of DSSCs.

Keywords: *Binary Metal oxides, Organic dye, Cyclic Voltammetry, Electronic Device*

B 041

Enhanced Performance of Cu Doped ZnO Nanoflower as Electrode Material For Supercapacitor Application

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ABSTRACT

Supercapacitors, as advanced energy storage devices, continue to be at the forefront of research due to their high power density, rapid charge/discharge capabilities, and long cycle life. In this study, we present the synthesis and characterization of copper-doped zinc oxide (Cu-ZnO) nanoflowers as a promising electrode material for supercapacitor applications. The Cu-ZnO nanoflowers were synthesized via a simple and cost-effective hydrothermal method, incorporating varying concentrations of copper to modulate their electrochemical performance. Structural and morphology analysis such as (XRD, FTIR, SEM, TEM and XPS) and electrochemical evaluation indicate that Cu-ZnO nanoflowers possess promising attributes, including high specific capacitance, excellent rate performance, and long-term cycling stability. These findings suggest that Cu-ZnO nanoflowers hold substantial promise as effective electrode materials in supercapacitor applications, contributing to advancements in energy storage technology.

B 042

Solvent-Free, One-Pot Synthesis of Tungsten Semi-Carbide for Stable and Self-Hydrating Short Side Chain-Based Polymer Electrolyte Membrane for Low Humidity Hydrogen Fuel Cells

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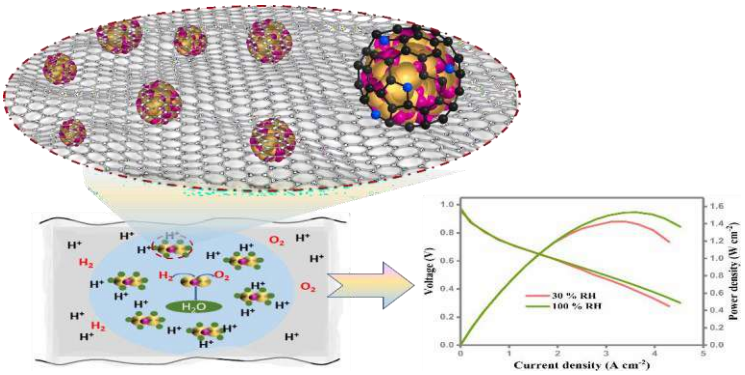
ABSTRACT

Polymer electrolyte membranes (PEMs) enable rapid and selective ionic transport at low relative humidity (RH), crucial for energy conversion devices like hydrogen fuel cells. Herein, we present a facile and solvent free synthesis of tungsten semi-carbide (W_2C@NC) and its incorporation onto short side chain (SSC)-based membrane matrix to facilitate water holding and water-assisted humidification generated by the reaction of cross-over gas molecules. It is demonstrated that addition of W_2C@NC facilitates membrane hydration via in situ water generation thus preventing fuel crossover across the membrane. In addition, W_2C@NC contributes towards low humidity polymer electrolyte fuel cell (PEFC) operation. The study revealed minimal differences in cell performance between fully humidified and low RH conditions for composite membranes, with a noteworthy improvement in performance observed even under completely dry conditions compared to pristine membranes. Apart from good thermal and mechanical stabilities, 81% of initial OCV and 72.86% of current density was retained even after 100 h of accelerated stress test (AST), which opens further perspectives for development of perfluoro sulfonic acid (PFSA) based low RH proton exchange membrane fuel cells (PEMFCs).



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B 043

Fabrication of Laser-Induced Graphene-Based Micro-Supercapacitor with Fractal Architecture

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ABSTRACT

As the electronic market is trending towards portable and miniature devices, it is imperative to design energy storage devices that easily enable on-chip integration. In-plane micro-supercapacitors (MSC) cater to this need with high power density, long cycle lifetime, flexibility and integrability with other circuits. Interdigital electrode design is a widely adopted structure for in-plane micro-supercapacitors. Very little research has been reported about other patterns of electrodes. Here, we report fractal-based electrode designs of micro-supercapacitors fabricated by means of laser inscription. Interdigital and fractal-based (Hilbert, Moore, and Sierpinski) electrode structures are scribed on polyimide film using a laser scribing unit. PVA-H_2SO_4 gel-based electrolyte is coated on the planar electrode structure. The electrode connections are made using copper tape. The performance of the synthesized MSCs is analyzed by means of cyclic voltammetry, galvanostatic charge/discharge and electrostatic impedance spectroscopy. From the analysis, it is seen that the areal capacitance of fractal MSC is higher than that of interdigital MSC. This is attributed primarily to the fringing effect of the electrostatic field in fractal electrode structure. Another reason is the slight increase in the area of the interface between the electrode and electrolyte.

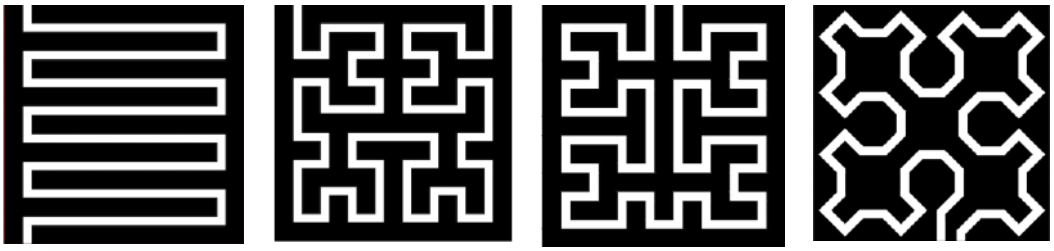

Fig.1. Schematic representation of (a) interdigital (b) Hibert (c) Moore and (d) Sierpinski MSC structure

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B 044

Preparation of $ZnFe_2O_4$/RGO Layered Heterostructures for Symmetric Device Performance Analysis

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ABSTRACT

Composite supercapacitive electrode materials exhibit various advantages in comparison to their individual counterparts. The combined synergistic effect of both individual materials balances their shortcomings and show an improved electrochemical performance. In this work, we have synthesized layered heterostructures of $ZnFe_2O_4$ and RGO on nickel foam via a facile hydrothermal route. The synthesized electrode material shows an exceptional performance with specific capacitance of 1029 F/g. These composite electrodes were then utilized for fabrication of symmetric supercapacitive device. The results obtained indicate that $ZnFe_2O_4$/RGO has a great potential to be employed as a supercapacitive electrode.

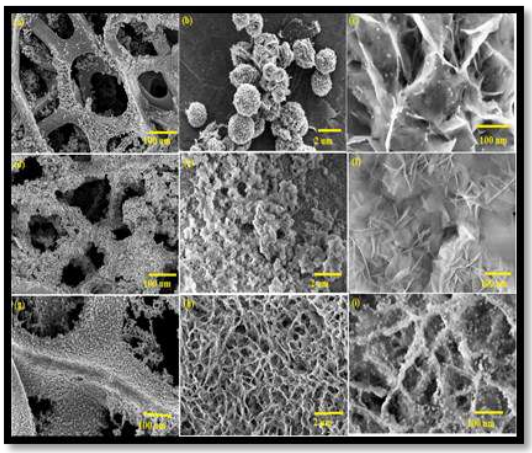

Fig.1. SEM micrographs of $ZnFe_2O_4$/RGO layered heterostructures

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B 045

Hexagonal Iron Phosphide Nanorods for Supercapacitor Utilization: Investigating the Dynamics of Charge Storage

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ABSTRACT

In this work, we have achieved the successful synthesis of iron phosphate through the utilization of a straightforward and cost-effective hydrothermal method. This approach was not only efficient but also environmentally friendly, aligning with the principles of sustainable materials synthesis. Our work involved a meticulous analysis of the resulting material's structural and morphological attributes, which conclusively revealed the formation of hexagonal nanorods of iron phosphate, primarily in the $Fe_2O(PO)_4$ phase. This hexagonal structure is of particular interest due to its potential impact on the material's electrochemical properties. One of the most compelling aspects of our study was the exceptional supercapacitive performance exhibited by the iron phosphate material. It displayed a specific capacitance of 190.58 mF/cm^2 when subjected to a current density of 1 mA/cm^2, emphasizing its suitability for energy storage applications. Additionally, the material demonstrated a remarkable energy density of 2.12 µWh/cm^2 under a power density of 200 µW/cm^2, further highlighting its practical relevance in the realm of energy storage devices. To gain a more profound insight into the electrochemical mechanisms governing this outstanding performance, we conducted a rigorous examination of the charge storage kinetics of the electrode, employing power law equations. This analytical approach allowed us to elucidate the underlying principles responsible for the material's superior capacitive behavior. Furthermore, we transitioned from fundamental research to practical application by fabricating a supercapacitor device and subjecting it to comprehensive electrochemical characterizations. Our findings collectively underscore the substantial promise of iron phosphate as a pivotal material for advanced energy storage applications, with the potential to revolutionize the landscape of energy storage technologies.

Keywords: *Iorn Phosphate, Hydrothermal method, Charge storage kinetics, supercapacitor device.*

B 046

Exploring Supercapacitor Performance of the novel Quaternary CuMnAg-Pd Composite: Emphasizing Charge Storage Kinetics and Performance Assessment

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ABSTRACT

This paper introduces a novel quaternary CuMnAg-Pd material for potential utilization in supercapacitor applications. The CuMnAg-Pd composite was synthesized via a hydrothermal method. The investigation primarily focuses on the comprehensive analysis of the inclusion of Ag and Pd in the CuMn oxide compound. The structural and morphological changes resulting from the introduction of Ag and Pd in the CuMn oxide compound were elucidated through X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses. These characterization techniques revealed the formation of a mixed phase comprising Ag_3O, $Cu_{1.5}Mn_{1.5}O_4$, and PdO compounds. Furthermore, SEM images clearly depicted the transition from nanoworms in CuMn Oxide to nanospheres in CuMn-Ag and nanoplates in CuMn-Pd, culminating in nanoflakes for the CuMnAg-Pd composite. Electrochemical analyses were conducted using a three-electrode system in a 2M KOH electrolyte. Remarkably high specific capacitance (3441.7 mF/cm^2), along with impressive 0.81 mWh/cm^2 energy density at 13 mW/cm^2 power density, was calculated at 20 mA/cm^2 current density. Stability testing was performed over 10,000 cycles, demonstrating a capacitive retention rate of 85%. The exceptional electrochemical performance can be attributed to the enhanced electrical conductivity conferred by the presence of Ag and Pd, which effectively mitigated sluggish electron transfer rates in the CuMnOxide electrodes. Additionally, the electrical double-layer capacitance (EDLC) charge storage mechanism within Ag_3O and PdO compounds contributed to supplementary EDLC-type charge storage. To assess the practicality of this innovative quaternary CuMnAg-Pd electrode material, a supercapacitor device was fabricated, which exhibited highly favourable supercapacitive properties. In summary, this electrode material presents a promising avenue for advancements in the field of supercapacitors.

Keywords: *CuMnAg-Pd composite, Mixed-phase formation, Electrochemical performance, Practicality assessment.*

B 047

Three-Dimensional Porous Graphene Intercalated with the CuFe2O4 Nanowire Architectures for Supercapacitor Applications: Electrode Modification and Its Catalytic Properties

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ABSTRACT

As energy storage devices, supercapacitors have recently attracted a lot of attention due to their unique characteristics. Metal ferrite is a new type of porous material that can have a large pore volume, excellent chemical stability, and a large specific surface area. In this study, one-dimensional $CuFe_2O_4$ nanowires were prepared and pursued by electrospinning methods. Three-dimensional graphene was synthesized by hydrothermal methods. For supercapacitor applications, a three-dimensional graphene oxide/Metal ferrite ($CuFe_2O_4$) nanowires composite was prepared using a simple hydrothermal technique. The structural formation of the prepared materials was used to establish by X-ray diffraction, Raman spectroscopy, Fourier transform-infrared spectroscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and transmission electron microscopy. To examine the electrochemical efficiency of the electrode through cyclic voltammetry (CV), self-discharge, galvanostatic charge-discharge, cycle stability, and electrochemical impedance spectroscopy. The 3DGO/$CuFe_2O_4$ composite-coated Ni-foam electrodes will apply for supercapacitor studies. We exhibited high specific capacitance, current density, and better charge-discharge cycling stability due to the substantial effect of capacitive behavior.

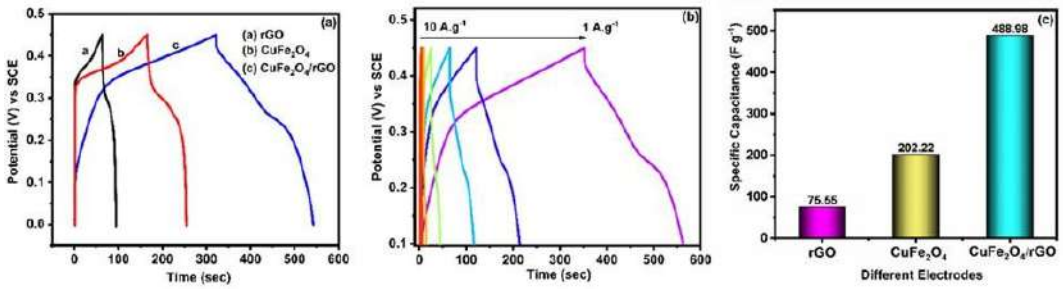

Fig. 1 charge-discharge curves of $CuFe_2O4$, 3D-RGO, and $CuFe_2O4$\|3D-RGO composites, (b) charge- discharge curves of $CuFe_2O_4$\|3D-RGO composites with different current density, and (c) specific capacitance of different electrode materials.

B 048

Bimetallic Iron-Cobalt Phosphide Nanosheets on Nickel Oxide Nanoparticles for Improved Glucose Oxidation Reaction

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ABSTRACT

Glucose fuel cells (GFCs) are chiefly fascinating due to their renewability, non-toxicity, low cost and free availability in plants or by waste biomass conversion. In recent years, GFCs have drawn great attention because they can provide implantable power sources with body fluids. Herein, we demonstrate hierarchical three-dimensional (3D) iron-cobalt phosphide ($Fe_{1-x}Co_xP$) nanosheets on nickel oxide nanoparticles as an electrocatalyst for improved glucose oxidation reaction (GOR) under alkaline electrolyte. The $Fe_{1-x}Co_xP$ nanomaterial-based anode, as it has been synthesized, demonstrates outstanding catalytic activity towards glucose oxidation with a low oxidation potential, high current density, high mass activity, and long-term durability. The $Fe_{1-x}Co_xP$ nanomaterial delivers a higher catalytic current density with a less positive shift, respectively, when compared to FeP, CoP, NiO, and commercial Pt/C electrodes. The Earth-abundant $Fe_{1-x}Co_xP$ nanomaterial's enhanced catalytic activity may be attributed to its unique architecture, which includes a less agglomerated structure, a high electrochemically active surface area (ECASA), a small pore size, combined active sites of iron and cobalt cations, and an environment that is conducive to an enhanced electron transfer process between analytes and electrodes. The current anode material can directly transfer electrons to the electrode surface, eliminating the need for mediators and enzymes.

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B 049

Electrochemical Measurements of Conducting Polymer Hydrogel for Supercapacitor Performance

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ABSTRACT

Due to the high energy crisis, energy storage technologies have been in great demand in this modern society. Among different energy storage devices, supercapacitors have attracted extensive attention from scientists because of their unique features such as fast charge-discharge capability, high power density, ultra-long durability, and environmental friendliness. Conducting polymers have emerged as prominent choices for the high electrochemical performance of supercapacitors. However, due to low mechanical strength and less adsorbing capabilities, suffers from poor cycling stability. To overcome these drawbacks, hydrogel offers a uniform interconnectivity with long mechanical durability. We have synthesized PEDOT: PSS hydrogel with a three-dimensional cross-link network and high swelling ratio allowing fast charge transport of ions during electrochemical measurements. Cyclic voltammetry, galvanostatic charge-discharge, and impedance of PEDOT: PSS hydrogel have been performed. The specific capacitance of PEDOT: PSS hydrogel is significantly higher than pristine PEDOT: PSS with better cycling stability.

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B 050

Synergetic Effects of Biomass Carbon integrated Tungsten Oxide: An Effective Hybrid Cathode for Deep Cyclable Aqueous Zn-Ion Battery

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ABSTRACT

Aqueous Zinc-ion batteries (ZIBs) are considered to be one of the significant candidates for replacing lithium-ion batteries as they are abundant, environmentally safe and cost effective. Tungsten oxide (WO_3) is considered as one of the potential cathode materials for AZIB application. Due to its poor stability and low capacity its battery application is limited. In order to improve the stability of the hybrid cathode, herein we have integrated the biomass derived carbon network with WO_3 (WO_3@C) and designed a deep cyclable Zn-WO_3@C battery. The synthesized hybrid cathode WO_3@C was analyzed through different techniques like XRD (X-ray Powder Diffraction), SEM (Scanning Electron Microscope) and XPS (X-ray Photoelectron spectroscopy). The electrochemical studies were further carried out to check their specific capacity, energy density, power density and capacity retention for about 100 cycles. Thus, this work provides a valuable insight on the fabrication of Zn-WO_3@C AZIB battery that demonstrates a great potential for next-generation energy storage application.

Keywords: *Aqueous Zinc Ion Battery, WO_3, biomass carbon, hybrid cathode.*

B 051

High Performance Proton Exchange Nano Composite Membrane Incorporating Water Insoluble Phosphotungstic Acid- Graphitic Carbon Nitride Nanohybrid for PEMFC

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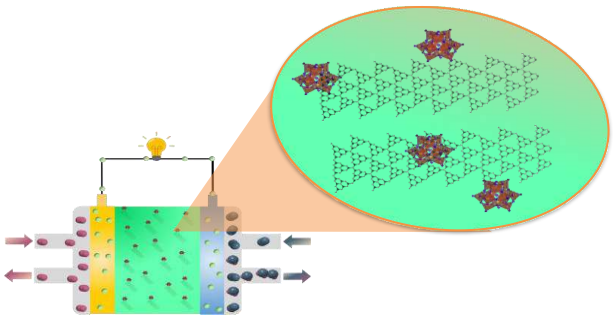
ABSTRACT

The integration of heteropolyacids is a promising avenue for the development of high proton-conducting membranes for energy storage and conversion applications. However, it's important to address the inherent hydrophilicity of heteropolyacids, which can lead to their leaching from the membranes, ultimately decreasing the fuel cell performance. In our research, we successfully crafted a proton-conductive membrane using a water-insoluble hybrid phosphotungstic acid (PCN). To enhance proton transport within the membrane, we introduced these PCN nanohybrids. They played a pivotal role in facilitating proton transport by combining the strong acidity of phosphotungstic acid (PTA) with the establishment of continuous 2D proton transport pathways. Consequently, our membrane exhibited an impressive proton conductivity of 0.228 S cm^{-1} at 80°C under 95% relative humidity. The real impact of our work became evident in the performance of fuel cells equipped with our Aquvion/PCN nanocomposite membrane. We observed a substantial 34% enhancement in fuel cell performance at an operating temperature of 60°C under 95% relative humidity. This improvement signifies a significant step forward in the field of energy conversion and storage.



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B 052

Enhanced Electrochemical Performance of Supercapacitors Using Photothermal Synthesis of Two-Dimensional Molybdenene

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ABSTRACT

Two-dimensional transition metal dichalcogenides (2D TMDs) have gained significant attention in recent years for their exceptional electrochemical properties, which make them promising candidates for supercapacitor electrode materials. Among these materials, molybdenene, a member of the TMD family, has emerged as a particularly intriguing choice for enhancing supercapacitor performance. This research article explores the use of photothermal synthesis as a novel approach to prepare molybdenene-based materials and demonstrates their potential to further improve the electrochemical performance of supercapacitors. The photothermal synthesis method involves the controlled irradiation of molybdenum precursor compounds, leading to the formation of high-quality molybdenene nanosheets. These synthesized nanosheets exhibit remarkable structural and morphological properties, which are essential for efficient charge storage in supercapacitors. The unique structural characteristics of molybdenene, such as a high surface area and excellent electrical conductivity, facilitate rapid ion diffusion and charge transfer, ultimately enhancing the specific capacitance and energy density of supercapacitors. In this article, we discuss the synthesis process, structural characterization, and electrochemical performance evaluation of photothermally synthesized molybdenene-based materials in supercapacitor applications. The results demonstrate that photothermally synthesized molybdenene can significantly improve the charge storage capacity and cycling stability of supercapacitors, making them an attractive choice for next-generation energy storage devices. This research paves the way for the development of advanced supercapacitors with enhanced electrochemical performance, contributing to the ongoing efforts to address energy storage challenges in various applications.

B 053

Formulation of Cobalt Dichalcogenides Nanostructures Electrodes for the Asymmetric Supercapacitor Devices

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ABSTRACT

The rapid development of high-density energy storage devices is highly significance to retort the recent energy storage demand and environmental concerns. The selection of electrode materials portrays extreme impact to improve the supercapacitor electrochemical characteristics. In recent times, two-dimensional metal dichalcogenides are the substantial substituent for supercapacitor electrode device fabrication. This work is targeted to prepare the cobalt-based chalcogenides ($CoTe_2$, CoS_2 and $CoSe_2$) nanostructures electrode material by the one-pot chemical kinetics for supercapacitor devices. The spectroscopic and microscopic studies were exclusively demonstrated the structural and surface properties of prepared $CoTe_2$, CoS_2 and $CoSe_2$. The assembled three-electrode measurement realized the enriched storage behavior with the specific capacitance of 548 Fg^{-1} at 2 Ag^{-1} applied current for the $CoSe_2$ electrode which is greater than its equivalent phase $CoTe_2$ (420 Fg^{-1}) and CoS_2 (363 Fg^{-1}) electrodes. Further, designed asymmetric device using the $CoSe_2$ anode and activated carbon cathode produced a maximum specific capacitance, high specific energy, and valuable retention behaviors.

B 054

Visualization Effect of CeP_2O_7 on The Structural, Thermal, and Transport Properties of NaH_2PO_4

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ABSTRACT

Solid acid composite NaH_2PO_4 /CeP_2O_7 were synthesized and characterized by a different molar ratio of NaH_2PO_4 and CeP_2O_7. The characterizations of the Solid acid composite were observed the thermal stability and conductivity in terms of X-ray diffraction (XRD) analysis, Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-Ray Analysis (EDX), Fourier Transform Infrared Spectroscopy (FTIR), Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA), and conductivity measurements. The amount of SDP, and CeP_2O_7 pressure used for pallet production and operating temperature. The composites powders were to form pellets of 3 mm thickness for conductivity measurement. CeP_2O_7 in the composites has a large effect on the conductivity measurement. The supertonic transition was identified at different temperatures of composites under atmospheric pressure. Thermal stability of the solid acid composites such as the temperature of dehydration, melting, and decomposition was investigated under environments atmospheric humidification.

Keywords: Solid acid composite, conductivity, thermal analysis, dihydrogen phosphate, fuel cell.

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B 055

Effect of Molybdenum Doped Nickel Ferrite for Energy Storage Devices

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ABSTRACT

Nickel molybdenum ferrite, a promising magnetic material, has been synthesized through the sol-gel method and comprehensively characterized using various analytical techniques. X-ray diffraction (XRD) analysis revealed the crystalline nature and crystal structure of the synthesized ferrite [1]. Vibrating sample magnetometer (VSM) was employed to investigate the magnetic properties of the material, unveiling its ferromagnetic behavior with a notable saturation magnetization [3].Ultraviolet-visible spectroscopy (UV) provided insights into the optical properties of the nickel molybdenum ferrite, revealing its wide band gap and potential for optoelectronic applications. Furthermore, Fourier-transform infrared spectroscopy (FTIR) was utilized to explore the vibrational modes and chemical bonding within the material, offering valuable information regarding its structural composition and functional groups. This multi-faceted study sheds light on the structural, magnetic, optical, and chemical characteristics of nickel molybdenum ferrite, paving the way for its potential use in diverse technological applications, including magnetic storage, sensing, photovoltaic devices and energy storage application like super capacitor.

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B 056

Innovative 3D-Based Metal-Organic Framework Used for Energy Storage Application

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ABSTRACT

Metal-organic frameworks (MOFs) are becoming increasingly attractive as electrode materials for supercapacitors because of their distinctive characteristics, including a large surface area, adjustable pore structure, and versatile functions. This article provides a thorough summary of the latest developments in supercapacitors that are based on Metal-Organic Frameworks (MOFs). We explore many approaches to improve the electrochemical efficiency of MOFs, such as modifying the pore structure, introducing heteroatoms, and combining with conductive materials. We additionally emphasize the pivotal parameters that impact the capacitance of electrodes based on Metal-Organic Frameworks (MOFs), including the specific metal ions, organic ligands, and electrolytes. Lastly, we address the obstacles and outlooks of supercapacitors based on MOFs.

Keywords: *metal-organic framework, energy storage, supercapacitor, surface area*

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B 057

Electrochemical Performance of g-C_3N_4 Embedded NiO Nanocomposite Anodes for Lithium-ion Batteries

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ABSTRACT

The combination of two-dimensional layered heterostructures with transition metal oxide electrodes has attracted considerable attention. In this work, facile hydrothermal method is adopted to produce graphitic carbon nitride-embedded Nickel oxide (gC_3N_4-NiO) nanocomposites and tested their electrochemical performance against Li/Li^+ half cells. Formation of gC_3N_4-NiO nanocomposite is confirmed through various structural analysis techniques, such as XRD, FTIR, and XPS. The scanning electron microscopy image reveals the existence of spherical gC_3N-NiO nanocomposites. Lithium diffusion kinetics is studied using cyclic voltammetry and electrochemical impedance spectroscopy (EIS) measurements. Compared to other NiO based nanocomposite anodes like NiO-GNF, Ni-NiO-G & NiO-rGO, NiO-G, and Graphene coated 3-D NiO-Ni , the gC_3N_4-NiO versus Li/Li+ half-cell deliver an initial discharge capacity of 982 mAh g^{-1} at a 0.1C rate [1-4]. The gC_3N_4-embedded NiO anodes exhibited excellent electrochemical performance and cyclability (200 cycles). The results indicate that the presence of nitrogen atoms in gC_3N_4 promotes electron transport and enhances the structural stability of gC_3N_4-NiO anodes.

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B 058

Morphologically Tuned Cu-based MOF Nanoparticles for Efficient Electrochemical Hydrogen Evolution Reaction

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ABSTRACT

To address the global energy crisis, the scientific community has made extensive efforts to produce hydrogen using eco-friendly methods. One of the most popular methods is electric-driven water reduction, which requires alkaline electrolyzer cells. In recent years, metal organic frameworks (MOFs) have been explored as a potential electrocatalyst in the electrolyzer cell for hydrogen evolution since they possess a high π electron conjugated system. On the nanoscale, they exhibit high electrocatalytic activity and electrochemical stability for the hydrogen evolution reaction (HER) due to the large exposed sites and fast charge transfer. Owing to the above-mentioned advantages, we have reported the facile synthesis of a Cu-based MOF (CuBDC) via the hydrothermal [1] and solvothermal routes [2]. This transition metal-based MOF nanostructure shows excellent electrocatalytic activity due to the high concentration of sp^2 bonds in the BDC organic linker. The MOF so produced is a cheaper, more stable alternative to the most explored Pt-based electrocatalyst in alkaline medium. The best sample exhibits a low tafel slope at a 10 mV/s scan rate. Due to its electrochemical and water-splitting properties, the as-synthesised material is suitable for a variety of applications.

Keywords: *Cu based MOF (CuBDC), Hydrothermal method, Solvothermal method, Electrocatalysis, Hydrogen evolution reaction (HER).*

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B 059

Morphology-Tailored Nickel and Cobalt Metal-Organic Frameworks and Their Metal-Oxide Derivatives: A Comprehensive Study on their Performance as Supercapacitor Electrodes

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ABSTRACT

Morphology is a critical factor that determines the electrochemical performance of a material through attributes such as specific surface area and active surface sites. Herein, we report the binder-free synthesis of 1D, 2D, and 3D Nickel and Cobalt metal-organic frameworks and their metal oxide derivatives via change of organic linkers, reaction time, and temperature. Comparing the 1D, 2D, and 3D morphologies, 2D-MOFs and their metal oxide derivatives, due to the impressive nanosheet structure, exhibited comparatively better electrochemical performance. Among them, 2D-NiO displayed the highest specific capacitance of 1376.3 Fg^{-1} at 1 Ag^{-1} with a good cyclic stability of 93.5% at 5 A g^{-1} after 5000 cycles. The exceptional specific capacitance and reliable cycling performance can be attributed to the homogeneous assembly of nanoparticles into a distinctive sheet-like structure with a high surface area which enhances the contact area between the active material and the electrolyte, thereby facilitating material utilization.

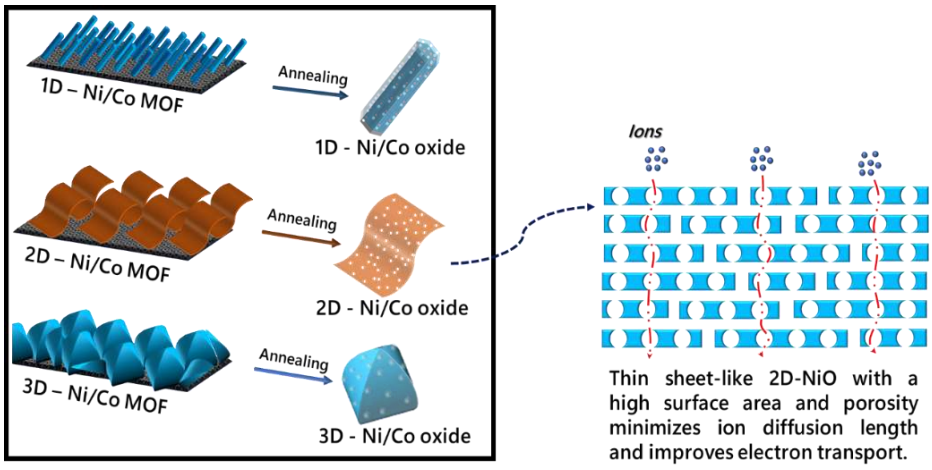

Figure. Schematic Diagram of Formation of Metal Oxide Derivatives from 1D, 2D, and 3D MOF

B 060

Polyaniline-Wrapped Hierarchical Architecture of $CuCo_2S_4$ for High-Performance Asymmetric Supercapacitor Applications

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ABSTRACT

Supercapacitors have garnered significant attention as energy storage devices due to their high-power density and long cycle life. Developing materials with enhanced electrochemical performance is crucial for advancing their practical applications. In this study, we report a novel electrode material consisting of a polyaniline-wrapped hierarchical architecture of $CuCo_2S_4$ for high-performance asymmetric supercapacitor applications. The hierarchical architecture of $CuCo_2S_4$ was synthesized via a simple solvothermal process with water and glycerol as a solvent. Polyaniline (PANI) was deposited through a simple electrochemical process. The conformal deposition of polyaniline on the $CuCo_2S_4$ surface not only enhances the electrical conductivity but also provides pseudocapacitance, resulting in improved overall electrochemical performance. The electrode of $CuCo_2S_4$ covered with polyaniline shows over 40% enhancement in the specific capacitance. The specific capacitance increases from 931 F/g obtained for $CuCo_2S_4$ to 1268.7 F/g through the wrapping of conducting polyaniline. The electrode also enables prolonged cycling stability with a 90.7% capacitance retention over 10000 cycles. Moreover, the asymmetric supercapacitor constructed using the polyaniline-wrapped hierarchical $CuCo_2S_4$ as the positive electrode and an activated carbon-based negative electrode exhibited high energy density and power density, making it a suitable candidate for various energy storage applications. This work offers a promising solution for addressing the growing demand for efficient and reliable energy storage systems in emerging technologies and renewable energy applications.

B 061

A Facile Synthesis of Coconut Shell Derived Activated Carbon to Enhance the Supercapacitor Performance

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ABSTRACT

Activated carbon gained a special attention towards energy storage application due to its unique properties such as excellent adsorption and retention capacity due to a large number of well-ordered pores. Considering the usage of activated carbon, industry demands a simple and ecofriendly synthesis approach by using biomass. In this work, coconut shells were utilized as the primary source material to extract activated carbon through a KOH activation process. The experimental characterization has been performed using XRD, FESEM, EDX, XPS and BET surface area techniques to study the various characteristics such as structure, morphology, chemical composition, specific surface area and pore structure of the coconut shell activated carbon (CSAC) and commercially procured activated carbon (CAC). X-ray diffraction confirms the hexagonal crystal structure of CSAC. The FESEM shows an ordered surface with uniform pores where BET analysis complements FESEM findings by showing an excellent specific surface area with an average pore size in the order of 4 nm. The total pore volume obtained for CSAC is slightly more than CAC which can be implemented towards supercapacitor application. EDX and XPS confirms the chemical compositions present in the CSAC and CAC. The presence of carbon has significantly increased in the CSAC by following this unique synthesis process. The device characterization has been performed by using Cyclic Voltammetry (CV), Galvanostatic Charge–Discharge (GCD) and Electrochemical Impedance Spectroscopy (EIS) techniques in 6M aqueous KOH solution. The potential window obtained for CSAC is about -0.5V to +1.5V which is higher than CAC. All other electrochemical characteristics of CSAC was observed to be better than CAC.

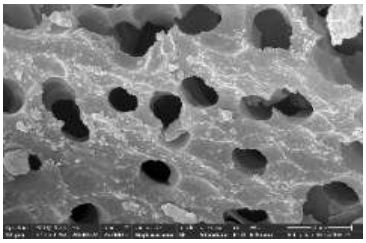

Fig.1. Synthesized CSAC with highly uniform pores

Keywords: *Activated carbon, Coconut shell, Supercapacitor, Pores, Cyclic Voltammetry, GCD, EIS.*

B 062

Unlocking The Potential of Nuclear Magnetic Resonance for Comprehensive Characterization of Metal-Organic Frameworks

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ABSTRACT

Metal-organic frameworks (MOFs) are a fascinating class of materials in materials science with a wide range of potential applications. Nonetheless, their intricate properties and behaviour when accommodating various guest molecules still need to be fully comprehended. Solid-state nuclear magnetic resonance (SSNMR) is a valuable analytical tool in studying MOFs, offering valuable insights alongside X-ray diffraction (XRD). In our research, we delve into three critical aspects of SSNMR in MOF characterization, explicitly focusing on examining metal centres, probing linker molecules, and exploring guest interactions. MOFs, due to their low densities and the presence of quadrupolar nuclei, pose specific challenges in SSNMR analysis. We undertake a thorough examination of local metal structures, addressing issues such as distinguishing distinct metal sites, understanding disorders related to metal atoms, refining the local metal geometry, exploring activation and adsorption effects, and monitoring in-situ phase changes. Characterizing organic linkers using 1H and 13C SSNMR complements the data obtained from XRD, contributing to a more complete understanding of MOF structural elucidation. We employ high-field magic-angle spinning (MAS) experiments with ultrafast spinning rates and isotope dilution to yield ultrahigh-resolution 1H MAS spectra, which enhance our knowledge of the local environment of hydrogen within MOFs. Moreover, MOFs are important in charge carrier storage, particularly in supercapacitor applications. Using 13C and 1H, SSNMR provides a comprehensive understanding of charge carrier storage mechanisms, ultimately contributing to improved performance and practical applications of MOFs in supercapacitors. This research not only advances our understanding of MOFs but also opens the door to their broader utility in supercapacitor technology.

B 063

Hydrothermally Synthesized Layered Vanadium Oxide as Electrode Material for Aqueous Asymmetric Supercapacitors

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ABSTRACT

Herein we prepared the Layered Vanadium Oxide (LVO) through the hydrothermal method as an electrode material for supercapacitor application. The prepared material was evaluated by XRD, FE-SEM, HR-TEM, and XPS to analyze its physiochemical properties. The electrochemical performances were evaluated by Cyclic Voltammetry (CV), Galvanostatic Charge-Discharge (GCD), and Electrochemical Impedance Spectroscopy (EIS). The prepared electrode material exhibited a better specific capacity of 549 C g^{-1} at 1 A g^{-1} current density with capacity retention of 79% at 10 A g^{-1} current density. Then the LVO was used as a positive electrode and Activated Charcoal (AC) as a negative electrode to construct an aqueous asymmetric supercapacitor (LVO//AC) using 3 M KOH as electrolyte. The fabricated device delivered a specific Energy Density (ED) of 98.75 W h kg^{-1} at a Power Density (PD) of 2.25 kW kg^{-1}. And stored a specific capacity of 316 C g^{-1} at 1 A g^{-1} current density with an initial capacity retention of 87 % even after 10000 cycles at a current density of 10 A g^{-1}.

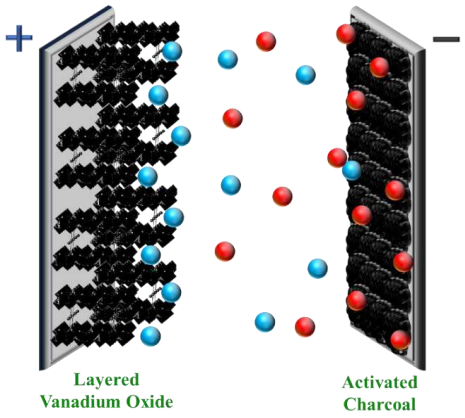

Figure. Charge storage mechanism of asymmetric (LVO//AC) device

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B 064

Exploring the Impact of Carbon Nanotubes Incorporation in Cobalt Zinc Mixed Ferrite

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ABSTRACT

Cobalt-Zinc ferrite have attracted considerable interest owing to its versatile properties, rendering it applicable across diverse fields such as electronics, telecommunication and material science. This study explores the impact of incorporating different Carbon Nanotubes (CNTs) compositions into $Co_{0.7}Zn_{0.3}Fe_2O_4$ ferrite. CNTs are known for their distinctive properties be they electrical, mechanical or thermal properties, suggesting their potential to enhance the overall performance of ferrite materials. In this work, cobalt-zinc ferrite with composition $Co_{0.7}Zn_{0.3}Fe_2O_4$ was synthesized using the chemical co-precipitation method and ferrite nanocomposites with CNT were synthesized using the ultra-sonication method. The influence of CNTs on different properties of ferrite nanoparticles have been investigated using different characterization techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), High-resolution transmission electron microscopy (HRTEM), Vibrating sample magnetometer (VSM), Electron paramagnetic resonance (EPR) spectroscopy etc. XRD results confirmed that the synthesized nanocomposites are crystalline in nature and as we increased the composition of CNT, crystallite size decreased. Fourier transform infra-red spectroscopy (FT-IR) confirmed the presence of bonds associated with spinel structures. The magnetic properties of the synthesized samples were explored using a vibrating sample magnetometer (VSM) and electron paramagnetic resonance (EPR) spectroscopy. The effect of adding CNTs with cobalt zinc mixed ferrite has a major influence on its magnetic properties. The maximum magnetization was obtained for CNTs percentage as 10%. Lande g factor was calculated using EPR. HRTEM analysis revealed that the ferrite nanoparticles and CNTs were well mixed and cobalt zinc ferrite nanoparticles were attached to MWCNT. The results show that the synthesized nanocomposite of cobalt zinc ferrite incorporated with CNTs holds promise for the development of advanced nanocomposite material having versatile applications.

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B 065

Urchin-Like α-MnO_2 And 2D g-C_3N_4 Composite Electrode for High-Performance Supercapacitors and Electrocatalytic Water Splitting

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ABSTRACT

In the quest for sustainable energy storage and conversion technologies, the development of advanced electrode materials is paramount. In this study, we present a novel urchin-like α-MnO_2 and two- dimensional graphitic carbon nitride (2D g-C_3N_4) composite electrode designed for high-performance supercapacitors and electrocatalytic water splitting. The unique architecture of the composite electrode is characterized by the urchin-like α-MnO2 nanostructures serving as a scaffold for the uniform deposition of 2D g-C_3N_4, thereby capitalizing on the synergistic effects of both components. The electrochemical performance of the composite electrode was systematically investigated. In supercapacitor applications, the urchin-like α-MnO_2/g-C_3N_4 electrode exhibited outstanding specific capacitance, exceptional rate capability, and remarkable cycling stability, making it a promising candidate for high-performance energy storage devices. Furthermore, the electrocatalytic properties of the composite electrode were assessed for water splitting. The α-MnO_2/g-C_3N_4 composite demonstrated superior catalytic activity with reduced overpotential, enhanced reaction kinetics, and robust long-term durability, suggesting its potential for renewable hydrogen generation. This study offers valuable insights into the design and performance of composite materials for supercapacitors and electrocatalytic water splitting, paving the way for clean and efficient energy technologies.

B 066

Ni@CoFe-MOF Electrode Materials as Advanced Electrodes for High-performance Hybrid Supercapacitors: Fabrication and Electrochemical Insights

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ABSTRACT

Metal-organic frameworks (MOFs) have attracted significant attention for their hybrid supercapacitor applications due to their remarkable tunability, porous characteristics, customizable chemical compositions, controllable crystal structures, and adaptable geometric morphologies. The predominant electrochemical double-layer capacitance originating from the organic framework is enhanced by the augmented pseudocapacitance arising from mixed metal-organic frameworks. In this study, we have devised a practical method to enhance the electrochemical properties of MOFs by introducing Ni^{2+} into the CoFe-MOF through a hydrothermal process. A hybrid supercapacitor was assembled, employing Ni-doped CoFe-MOF as the anode and activated carbon, along with KOH as the electrolyte. The nanostructured Ni-doped CoFe-MOF offers abundant electroactive sites and shortens electron transfer and electrolyte diffusion pathways. Consequently, this results in exceptional electrochemical performance, characterized by increased capacitance at low current densities. Additionally, it demonstrates superior rate capability and exceptional cyclic stability, coupled with impressive energy and power densities. These findings open the door to employing them as promising electrode materials in the next generation of hybrid supercapacitors.

Keywords: *MOF, hybrid supercapacitor, energy density, pseudocapacitance, energy storage*

B 067

Hyparrhenia Hirta Derived Hierarchical Porous Activated Carbon for High-Performance Symmetric Supercapacitor Applications

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ABSTRACT

This study reports on the valorization of Hyparrhenia hirta waste into a valuable electrode material for high-performance supercapacitor application. Activated carbons (ACs) with tailorable porous texture are turned from Hyparrhenia hirta via hydrothermal and microwave activation. The hydrothermal followed by microwave irradiated-activated carbon (HSW) shows meso/microporous texture with a high specific surface area of ~ 991 $m^2 g^{-1}$, a pore size of 3.09 nm in diameter. The HSW electrode shows the highest specific capacitance (Cs) of ~ 508.9 F/g at 2 A/g in 1 M Na_2SO_4 aqueous electrolyte (three-electrode configuration), with an outstanding cyclability of 84.6% over 10,000 charge/discharge cycles at 10 A/g. The fabricated solid-state symmetric supercapacitor exhibits Cs ~ 75.3 F/g at 3 A/g with a high energy density of ~ 26.7 W h/kg at a power density of ~ 1298.9 W/kg as well as excellent cyclability up to 10,000 cycles. The auspicious outcomes strongly ensure a high possibility of eco-friendly electrode materials for supercapacitor application.

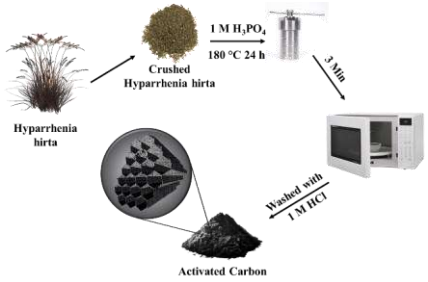

Fig. Schematic illustration of Activated Carbon synthesis

Keywords: *Activated carbon; Bio-mass; Microwave; Hydrothermal technique; Supercapacitor;*

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B 068

Intercalation of Au@Bi_2S_3 into MXene Nanosheets: A Facile Approach for High-Performance Supercapacitors

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ABSTRACT

In pursuit of efficient and sustainable energy technologies, there is an increasing demand for the development of advanced components that can improve energy conversion and storage processes. In this work, a simple and scalable hydrothermal technique was used to synthesis Bi_2S_3 nanoparticles while HF-etching technique was used for Ti_3C_2 nanoparticles. Ti_3C_2's excellent electrical conductivity is well-known and essential for rapid and effective charge transfer inside the electrode material. Ti_3C_2 is characteristic of MXenes which has a high surface area and hence, greater number of active sites for electrochemical reactions. Contribution of pseudocapacitive materials like Bi_2S_3 to total capacitance may give the device a better energy density than EDLCs. A hybrid supercapacitor can improve energy storage efficiency by combining Ti_3C_2's electric double-layer capacitance with Bi_2S_3's pseudocapacitance. When put together, these components may produce a supercapacitor with high cycle stability, making it ideal for prolonged and repeated usage. The doping of Au nanoparticles was done after the intercalation of Ti_3C_2 with Bi_2S_3 nanoparticles. The material was characterised using XRD to establish its crystallinity and crystallite size. SEM, TEM, and SAED patterns revealed the sheet-like structure of Ti_3C_2, flower-like structure of Bi_2S_3 nanoparticles, and low-concentrated dopant using EDAX. Synergy between the high conductivity and surface area of Ti_3C_2 and the unique properties of Au-Bi_2S_3, such as its high charge carrier mobility and electrocatalytic activity, are achieved. The technique of alteration is eco-friendly, and therefore it contributes to the ongoing efforts to develop sustainable and efficient materials for the ever-growing global energy demand.

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B 069

Dual Heteroatom Doped Carbon Nanotubes Supported Iron Doped Nickel Phosphide for improved Oxygen Evolution Reaction

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ABSTRACT

The purpose of energy conversion demands oxygen evolution reaction through electrolysis of water for fuel cells, rechargeable metal air batteries etc. It is must to employ an active and stable electrocatalyst to overcome the sluggish kinetics of oxygen evolution reaction. Transition Metal Phosphides has got more attention by the usage for OER instead of non-noble metals. Upon them, Nickel Phosphide is well known for OER owing to its abundance and high activity. Currently, Iron Nickel based catalysts have shown effective activity towards OER in alkaline media. In addition to this, creating support with carbonaceous material attributes to the higher conductivity and to expose more active sites which leads to the enhanced electrochemical performance. Hence this provides idea for forming hybrid dual hetero atom doped carbon composites with metal phosphides. In this regard, we have reported N doped Carbon Nanotubes supported Iron doped Nickel Phosphide using hydrothermal method followed by phosphatization. Furthermore, the optimized Fe doped Ni_2P/N,S-CNT displayed a OER electrocatalytic performance with a overpotential of 290 mV at 10 $mAcm^{-2}$ and a Tafel slope of 80 $mVdec^{-1}$ in 1M KOH alkaline electrolyte.

Keywords: carbon nanotubes, phosphides, heteroatom, dual doping

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B 070

Hydrothermally Synthesized Tin Cobalt Sulfide Enhanced with Pyrrole as an Electrode for Improving Supercapacitor Performance

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ABSTRACT

Supercapacitors are preferred because of their features like environment friendliness, high specific power, long life, and fast charging. Herein, we report the synthesis of Tin Cobalt Sulfide (TCS) enhanced with polymer addition as electrodes for high-performance supercapacitors. The Tin Cobalt Sulfide was synthesized by hydrothermal method. It is composited with pyrrole by chemical oxidation reaction and their morphological, structural, and elemental analysis was done by XRD, SEM TEM, and XPS analysis. Electrochemical studies of Pyrrole, TCS, and their composites were examined in detail. TCS@Ppy exhibits electrochemical performance with high-capacity value and very good redox reversibility than other pristine electrodes. TCS@Ppy composites exhibit a high specific capacity of 300 C/g at 1 A/g and a noticeable cycling capabilityof 85 % capacitance retention at 20 A/g after 10,000 cycles in three-electrode system.

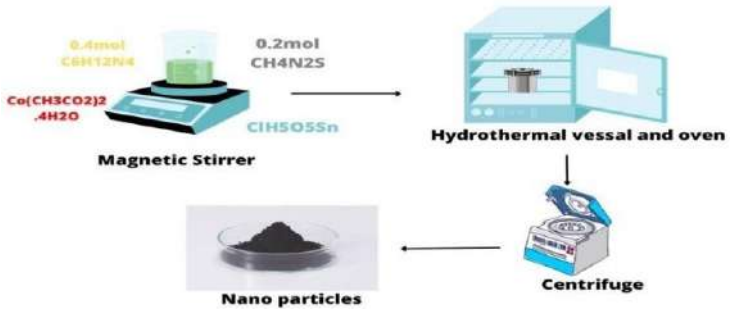

Figure. Schematic Diagram of formation of Tin Cobalt Sulfide References

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B 071

Effectiveness of Activated carbon Decorated Graphene Oxide Electrode inHigh Performance Supercapacitor Application

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ABSTRACT

Porous carbon derived from biomass has gained increasing interest as a cost-efficient, eco-friendly, and sustainable energy storage solution. In this study, we produced porous activated carbon from biomass using a two-stage process. Initially, the sample underwent preheating, after which it wasactivated through a microwave activation method. The activated carbon (AC) was then composited withGraphene oxide (GO) at different ratios. The AC/GO sample was used as an electrode in a supercapacitor application. We optimized different ratios of AC/GO composites and found that the onewith the highest electrochemical performance was 260 F/g at 2 A/g. with a good capacitance retention rate after 10,000 charge/discharge cycles. This work presents a simple and feasible approach for converting renewable biomass waste into cost-effective and high-performance supercapacitor electrodes suitable for real-time applications.

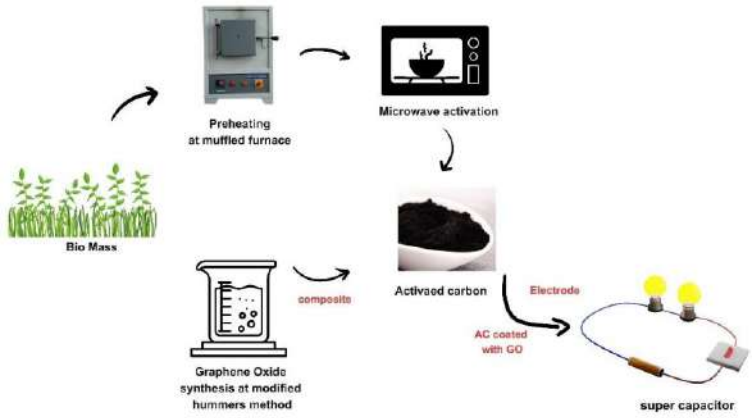

Fig. Synthesis of AC decorated GO oxide supercapacitor application

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B 072

Lithium Ion Transport Studies of Lithium Aluminium Titanium Phosphate (LATP) Based Blend Polymer Electrolyte Composites Systems

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ABSTRACT

Solid-state electrolytes (SSEs) are a promising alternative to liquid electrolytes, as they are non-flammable and have a higher energy density. However, the ionic conductivity of SSEs is typically much lower than that of liquid electrolytes. In the present study, we investigated the lithium-ion transport properties of $Li_{1.3}Al_{0.3}Ti_{1.7}(PO4)_3$, i.e. Li Al Ti phosphate (LATP) ceramics, complexed with polymers of different molecular weight phase (Blend Solid Polymer Electrolyte or BSPE). The LATP ceramics were prepared by solid state reactions at 950 °C, and subsequently ball milled and later pelletized for further electrical and structural characterizations. Blended solid polymer electrolytes (BSPE) were prepared by mixing different molecular weight polymers PEO_6 (M_w = 1 × 10^6 g/mol) and PEO_5 (M_w = 1 × 10^5 g/mol), and complexed with LATP ceramic phase.

The conductivity and dielectric studies at different temperatures were carried out on the LATP ceramic and BSPE systems using impedance spectroscopy in the frequency range 0.1–10^6 Hz. The structural, phase, surface morphology and elemental composition analysis were carried out using X-ray diffraction, scanning electron microscopy (SEM) coupled with Energy-dispersive X-ray spectroscopy (EDS) respectively. Impedance data have been studied, scaled and analyzed under conductivity and modulus formalisms over wide ranges of frequency and temperature for both LATP and BSPE systems. The analysis of the scaled formalisms indicates that both the conductivity and the structural relaxation mechanisms are temperature-independent for the above systems. Results obtained will be presented.

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B 073

Investigating the Electrochemical Performance of Carbon Assisted Mixed-Phase of $Mn_3O_4/MoMn_2P_{12}$ Catalyst for Hybrid Supercapacitor Applications

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ABSTRACT

Electrode materials with efficient electrochemical properties are always desirable for high-energy storage devices. In this research, due to the attractive attributes of Mn/MoMn hybrid oxide and phosphide composite (MnO@MoMnP) assisted with different activated carbon composites such as coconut charcoal (CC) and drumstick seed husk charcoal (DC) have been synthesized via hydrothermal process and used as electrode for supercapacitors. The outcome has been compared with the corresponding bare MnO@MoMnP. XRD analysis confirmed that the synthesized catalyst exhibited a mixed-phase structure resembling Mn_3O_4 and $MoMn_2P_{12}$. The structure, morphology, and composition of the synthesized materials are studied by XRD, SEM, TEM, and XPS measurements. The electrochemical studies have been carried out in 6 M KOH electrolyte and the findings from the cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), impedance plot are investigated. For three electrode system MnO@MoMnP/CC and MnO@MoMnP/DC composites exhibit significantly improved specific capacitance (C_s) of 573 F/g and 676 F/g at 1A/g respectively, which is higher than bare MnO@MoMnP specific capacitance (419F/g at 1A/g). Fabricated asymmetric supercapacitor with MnO@MoMnP/CC and MnO@MoMnP/DC composite also exhibit higher specific capacitance (C_s) of 63 F/g and 76 F/g at 1A/g respectively. Based on the findings we demonstrate that MnO@MoMnP/DC is a potential option for low-cost electrodes in hybrid supercapacitors.

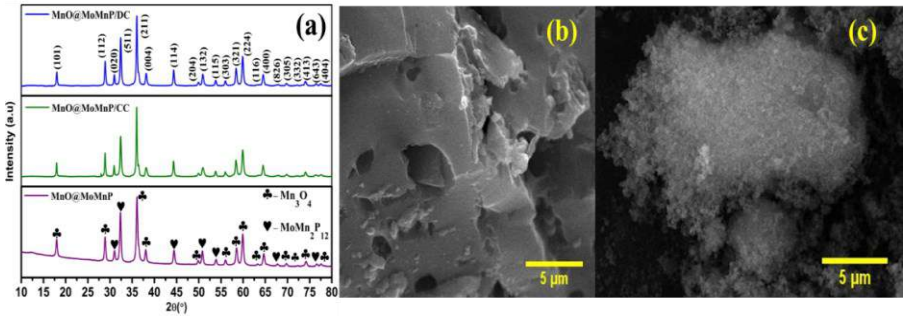

Fig.1: (a) XRD pattern of Bare MnO@MoMnP, MnO@MoMnP/CC, MnO@MoMnP/DC (b-c) SEM image of drumstick seed husk charcoal (DC) and MnO@MoMnP/DC composites.

B 074

A mini review on the applicability of nanostructured tungsten trioxide as supercapacitor electrode material and its overall performance analysis

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ABSTRACT

Energy storage devices are studied extensively due to the increased depletion of fossil fuels in connection with accelerated global economic growth. Batteries and supercapacitors (SCs) are the primary choices owing to their attractive efficiency, stability, and environmental friendliness. The scientific community has recently paid immense attention to the design and development of hybrid supercapacitors, which combine the mechanism of both batteries and SCs, thus potentially supplying both high energy and power density. Transition metal oxide (TMO)-based electrodes are extensively studied for the same which facilitates a faradic charge transfer mechanism[1]. Among the TMO, tungsten trioxide (WO_3) has continually received attention due to its low cost, abundance in nature, pseudocapacitance behavior, fast charge/discharge characteristics, excellent charge transport features, and good resistance to electrochemical corrosion[2]. WO_3 has many oxidation states which can offer intriguing redox reactions at the surface of the active material. Recent reports suggest that the use of WO_3 as the electrode material in devices such as symmetric supercapacitors (SC) and asymmetric supercapacitors (ASC) can enhance the specific capacitance significantly[3]. However, it is also evident from the literature review that WO_3 suffers from low specific surface area and low energy density coupled with poor electron conductivity[4]. This mini-review focuses on the reported works (in the last five years) with WO_3 as electrode material for supercapacitor applications. We have analysed in detail the pros and cons associated with the use of this material and changes in the electrochemical parameters with sizes and morphology of the nanostructures. A comparative study with other TMOs as electrode material has also been provided here. It will provide a roadmap to mitigate the associated problems and scope of future works with this material.

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B 075

Antimony-Graphene and Antimony-Aluminium-Graphene Composite Anode Materials for High-Capacity Secondary Battery Systems

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ABSTRACT

Though Lithium-ion batteries (LiBs) are the most popular energy storage devices at present, focus is towards replacing Lithium ions with alternate energy storage systems because of its availability, cost, toxicity and processing difficulties. Researchers are also working extensively with other alkali metal ions like sodium, and potassium as a replacement to more reactive lithium ions. Another promising candidate for large-scale energy storage is Al-ion batteries (AIBs), as it offers many advantages such as low cost, high availability and low flammability with higher capacity. As an essential role in AIBs, efforts have been dedicated to explore suitable anode materials over the past decade.

In the present study antimony-graphene (Sb-C), and antimony- aluminium- graphene (Sb-Al-C) based composite materials were synthesized as anode materials using pre-calculated (based on weight% and molar ratios) quantities of constituent raw materials followed by wet ball milling, in suitable solvent media. Samples of both the compositions were analysed after 20 hours, and 50 hours of ball milling. The influence of pulverising time on the composition powders on particle size (sub-micron), morphology, homogeneity, and phases were studied from the inputs of particle size analyser, SEM, EDS, and XRD. The effects of aluminium addition to the Sb-C composition and ball milling time on the ionic conductivities (with varying temperatures) were studied. The results were analysed and related to the existing literature on the subject. The results showed variation in the electrical characteristics attributable to the morphological changes during ball milling, and also due to the addition of aluminium.

B 076

Activated Carbon by Hydrothermal Carbonization of Corncob and its Application as a Supercapacitor Electrode

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ABSTRACT

Supercapacitors with carbonaceous electrode materials represent an efficient energy storage system with a long lifetime and high-power density. In this study, the activated carbon from Corncob biomass is synthesized by hydrothermal carbonization (HTC) with and without activating agents. The dried Corncob powder is loaded with an activating agent ($ZnCl_2$, H_3PO_4, KOH) during the hydrothermal treatment at 200 °C for 7 h and further followed by carbonization. The treatment with the activating agent decomposes and facilitates the generation of oxygen-containing functional groups on the precursor sample, which helps to enhance the porosity and electrochemical performance of the sample. The X-ray diffraction patterns show peaks at around 24-26° and 43°, corresponding to prepared carbon samples' amorphous and graphitic phases [2]. The morphology examination of the samples by SEM revealed more meso and macro pores when treated with the activating agent than those obtained without the activating agent. Two distinct peaks, D and G bands, are observed in the Raman spectroscopy [3]. Overall structural and electrochemical properties are elaborated in the results and discussion section.

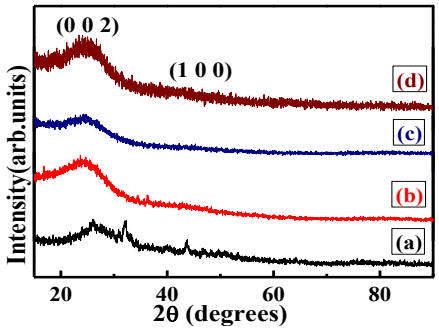

Fig.1. X-ray diffraction patterns of prepared samples ((a)-(d))

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B 077

A Comparative Study on RuO_2 Electrode Fabricated on Different Substrates for Supercapacitor Applications.

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ABSTRACT

Strong research efforts are right now focused on supercapacitors based on metal oxides, such as ruthenium oxide (RuO_2), mostly because of their capability to maintain high power density along with high energy density. In this work, the hydrothermally synthesized RuO_2 is coated on different substrates (stainless steel, nickel foam, carbon cloth, and Electrospun carbon fiber) to be used as the electrodes for asymmetric supercapacitors, and a comparative study of their charge storage mechanism and capacitive behavior is studied. The RuO_2 showed different yet peculiar specific capacitances on different substrates, which reflected the importance of analyzing the substrate materials. The prepared RuO_2 was analyzed using SEM, XRD, Raman spectroscopy, and FT-IR spectroscopy. Then, an asymmetric supercapacitor is fabricated by coating RuO_2 on electro-spun carbon nanofiber. The carbon nanofiber laminates were prepared by electrospinning carbonized and chemically activated peanut shell powder. The prepared RuO_2 was coated over the electro-spun carbon nanofiber–stainless steel laminates to obtain electrode-current collector assembly. This novel electrode is also compared with all other substrates. The performance of the electrode was studied by Cyclic Voltammetry (CV), Galvanostatic charging and discharging techniques (GCD), Electrochemical Impudence spectroscopy (EIS), etc. CV results of the NiF/RuO_2 electrode showed high specific capacitance compared to metal oxide-based electrodes and exhibited wide operating potential windows, significantly enhancing its capacitive behavior. The Cp value of the NiF/RuO_2 electrode was reported to be 186.98 F/g and 160.02 F/g for CV and GCD analysis, respectively.

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B 078

Morphology Modulation of Cobalt Bismuth Oxide through Solvothermal for Supercapacitor Application

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ABSTRACT

In this work, novel cobalt bismuth oxide (CBO) with three different morphologies (micro sheets, nanosheets and nano-needles) were successfully synthesised by solvothermal method and used as active electrode materials for supercapacitors. The prepared samples' crystal structure, morphology and surface were analyzed using various techniques. The electrochemical tests showed that the nanoneedle CBO electrode exhibited a better supercapacitive performance than others in a 6M KOH solution. The specific capacitance was 535.8 Fg^{-1} at a current density of 0.5 Ag^{-1}, however, the capacitance of micro sheets was only 246.3 Fg^{-1}, and nanosheets were 378.3 Fg^{-1} under the same conditions. Furthermore, at a current density of 3 Ag^{-1}, the capacitance retention of the nanoneedle CBO electrode remained at 85% after 2000 cycles. In contrast, the micro sheet and nanosheet electrode retention was only 67% and 74%, respectively. The peculiar structure of nanoneedle CBO, which affords a highly porous structure and an enhanced specific surface area, helps to explain these results.

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B 079

Study of Electrical and Dielectric Properties of Mixed Phase Tungsten Oxide Nanostructures

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ABSTRACT

WO_3 nanostructures were successfully synthesized via facile co-precipitation method with different amounts of Hydrochloric acid. The different crystalline forms of these nanostructures were investigated by XRD. XRD illustrated the presence of different phases in various samples with different amount of Hydrochloric Acid. Subsequently, the effect of Hydrochloric acid amount on dielectric constant, ac conductivity, impedance, and electric modulus of WO_3 nanostructures was observed. It could facilitate notable highest value of Dielectric Constant for minimum amount of acid with the formation of mixed phase. The significant results of ac conductivity and impedance of this sample emphasises on its further application in energy storage devices to improve parameters like cyclic stability, power density, heat generation.

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B 080

Electrocatalytic Performance of Synthesized PdCu/N,S-MWCNT Nanoparticles towards Oxidation of Methanol

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ABSTRACT

Fuel cells are gaining significant attention due to the ability of converting the chemical energy to electrical energy. Direct Methanol Fuel Cells (DMFCs) are electrolyte nature-based fuel cells, which utilizes high energy density of fuel such as methanol to produce highly efficient energy with water and carbon dioxide as the byproducts. Here, two half-cell reactions, methanol oxidation reaction (MOR) occurs at the anodic side and oxygen reduction reaction (ORR) occurs at the cathodic side of DMFCs. However, MOR significantly influence the performance of DMFCs due to the six electrons transfer mechanism. Pt-based electrocatalysts are known as best electrocatalysts for MOR, however it is highly poisoned by electrocatalyst intermediates such as carbon monoxide and also suffers from a major drawback such as high cost. In order to replace Pt-based electrocatalysts, various research groups reported Pd-based electrocatalyst towards MOR with similar performance and at low cost. Further, to reduce the cost and improve the performance towards MOR, PdM-based materials were reported, where M (Cu, Ni, Co, Mo, etc.). Herein, a PdCu alloy incorporated N,S doped MWCNT (PdCu/N,S-MWCNT) was synthesized and employed as an electrocatalyst towards MOR. PdCu/N,S-MWCNT were characterized by various techniques. Further, electrochemical studies of the synthesized electrocatalyst were performed in 1 M KOH as the electrolyte. Upon addition of 1 M methanol, electrocatalyst shows two oxidation peaks and resulting in high performance. Stability of the electrocatalyst was performed using chronoamperometric analysis. It has been observed that the novel electrocatalyst PdCu/N,S-MWCNT could efficiently enhance the electrochemical activity towards MOR.

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B 081

A Faster Microwave-Assisted Hydrothermal Synthesis of Low-Cost Conversion Type $ZnMn_2O_4$ Anode Materials for High-Performance Lithium-Ion Batteries

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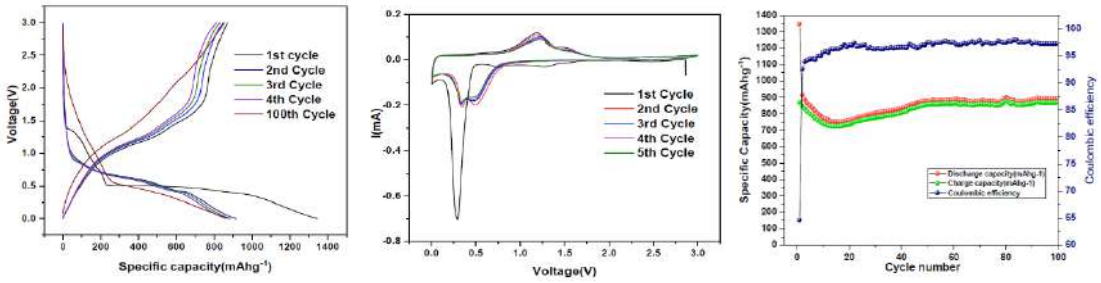
ABSTRACT

$ZnMn_2O_4$ can be considered one of the most promising anode materials for lithium-ion batteries (LIBs) because of its high theoretical capacity and low discharge potential. We have synthesized $ZnMn_2O_4$ bundled nanocubes by microwave-assisted hydrothermal method and characterized them. Structural analysis of the prepared samples was carried out by powder X-ray diffraction (XRD), confirming the formation of $ZnMn_2O_4$ nanoparticles. 2032 coin cells were fabricated using $ZnMn_2O_4$ as the anode, and the corresponding electrochemical performance was analyzed. We also recorded cyclic voltammetric studies for reversibility in capacitance. Subsequently, charge-discharge studies in the voltage range of 0.01 to 3.0 V versus Li/Li+ at a sweeping rate of 0.01 mVs−1 at room temperature were also examined. From the charge-discharge curve, it is obtained that discharge capacity reached about 895.8mAh g^{-1} after 100 cycles at a current density of 100mAg^{-1}. Coulombic efficiency has increased from 92 to 97% from 1st to 100th cycle. A drop in discharge capacity from 1346 mAhg-1 to 895.8 mAhg-1 has been observed after 100 cycles.



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B 082

Electrochemical Performance of Hydrothermally Synthesized $NiFe_2O_4$ Nanoparticlesunder Different Conditions as Anode Material for Lithium-ion Batteries.

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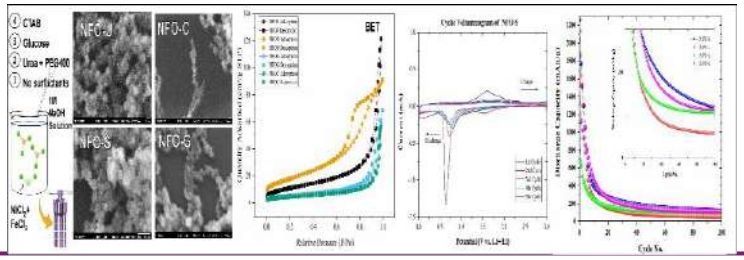
ABSTRACT

The search for better anode material which can replace graphite in Lithium-ion Batteries has made it to the Transition metal oxides with high theoretical capacity. Nickel Ferrite ($NiFe_2O_4$) is a metal oxide with exceptional electrochemical performance, eco-friendliness, and affordability. The large volume change during continuous charge-discharge cycles is a major drawback of $NiFe_2O_4$ as an anode. Nanoengineering the $NiFe_2O_4$ increases the surface area and porous volume, which improves the electrochemical performance. In this study, $NiFe_2O_4$ nanoparticles are synthesised under four different conditions through the hydrothermal method. The phase formation of NiF_2O_4 samples is confirmed by XRD and Raman spectroscopy. The morphology of $NiFe_2O_4$ samples is studied through SEM-EDX, and the surface and porosity are analysed with N_2 adsorption-desorption studies. The electrochemical performanceof the $NiFe_2O_4$ samples as anode material in Lithium-ion batteries is studied and compared by Cyclic Voltammetry, Charge-discharge study and Electrochemical Impedance Spectroscopy. By comparison, the $NiFe_2O_4$ hydrothermally synthesized without any surfactants at 180°C (NFO-S) shows the best specific capacity throughout the 100 cycles of charge-discharge. NFO-S has an excellent first-discharge capacity 2258 mAh/g at a current density of 100mAh/g. The Cyclic voltammogram of the $NiFe_2O_4$ samples explains the redox reactions inside the cell and their reversibility. The analysis of Nyquist plots before and after cycling interprets the decline in specific capacity over the charge-discharge. The large surface area and porevolume of NFO-S lessen the charge transfer resistance, increasing the capacity.



B 083

Instigate of Punica Granatum, Vitis Vinifera, Hibiscus Sabdariffa & Spinach Oleracea Based Photo Sensitizers in the Efficiency of Dye Sensitized Solar Cell

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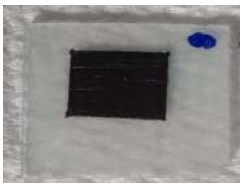
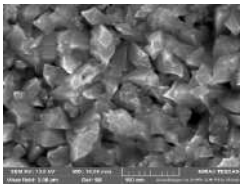
ABSTRACT

In our present work, fruits based organic dyes were prepared to act as photo sensitizers for DSSC applications. The dye extract from Punica granatum, Vitis vinifera (DYE I) consists of anthocyanin and Hibiscus sabdariffa & Spinach oleracea (DYE II)consists of chlorophyl pigment. DYE II is the mixture of anthocyanin and chlorophyl pigment. Two DSSC are fabricated as DSSC-1 (MTO/TiO_2/Anthocyanin dye/graphite) and DSSC-2 (FTO/TiO_2/Anthocyanin and Chlorophyll mixed dye/graphite). Screen printing technique is used for the coating of TiO_2. Magnesium Tin Oxide is used as the TCO substrate. Optical properties of the natural anthocyanins dyes in plants have been studied. From XRD, the prepared magnesium tin oxide and TiO_2 phase films show tetragonal structure. The grain size and thickness of the prepared TiO_2 film varies from 5.29µm and 5.96µm & 4.82µm & 8.99µm. The maximum percentage of transmission is observed in the range of 85% in the entire ultraviolet region for mixed natural dyes (DYE II) and 80% for fruit based natural dyes (DYE I). The optical band-gap energy values for the DYE I and DYE II were found to be 3.83 and 3.80 eV, respectively, and the transitions were found to be direct allowed. Each layer in the solar cell is investigated. Through EIS measurement, DYE II's resistivity values are less than DYE I's. The combination of Anthocyanin and chlorophyll mixed natural dyes [DSSC II] shows a maximum efficiency of 0.53% compared to anthocyanin-based cell, 0.22% (DSSC I), which is due to less sheet resistance.

B 084

Screen-Printed Silver-Zinc Rechargeable Micro Batteries Using Silver Nanoparticles Modified Graphene Nanocomposite

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ABSTRACT

Screen-printed micro batteries symbolize a significant advancement in energy storage at the micro-scale. These micro-batteries are progressing in areas like wearable electronics, medical implants, and more by integrating advantages such as compact sizing, effective energy conversion, and minimal ecological footprint. Silver-zinc rechargeable batteries are safe and will be an alternative to the existing lithium batteries. This work presents the fabrication of a screen-printed silver-zinc micro battery using graphene silver nanocomposite. The electrodes are screen-printed and electrochemically analyzed using various techniques. A solid-state micro battery was fabricated with a gel electrolyte, and the conditions were optimized. The battery showed an open circuit potential (OCP) of 1.8 V, a high specific capacity of 91.11 mAh/g, with a specific energy of 170.375 mWh/g and a specific power of 43.384 mW/g.

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B 085

Synthesis of Cerium-Cobalt Double Hydroxide Nanomaterials and Its Application inFlexible Supercapacitors

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ABSTRACT

This work presents the fabrication of a flexible supercapacitor with cerium-cobalt-layered double hydroxide nanomaterials. The layered double hydroxide nanomaterials are synthesized by the urea hydrolysis method. The material was thoroughly characterized electrochemically and has shown good pseudocapacitive behaviour. The response of the LDH was compared with the hydroxides of the individual metals, and the synergistic combination of cerium and cobalt was evident from the responses. Screen-printed capacitor with gel electrolyte was fabricated and has shown a high areal capacitance ofmF cm^{-2} with 0.625 µWh cm^{-2} areal energy density and 25.7 µW cm^{-2} areal power density. Excellent capacitance retention was observed even after 5000 charge-discharge cycles. The capacitor fabricated could withstand various bending cycles and retain the capacitance.

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B 086

Nitrogen and Sulphur co-doped Graphene Enwrapped with Mo doped Ni–Fe-Layered Double Hydroxides as an Efficient Electrocatalyst for Oxygen Evolution Reaction

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ABSTRACT

Developing highly active and precious-metal-free catalysts for the oxygen evolution reaction (OER) is of great significance to the development of electrochemical water splitting and metal–air batteries. NiFe-based layered double hydroxides (LDHs) are among the most efficient oxygen evolution reaction (OER) catalysts in alkaline medium. However, the poor conductivity hinders the electrochemical performance of the material. Therefore, the present work is focused on increasing the electrochemical performance of layered double hydroxide nanosheet compositing with conducting carbon material. Nitrogen sulphur doped graphene provides improved electrical conductivity and stability. Herein, we synthesize Mo doped Nickel-iron layered double hydroxides composited with Nitrogen sulphur doped graphene by a simple hydrothermal method. Mo doping increases the Ni^{3+} catalytic active site and found to be very effective in decreasing the overpotential. The synthesized Mo-NiFe LDH/N, S rGO exhibits low overpotential of 258 mV at 10mA/cm^2 and a low Tafel slope of 52mV dec^{-1} in 1 M KOH alkaline electrolyte. This work will provide new insights in developing a low cost and efficient electrocatalyst for water oxidation reaction.

Keywords: *Electrocatalyst, water electrolysis, layered double hydroxide, N, S rGO*

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B 087

Effect of Calcination Temperature in Zinc Phosphate Materials to Elevate Supercapacitor Applications

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ABSTRACT

Global attention to sustainable energy systems has increased as a result of the progressive depletion of non-renewable energy sources and global warming. Consequently, there is a marked increase in demand for new technologies in the fields of energy conversion and storage, especially for efficient energy storage devices like supercapacitors and rechargeable batteries. In situations where uninterruptible power supplies and load-leveling are necessary, supercapacitors can offer high power density, fast charge-discharge rate, and long cycle life in comparison to batteries with high energy density.

An increasing variety of people are intrigued by utilizing Transition Metal Phosphates (TMPs) as a potential supercapacitor electrode due to their significant redox-active functionality, high electrical conductivity, outstanding chemical and thermal stability, low cost, and layered structure. Furthermore, it has been found that by tweaking the native atomic formation, TMPs can draw in more water molecules than conventional metal oxides, hence improving their electrocatalytic ability. The superior electrochemical performance of TMP over metal oxides can be attributed to the strong P–O bonding and metal ion contribution, leading to improved conductivity yet preserving high mechanical stability. TMPs have unique electrochemical characteristics and a wide potential window because of the oxygen present in them.

A conventional hydrothermal process was used to synthesize the zinc phosphate nanopowder, which was then calcined at an array of temperatures to examine the effects on structure, morphology, and electrochemical characteristics. This study made use of XRD, FTIR, Raman Spectroscopy, SEM, TEM, BET, XPS, TGA characterizations, and electrochemical studies (CV, GCD, EIS).

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B 088

ZnSe@ZnO Heterostructures Constructed as an Electrocatalyst for Enhanced Supercapacitor Performance

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ABSTRACT

Energy crisis and depleting energy resources have triggered into plentiful efforts for the development alternative ways to cope up with the energy deficiency. Supercapacitor is one such energy storage device that plays an essential role in constant energy supply. Transitional metal selenides and their composites have undergone research in the recent times as potential candidates of supercapacitor devices due to their astounding physical, chemical and electrical properties. Selenium possesses an electronegativity lower than that of oxides and sulfur. This makes the chemical bond between the atom and the binding electrons weaker resulting in higher electrochemical activity that metal oxides or hydroxides. A ZnSe/ZnO composite has been synthesized by a facile hydrothermal method and investigated as a potential supercapacitor electrode in this work. The phase purity and morphology of the synthesized materials were examined through basic characterization techniques such as XRD, FESEM, FTIR etc. The composite material ZnSe/ZnO delivered high specific capacitance in the charge-discharge profile and stable long cycle life retaining 92.3% over 2000 cycles. Moreover, the composite structure ZnSe/ZnO enhances electrochemical performance by offering additional electrolyte ions and electron mobility. Therefore ZnSe/ZnO composite can be utilized as a promising candidate for supercapacitor applications.

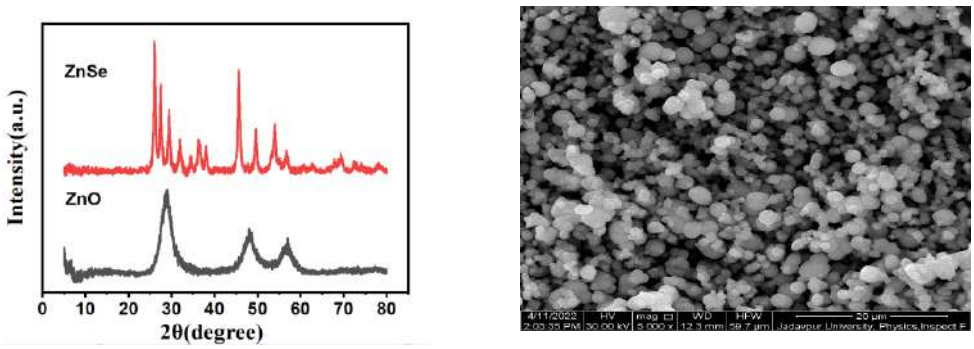

Fig 1. (a) FESEM image of ZnSe nanostructure (b) XRD spectra of ZnSe and ZnO nanostructures.

B 089

Ru Doped FeNi PBA Supported N-Doped Reduced Graphene Oxide as An Efficient Electrocatalyst for Oxygen Evolution Reaction

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ABSTRACT

Water splitting electrolysis is a promising pathway to achieve the efficient hydrogen and oxygen production in terms of energy conversion and storage in which catalysis or electro catalysis plays a critical role. The development of active, stable, and low-cost catalysts or electro catalysts is an essential prerequisite for achieving the desired electro catalytic oxygen production from water splitting for practical use. For efficient water splitting, it is essential to develop inexpensive and super-efficient electro catalysts for the oxygen evolution reaction (OER). Herein, we report an Iron Nickel based Prussian Blue Analogues electro catalyst we here set a facile strategy to prepare Ru doped NiFe PBA supported N-doped graphene as an efficient electrocatalysts for oxygen evolution reaction. The prepared catalyst shows superior OER catalytic activity than precious metal catalyst of IrO_2, with a low overpotential of 290 mV for 10 mA cm^{-2} in 1M KOH alkaline medium. Ru-FeNi PBA/N-rGO exhibits considerable potential to replace noble metal-based catalysts due to its straightforward production technique and exceptional electrocatalytic capabilities. [Fe3Ni@reduced-graphene-oxide (rGO)] showing outstanding OER performance this electro catalyst displays low over potential 300 mV at high current density 100 mA cm−2 in 1 M KOH.

Keywords: *FeNi PBA, reduced graphene oxide, oxygen evolution reaction*

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B 090

Precision Engineering of Turbostratic Graphene through Varied Power and Precursor Materials via Rapid Flash Sintering

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ABSTRACT

Two-dimensional materials find extensive application across various fields, notably in areas such as gas sensing, electronics, and energy storage. Herein, we present a systematic investigation into the synthesis and characterization of 2D-turbostatic graphene, achieved through varying power levels (50 – 400 Volts) using a capacitor bank and employing diverse precursor materials like carbon black, mushrooms, and tires via the rapid flash sintering. The resulting graphene samples were subjected to a multi-technique analysis like XRD, SEM, and Raman, and their turbostratic structure, sheet-like morphology, and functional attributes were determined. This study highlights the significance of precise parameter control in flash Joule heating for customizable graphene for energy applications.

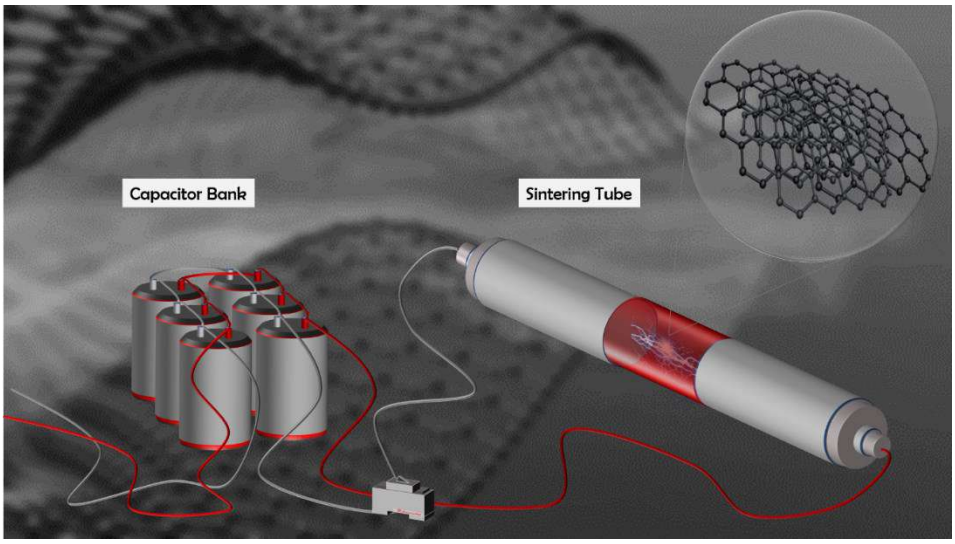

Figure. Schematic Diagram of Rapid Flash Sintering

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B 091

Synthesis and Characterization of Pi conjugated Conductive 2D Metal-Organic Frameworks (c-MOFs) as Electrocatalysts for Oxygen Evolution Reaction.

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ABSTRACT

Among the finding high performance electrocatalysts, the 2D conductive metal-organic frameworks (c-MOFs) were synthesized by microwave assisted reaction and developed new electrocatalysts for oxygen evolution reaction (OER) which is mandatory application in electrochemical energy conversion and storage. Here, we constructed a series of monometallic M-CAT MOFs which can achieve by 4e- transfer process that suffers from sluggish kinetics of OER in alkaline electrolyte. During the reaction process, M-CAT is the main active component for OER to improve the efficiency of oxygen evolution. Also, these materials are undergone with structural and electrochemical changes during the electrochemical measurements. Furthermore, we studied variety of techniques to point out the important criteria for a good catalyst.

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B 092

Preparation and Characterization for Natural Polymer Electrolyte Guar Gum Blend PVA with Magnesium Chloride Using Energy Storage Application

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ABSTRACT

We propose a cost-effective and eco-friendly natural biopolymer electrolyte made of a Guar Gum (GG) blend with polyvinyl alcohol (PVA) and magnesium chloride ($MgCl_2$) has been prepared by using the solution casting technique. In the current study, biopolymer electrolytes were created using MgCl2 salt compositions at various concentrations. The increase in the amorphous nature of the polymer/salt complex has been confirmed by XRD analysis. Using a scanning electron microscope, the surface morphology, structure, polymer interaction, and water-absorbing capacity have been examined (SEM). Different Scanning Calorimetric (DSC) is a technique we use to study the thermal stability of the biopolymer electrolyte film. The highest ionic conductivity has been found by guar gum blends PVA with $MgCl_2$ using electrochemical impedance spectroscopy (EIS) analysis at room temperature. The present work highlights a novel biomass strategy to reduce the crystallinity of PVA and obtain a flame-retardant hybrid with Biopolymer GG: PVA: $MgCl_2$ Salt simultaneously, which provides opportunities for flexible electronics with greatly enhanced ionic conductivity and safety.

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B 093

Enhancement of Energy Storage Properties of Nitrogen doped $ZnMn_2O_4/Mn_2O_3$ Nanocomposite

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ABSTRACT

Due to their rate capabilities, higher power density than batteries, and higher energy density than traditional dielectric capacitors, supercapacitors have garnered a lot of attention. The highly efficient Ultrasonication assisted hydrothermal chemical reaction was used to synthesis the nitrogen doped $ZnMn_2O_4/Mn_2O_3$ composites as high capacitance electrode material for supercapacitor. In order to enhance their capabilities and electrochemical performance, hybrid or composite nanoscale Nitrogen doped $ZnMn_2O_4/Mn_2O_3$ should include extremely porous and electrically conductive elements. Nitrogen doped $ZnMn_2O_4/Mn_2O_3$ nanocomposite is synthesized and its morphological properties are investigated. The morphological, structural, and elemental content of the produced nanocomposite are studied by X-ray Diffraction Analysis, Raman Spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, and Energy Dispersive X-ray Analysis. Using three-electrode system, the electrochemical properties of the prepared composite material can be studied which includes Cyclic Voltammetry, Electrochemical Impedance Spectroscopy and Galvanostatic Charge/Discharge Cycling. The composite is expected to be a promising material for supercapacitor devices.

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B 094

Hydrothermal Synthesis of Mn_2O_3/g-C_3N_4 Nanocomposite for Supercapacitor Application

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ABSTRACT

A variety of transition metal oxides and their composites have been used in energy conversion and storage. Because of their various oxidative states, Mn_2O_3 and its composites are advantageous in redox reactions, they have been widely used in energy storage applications. Potassium permanganate and melamine, a polymeric layered material have been utilized in a one-step hydrothermal process to create Mn_2O_3/g-C_3N_4 nanocomposite. Hydrothermal technique is recommended because of its low temperature requirements and easy instrumentation. The hydrothermal process is used to create the Mn_2O_3/g-C_3N_4 nanocomposite and its morphological properties are investigated. The morphological, structural, and elemental content of the produced nanocomposite are studied by X-ray Diffraction Analysis, Scanning Electron Microscopy, Transmission Electron Microscopy, and Energy Dispersive X-ray Analysis. Various experiments including Cyclic Voltammetry, Electrochemical Impedance Spectroscopy and Galvanostatic Charge/Discharge Cycling are used to characterize the electrochemical properties of the Mn_2O_3/g-C_3N_4 nanocomposite. The composite is expected to be a promising material for supercapacitor devices.

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B 095

Multi-Interface MoS_2@Ni_3S_4-NiS Composite as An Efficient Electrocatalyst for Overall Water Splitting Over a Wide pH Range

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ABSTRACT

Hydrogen production by water splitting is a promising and inexpensive method for future energy requirements. Therefore development of a non-precious, stable, and highly efficient electrocatalyst is crucial for Hydrogen evolution reaction (HER) and Oxygen evolution reaction (OER). In this work, we prepared a multi-interface MoS_2@Ni_3S_4-NiS by a simple hydrothermal method. MoS_2 nanosheets grown on with Ni_3S_4-NiS increase the electrical conductivity and hydrogen adsorption sites, lead to higher catalytic activity for the HER and OER. MoS_2@Ni_3S_4-NiS exhibited an overpotential of 141 mV for HER and 231 mV for OER. The MoS_2@Ni_3S_4-NiS exhibits superior electrochemical performance compared to pure Ni_3S_4-NiS and also robust durability in alkaline medium. This work focuses on designing noble metal-free electrocatalysts and producing large-scale green hydrogen energy for the alkaline environment.

Keywords: MoS_2@Ni_3S_4-NiS, Hydrogen evolution reaction, Oxygen evolution reaction, Water splitting.

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B 096

Nanocomposites of Manganese Oxide as Anode and Cathode Catalysts for Anion-Exchange Membrane Fuel Cells

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ABSTRACT

Fuel cells (FC) are devices for converting chemical energy into clean electrical energy, so they have attracted intense research interest.[1] FC are of different types, within which the H_2/O_2 fuel cell receives particular attention due to its low operating temperature and high energy density. Due to the limitation of PEMFCs, anion exchange membrane fuel cells (AEMFCs) have been proposed as a potentially cheaper alternative. Using an alkaline electrolyte allows the use of non-PGM electrocatalysts with a broader selection of materials that are not acid-stable.[2,3] Blends of MnO_2 with carbon nanotubes decorated with Pd nanoparticles (NPs) were studied to evaluate the performance and the mechanism for the oxygen reduction reaction (ORR) and the hydrogen oxidation reaction (HOR), as cathodic and the anodic reactions that take place in anionic exchange membrane fuel cells (AEMFC). The MnO_2 shows catalytic activity for ORR. However, the loading of Pd enhanced the catalytic kinetic parameters such as E_{onset}, $E_{1/2}$, $J_{lim,}$ and K. When the catalysts were mixed with carbon support, a synergistic effect was observed due to the ohmic resistance in the cell decreased. On the other hand, pure MnO_2 nanorods do not show catalytic activity towards HOR. When the NPs are deposited on the MnO_2, they exhibit catalytic activity. Finally, the blends were evaluated as anodic and cathodic electrocatalysts in an AEMFC. When used as cathodes, the Pd/MnO2: Pd/CNT showed a value of J of 197 mA cm-2. When the materials are used in the anode, the value of J_{lim} increases. The flooding of the cell was observed, and the low porosity of the catalyst led to the generation of large amounts of water, decreasing the performance of the fuel cell.

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B 097

Laser Induced Fast Fabrication of a Compositionally Complex Ball-In-Ball Type Metal Oxide Anode with Boosted Redox Reaction for Binder Free High-Capacity Li-Ion Batteries

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ABSTRACT

Addressing the inherent challenge of limited cyclability in conversion-type anodes is a crucial undertaking in the field of rechargeable lithium-ion batteries (LIBs). High entropy materials have demonstrated promising performances in terms of both high reversible capacity and cycle stability. In this study, we investigate the efficacy of a high entropy glycerate based on first-row transition metals (Fe, Co, Ni, Mn, and Cr) as an efficient Li-ion battery anode. The results show a high reversible capacity exceeding 500 mAh/g (0.1 A/g) over 270 cycles. Additionally, we present a novel approach involving the flash conversion of the high entropy glycerate (HEG) to a spinel phase high entropy oxide (HEO) using a CO_2 laser. The fabricated binder-free composite anode combines laser-induced reduced graphene oxide (rGO) and HEO ($(FeCoNiCrMn)_3O_4$) composites, exhibiting improved reversible capacity and cyclability. Morphological analysis indicates a morphological evolution of the HEG from microsphere to ball-in-ball type after laser treatment. Ex-situ XRD analysis reveals the persistence of the spinel structure within HEO, even during the delithiation process, accompanied by a partial transformation towards a rock salt configuration in the charge storage mechanism. The optimized composite (HEO@rGO) demonstrates a high specific capacity of ~794 mAh/g after 100 cycles and ~530 mAh/g after 200 cycles at 0.1 A/g and 0.5 A/g current, respectively. The undulating nature of the cycling stability profile is correlated with variations in charge transfer resistance and lithium diffusion throughout the cycling process.

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B 098

Investigation of the Dielectric Characteristics of a Mucilage-Based Biopolymer (Hybanthus Enneaspermus) Electrolyte Used in Energy Storage Devices

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ABSTRACT

Our ecosystems are being impacted by the excessive usage of fossil fuels, which will be exhausted in a few decades. Researchers are looking into alternate sources to avoid this problem. The electrochemical device is one type of resource that has successfully overcome these problems. Electrochemical devices are those that use electrical energy to start chemical reactions or employ chemical reactions to produce electricity. Actuators, batteries, fuel cells, sensors, and supercapacitors are examples of electrochemical devices. The anode, cathode, and electrolyte are their three primary parts. Electrolytes are the main topic of our attention. Liquid-based electrolytes were previously utilized, but it has drawbacks including flammability, leaking, and the requirement for a specific type of separator. Liquid electrolytes were replaced by solid polymer electrolytes. Among them, naturally derived polymer is the one which attracted more than synthetic. Mucilage-based polymer electrolytes were synthesized using the solution cast technique. Hybanthus enneaspermus leaves (HEL) powder and lithium nitrate salt were utilized in this study. The various salt concentrations (0.075g, 0.150g, 0.225g, and 0.300g) were combined with one gram of HEL powder. The X-ray diffractometer (XRD) verifies the material's amorphous nature. Their amorphous nature increased with the increase in salt concentration. Fourier transform infrared spectroscopy (FTIR) confirms that salt and leaves have been properly combined. Electrochemical studies were carried out using electrochemical impedance spectroscopy (EIS). The membrane's dielectric properties were thoroughly examined by the dielectric instrument. The obtained highest conductivity of the membrane is in the order of 10^{-5} S/cm. Our results suggest this membrane can be used in lithium battery applications.

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B 099

Synthesis of NiO Based Carbon Allotrops Nanohybrids and Camparing The Efficency of Various Carbon Allotropes with p-type DSSC

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ABSTRACT

Semiconductors of p-type have a large optical band gap and high ionization potential however these semiconductors face low hole transfer rate and recombination, which results in low efficiency of cell as compared to n-type dye sensitized solar cell (DSSCs). NiO (nickel oxide) nanotube is a good candidate for p-type DSSC. Therefore, NiO nanotubes were synthesized by sol-gel method. Some of the nanomaterials reported for enhancing the efficiency of p- type DSSC with NiO are carbon allotropes like functionalized multiwalled carbon nanotubes (f-MWCNTs), reduced graphene oxide (RGO), graphene quantum dots (GQD) and fullerene(C_{60}). Composites of NiO and carbon allotropes were synthesized with MWCNT, RGO & GQD as NiO@MWCNT, NiO@RGO and NiO@GQD and NiO@fullerene. These composites of NiO/carbon allotropes can provide more surface area for dye adsorption, decrease recombination and higher electrochemical performance than pristine NiO nanotubes. Composites enhance the open circuit photovoltage (V_{oc}) and short-circuit photocurrent (I_{sc}), hole transportation which improves the power conversion efficiency (PCE) of the cell. Morphological conformation was obtained from FE-SEM (field emission scanning electron microscopy) and TEM (transmission electron microscope). To conform the synthesis of NiO nanotubes, f-MWCNT, RGO, GQD, functionalized fullerene and their nanocomposites FTIR, XPS and RAMAN have been done. Diameters of NiO nanotubes was found to be between 300-500nm whereas RGO, GQD and OMWCNT were found to be of 2nm, 100nm and 50nm. From the electrochemical measurements such as (electrochemical impedance spectroscopy) EIS, mott-Schottky analysis, J-V profile, OCVD spectra, and IPCE plots comparing the efficiency of the device which will be discussed at the time of presentation.

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B 100

Construction of Co_3O_4/Fe_3O_4/RGO Ternary Hybrid Nanocomposite for Electrochemical Supercapacitor Applications

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ABSTRACT

The demand for high-performance energy storage devices has stimulated significant interest in the searching and development of advanced electrode materials for electrochemical supercapacitors. In this study, we present the synthesis and characterization of a novel Co_3O_4/Fe_3O_4/reduced graphene oxide (RGO) ternary hybrid nanocomposite designed for superior electrochemical supercapacitor applications. The fabrication of the ternary nanocomposite was achieved through a precisely controlled chemical oxidation process. The resulting ternary hybrid nanocomposite exhibits synergistic effects arising from the unique combination of Co_3O_4, Fe_3O_4, and RGO, leading to improved conductivity, enhanced electrochemical performance, and extended cycling stability. XRD, FESEM, TEM, FTIR, TGA, VSM and surface area analysis were employed to characterize the synthesized nanocomposite. The ternary magnetic composite showed a saturation magnetization of 21 emu/g and the estimated surface area of the composite is 229 m^2/g Electrochemical studies, such as CV and GCD measurements were conducted to assess the electrochemical performance of the ternary hybrid nanocomposite and showed in Fig.1. The results demonstrate promising possibilities for this nanocomposite as a high-performance electrode material for electrochemical supercapacitor applications.

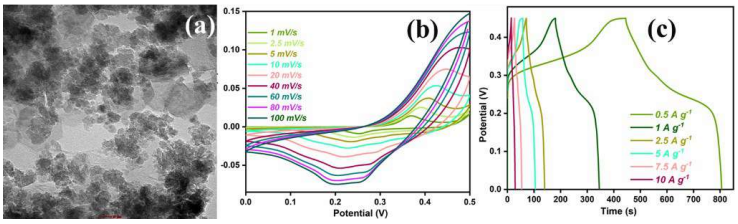

Fig.1. (a)TEM micrograph of, (b) CV, and (c) GCD curves of ternary electrode material.

B 101

Green Synthesis of Copper MOF for Electrochemical Reduction of CO2

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ABSTRACT

Increasing greenhouse gases in the atmosphere of our earth mainly consist of CO_2, which has caused the greenhouse effect, such as global warming and climate change. Therefore, it is necessary to develop technologies for mitigating carbon dioxide. Electrochemical reduction of CO_2 is the technique to reduce carbon dioxide, which converts into other chemicals, such as formic acid and methane. Moreover, the electrochemical reduction of CO_2 comprehends advantages such as lower overpotential and higher conversion at high current densities. Metal-organic frameworks (MOFs) will be profitable electrocatalysts for the electrochemical conversion of carbon dioxide because of their high surface area and effective absorption of CO_2. MOFs are synthesized by conventional procedures such as the hydrothermal method. However, DMF solvent is involved in this customary process, which is expensive and detrimental to the ecosystem. Herein, our group has researched the green synthesis of Cu-based MOFs using water-based solvent for the electrochemical reduction of carbon dioxide, which can be replaced with DMF solvent. The experiments for the electrochemical reduction of CO_2 such as linear sweep voltammetry (LSV), and cyclic voltammetry (CV) were implemented with an electrolyte in an H-type cell. The characterizations of Cu-based MOFs were analyzed with SEM, TEM, XRD, FT-IR, and XPS.

Keywords: Electrochemical reduction of CO_2, Cu-based MOFs (metal-organic frameworks), Green synthesis, Water-based solvent, LSV (linear sweep voltammetry), CV (cyclic voltammetry)

B 102

CuCo Double-Layered Hydroxide / Vanadium Carbide Nanocomposites: Nanoflower Structure for Optimised Electrocatalytic Water Splitting

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ABSTRACT

Electrochemical water splitting has shown great development potential as a green, renewable energy-producing technology in recent years. In the subject of water splitting, several materials have been discovered to work well as catalysts. Nevertheless, the fabrication of bifunctional electrocatalysts for the sustainable and effective simultaneous creation of oxygen and hydrogen remains a formidable problem. Here, as improved electrocatalysts for complete water splitting, we have successfully developed oxygen vacancies abundant CuCo layered double hydrooxide (CuCo-LDH) with vanadium carbide nano arrays (VC) loaded on copper foam. When the current density was 10 mA cm^{-2}, the CuCo-LDH/VC has exhibited outstanding overpotentials of 102 and 230 mV for the hydrogen evolution and oxygen evolution reactions (HER and OER) in alkaline medium, respectively, because of the bimetallic synergistic effect between the cobalt and copper and the unique hollow porous structure. After prolonged total water splitting for more than 12 hours, it also demonstrated exceptional durability. The study findings presented in this work offer comprehensive and clear insights into initial robust and effective multifunctional electrocatalysts for total water splitting, which is very relevant to practical applications of the water splitting process.

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B 103

Synthesis of Manganese Oxide Mn_2O_3 as electrode for Supercapacitors

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ABSTRACT

Among the various materials and composites used in energy conversion and storage, metal oxides have been utilized more than any other materials due to their pseudocapacitive nature. Manganese with its various oxidation states, it can form various metal oxides like MnO, MnO_2, Mn_2O_3 and Mn_3O_4. These oxides have various advantages like non-toxicity, cost effectiveness and abundance. One among this is Mn_2O_3 which have been utilized as anode for lithium-ion batteries. Hydrothermal method is used due to its simple instrumentation and low temperature operations. The as synthesised Mn_2O_3 nanomaterial is further characterized using various techniques including X-ray Diffraction Analysis, Scanning Electron Microscopy, Transmission Electron Microscopy and Raman Spectroscopy. On successful synthesis and characterization, Mn_2O_3 nanomaterial electrodes are prepared and studies like Cyclic Voltammetry, Electrochemical Impedance Spectroscopy and Galvanostatic Charge/Discharge Cycling will be done in order to test its performance for supercapacitor application.

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B 104

Role of Co-Doping on Ionic Conductivity of Ceria based Electrolyte for Low Temperature SOFC Application

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ABSTRACT

Doped Ceria has been one of the most explored alternatives of YSZ which, not only reduces the operating temperature but also, enhances the ionic efficiency due to its electro-catalytic property. The double valency property of ceria arising due to the oxygen non-stoichiometry ($CeO_{2-\delta}$), generates oxygen vacancies making it a potential electrolyte material. Rare Earth (RE) dopants like Gd^{3+} and Sm^{3+} have been reported to have high ionic conductivity at low temperatures. In the present study, synthesis of Sm-Gd co-doped ceria is performed by wet chemical route to ensure homogenous distribution, with the stoichiometry $Ce_{1-a}Gd_{a-y}Sm_yO_{2-0.5\delta}$ where a=0.20 and $0 \leq y \leq a$. Phase purity was obtained by calcining the precipitants at 650°C temperatures in air. The green bodies were formed by uniaxially pressing the calcined powder and then sintering in air at an elevated temperature of 1450°C. XRD and Raman spectroscopy confirmed the successful substitution of both the dopants and the presence of a single-phase cubic structure of the nanoparticles. Surface morphology using FESEM showed a highly dense microstructure (more than almost 97% density) and EDX confirmed the elemental composition. AC impedance spectroscopy (EIS) of the sintered pellets between 400-700°C temperatures revealed much higher conductivity than singly doped ceria.

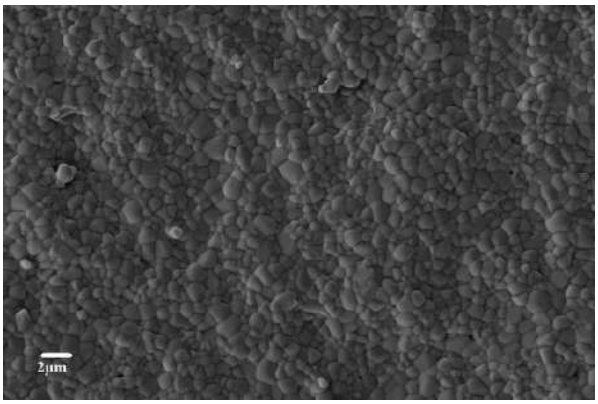

Figure 1. FESEM of 15-5SGDC sintered pellet

B 105

Polyaniline-Carbon Dot Nanocomposite for the Fabrication of Screen-Printed Flexible Supercapacitor

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ABSTRACT

Printed supercapacitors are ideal for the energy demand of flexible and portable electronic applications. Polyaniline (PANI) is a widely used conducting polymer to fabricate microsupercapacitors due to its unique structure, high energy density, good electrical conductivity, and low cost. However, the major shortcomings of PANI are the low cycling stability because of the eventual swelling or breaking of the structure and low specific capacitance. The composite materials of PANI with other nanomaterials like carbon dots (CD) increase its stability. This work aims to electrochemically synthesize PANI/CD nanocomposite and validate its capacitive performance. Initially, PANI was electrodeposited on the electrode surface by cyclic voltammetry from an electrolyte solution containing 20 mM aniline in 1 M H_2SO_4 medium. The areal capacitance at 2 mV s^{-1} was found to be 1982 mF cm^{-2} with an energy density of 7.12 mWh cm^{-2} and power density of 6.4 mW cm^{-2}. Further, 200 µL of the CD was added to the aniline solution, and PANI/CD nanocomposite was electrodeposited using CV, wherein an enhanced performance was obtained.

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B 106

Enhanced Energy Storage Capacities of hematite Fe_2O_3 doped with MoS_2 Nanostructures

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ABSTRACT

This study investigates the enhanced electrochemical performance of hematite (Fe_2O_3) as an anode material for batteries through doping with molybdenum disulfide (MoS_2). The synergistic effects of MoS_2 doping are examined, the synthesized hematite-MoS_2 composite demonstrates improved lithium-ion storage capabilities compared to pure hematite. The incorporation of MoS_2 promotes electrical conductivity and facilitates the negative effects of hematite's intrinsic properties, which include low electronic conductivity and significant volume expansion during cycling. As a result of its greater rate capacity and cycling stability, the composite is an effective choice for high-performance lithium-ion battery anodes. This research illustrates the synergistic effects of hematite and MoS_2 for advancing the performance of energy storage devices.

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Investigation of $BaTiO_3$/rGO composite for water splitting application

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ABSTRACT

Integrating advanced materials, such as Barium Titanate ($BaTiO_3$) and reduced graphene oxide (rGO), has opened new avenues for diverse technological applications. The use of BaTiO3 makes it a promising choice for electrochemical properties. $BaTiO_3$ holds immense potential for its application, offering unique properties and versatility. rGO because of its superior electrical conductivity, chemical stability, and large surface area has demonstrated considerable promise in energy storage applications. These properties can improve the efficiency of energy storage devices. This research aims to harness the unique properties of BaTiO3-rGO composites for hydrogen evolution reaction. The $BaTiO_3$-rGO composites have electrical, mechanical, and electrochemical properties, making them ideal candidates for HER application. The characterizations like XRD, SEM, TEM, FTIR, UV, and Raman confirm the presence of composite material, and this study investigates the synthesis and optimization of $BaTiO_3$-rGO composites to achieve enhanced electrochemical performance for hydrogen evolution reaction (HER) application.

Keywords: Barium titanate, Perovskite, Hydrogen evolution reaction, Electrocatalysis, reduced graphene oxide.

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Fabrication of Mixed Cation Perovskite Solar Cell Using Donor Acceptor Polymeric Hole Transport Layer

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ABSTRACT

Donor-acceptor based random copolymer-type hole transport materials (HTMs) are important in perovskite solar cells (PSCs) to achieve superior performance and highly durable[1-5]. The main objective of this study is to fabricate mixed-cation PSC using random copolymer of P(BDTT-PhC8TPD-TPD) (RCP-BPT) as the HTM (Figure 1). The RCP-BDT has deeper HOMO energy level (-5.41 eV), highly compatible with Cs-containing mixed-cation perovskite light absorber with HOMO energy level (-5.66 eV), HTM with gradient band alignment with perovskite is important for higher hole mobility in the PSCs. PSCs exhibit high power conversion efficiency and high durability.

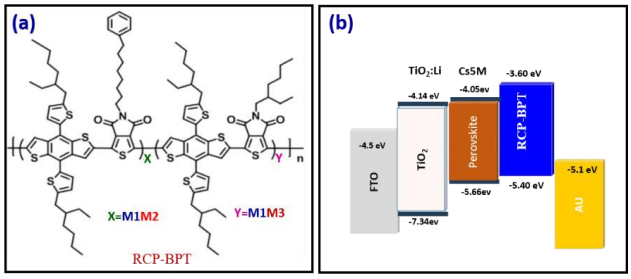

Figure 1. (a) Structure of RCP-BPT polymer and (b) energy diagrams of HTM with perovskite.

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Harnessing the Synergy of Cu-Co_3O_4/rGO for High-Performance Supercapacitors: AComprehensive Synthesis and Characterization Study

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ABSTRACT

In the modern period the expansion of secure and sustainable energy storage system is followed because of their extensive production and worldwide application, the device supercapacitor plays vital role with advantage of high-power density, fast charge and discharge, long cycling life and have acquired great academic and industrial attention. By optimizing the nanomaterial using synthesis approaches, the researchers have developed the superior mechanism to improve the electrode material. Here, Cu-Co_3O_4/rGO is the electrode material was synthesized by Co-Precipitaion method with large surface area and novel shapes. It is high theoretical capacity, environmental friendliness, natural abundance, low cost for the electrochemical performance of supercapacitor. It is high theoretical capacity, environmental friendliness, natural abundance, low cost for the electrochemical performance of supercapacitor. The prepared material was characterized with XRD, FTIR, UV-Vis, SEM, TEM, XPS, and BET to analyze their size, structure, and morphology and oxidation states of required nanoparticles. Hence, the article is reported that to control the issues of poor electrochemical stability, low conductivity and high rates of agglomeration are can control by Cu-Co_3O_4/rGO electrode nanomaterials that are effectively combined the metal oxides with carbon-based materials for enhance structure and specific area. The material is carried out with the electrochemical studies with CV, GCD and EIS to check the performance. Therefore, in the energy storage system the current challenges are faced that the prepared electrode material to promote high electrochemical performance supercapacitor electrodes in near future.

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B 110

Graphitic Carbon Nitride (g-C_3N_4) Blended CO_3O_4/Fe_2O_3 Nanoparticles as a Potential Supercapacitor Electrode

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ABSTRACT

In this work, a novel mixture of graphitic carbon nitride (g-C_3N_4) with Co_3O_4/Fe_2O_3 nanoparticles were synthesized using simple decomposition method. More specifically the composites were prepared by decomposing suitable proportion of metal complexes (Co, Fe) with varying concentration of graphitic carbon nitride (0, 5, 10 and 15 Wt%) at elevated temperature. The structural and morphological investigations reveals that this attractive nano-composite possess better crystalline nature and particle morphology. As a supercapacitor electrode, this material exhibits higher capacitance, lower charge transfer resistance and exhibits better cyclic stability. Further a two-electrode device was assembled and its electrochemical performance also detailed.

Keywords: Graphitic carbon nitride; Co_3O_4/Fe_2O_3; Electrochemical; supercapacitor; Energy storage

B 111

Designing and Fabrication of Binary Metal Oxide/Hydroxide Micro-/Nanoarchitecture as a High-Performance Electrode for Hybrid Supercapacitor Application

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ABSTRACT

Developing high-performance advanced electrode materials is significantly impacted by the design and construction of nano/microstructured materials. It has garnered significant attention in pursuing reliable and efficient energy storage devices. Herein, we reveal an efficient and straightforward approach to designing and fabricating binary metal oxide/hydroxide micro-/nanostructures using a hydrothermal technique. This investigation into the ratio between the binary metal oxide/hydroxide highlights its effects on particle size, structure, morphology, specific surface area, and electrochemical properties. Impressively, the binary metal oxide/hydroxide prepared at an equimolar ratio exhibits superior electrochemical performance as the supercapacitor electrode, with higher capacitance, better electronic conductivity, faster charge transfer, and low resistance. Moreover, the configured hybrid supercapacitor delivers excellent electrochemical performance, revealing outstanding capacitance, energy density, power density, and exceptional cyclic stability. Based on the above results, the binary metal oxide/hydroxide electrode is a potential candidate as a battery-type electrode material for enhancing the capacitive behavior in hybrid energy storage devices.

B 112

Earth abundant and non-toxic FeS and FeS_2 for energy conversion applications

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ABSTRACT

Iron sulphide (FeS) and iron disulphide (FeS_2) are the emerging compound materials considered in energy conversion and storage applications such as photovoltaics, water splitting, supercapacitor and battery due to its high photon absorption, good redox activity, stability of material and its abundance. In this work, we attempt to synthesize FeS and FeS_2 bulk material via mechanochemical process using ball milling. Elemental iron and sulfur source powders were subjected to wet milling for 48 hours at 500 rpm in presence of toluene medium and the ball-to-powder ratio was maintained at 15:1. In the powder milled to 24 and 48 hours showed the formation of FeS and FeS_2 phases respectively as confirmed by X-ray diffraction analysis. Further, an elaborate analytical characterization using Raman spectroscopy, scanning electron microscope, thermos gravimetry analysis, optical absorption analysis and photoluminescence measurements were done to examine the structural, morphological, and optical properties of the milled FeS and FeS_2 powder. Optical measurements showed high absorption in the visible region and the bandgap values are about 2.0 eV and 1.28 eV for FeS and FeS_2 respectively. In addition, electrochemical studies were performed to understand its suitability for water splitting.

Key words: Iron pyrite, solar absorber, optical properties

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B 113

The Multifunctional Electrochemical Properties of Sugarcane Baggase-Derived Activated Carbon for Li-S, K-ion, and Zn-Air Batteries

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ABSTRACT

The development of alternative Li- ion technologies is mandatory for future grid-scale and electric vehicle applications. Biomass-derived carbon can be used for various energy storage applications owing to its highly tunable properties. The present work, preparation of N-doped carbon, involves K_2CO_3 and urea as the activating agent and N_2 source, respectively. The observed two reflections from the X-ray diffraction correspond to (002) and (101) planes of graphite, revealing the dominant features of amorphous carbon. The less ordered graphitic structure of the NSAC-1:2 is in agreement with the Raman spectral results. FT-IR results confirm the presence of O-H, C-O, C=O, and amine functional groups in SAC and NSAC samples. The initial discharge capacity of the fabricated Li-S batteries (LSBs) using pristine SAC and N doped SAC (1:1, 1:2 &1:3)@GF coated separators are 1172.3 mAh g^{-1}, 1320.8 mAh g^{-1}, 724.6 mAh g^{-1} and 1280 mAh g^{-1}, respectively. Amongst NSAC (1:1)@GF yielded a higher specific capacity, excellent cycling stability, and better capacity retention due to the presence of multiple functional groups. While using the same carbon as the anodes for K-ion batteries (KIBs), nitrogen doping improved the charge transfer and promoted charge storage via K-ion adsorption. The GCD profile during discharge exhibited a slopy profile below 1.5 V, indicative of K-ion storage by adsorption. The N-doped carbon (27%) has exhibited better Initial Coulmbic Efficiency (ICE) than the pristine carbon (22%). At 20 mA/g, the K-ion cells delivered a reversible capacity of 190 and 210 mAh/g for SAC and NSAC (1:1). The performed Linear Sweep Voltammetry (LSV) at 1600 rpm evidences the NSAC is the most favorable in terms of limiting current density (1.8228 mA/cm^2), lower onset (0.842 V vs. RHE), and half- wave potential (0.4616 V vs. RHE) with minimal Tafel slope (154 mV/dec). Thus, nitrogen-doped sugarcane bagasse-derived activated carbon is a suitable candidate for a better separator modifier to hinder polysulfide shuttling in LSBs, anodes for KIBs, and air cathode in MABs.

B 114

Enhanced photocatalytic water splitting using Bi_2O_3/MnO_2 impregnated on ordered mesoporous carbon

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ABSTRACT

In order to meet the escalating energy demand and the declining fossil fuel reserves, it is the need of the hour to find a reliable source of energy with minimum environmental pollution. Hydrogen is considered as one of the promising clean fuel that serves as an input in fuel cell technology. The demand for highly pure hydrogen shifts the source of hydrogen from fossil fuel to other resources. Hydrogen production from splitting of water is a promising technology to produce pure hydrogen. The challenge lies in overcoming unfavourable thermodynamics, slow kinetics, presence of dissolved oxygen, possibility of backward reaction, and competing side reactions. Artificial photosynthesis with a suitable photocatalyst can split water efficiently by capturing solar light. Mesoporous (pore size: 2–50 nm) supported metal oxide photocatalysts are found to be visible light active photocatalysts because of their high surface area and stability. Modified mesoporous carbon is an active photocatalyst with low bandgap. In this study, mesoporous carbon prepared from hard template method using SBA-15 was used as a support, and metal oxides such as Bi_2O_3 and MnO_2 are deposited on mesoporous carbon by wetness impregnation method. All the catalysts were characterized to understand the physico-chemical properties by XRD, BET, FT-IR, SEM, TEM, UV-Visible DRS etc. The photocatalytic water splitting was carried out in a photoreactor. The effect of metal oxide loading, catalyst weight, time, and temperature was optimized. The products were analysed by gas chromatograph using TCD detector. The electrochemical studies of the photocatalyst was also carried out.

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B 115

Electrodeposited composites of Vanadium oxide with polyaniline nanostructures for Supercapacitor Application

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ABSTRACT

Vanadium pentoxide (V_2O_5) is a potential material for energy storage devices due to its good redox characteristics and high theoretical specific capacitance. In this paper, we look at how an electro-deposition process may be used to make V_2O_5/PANI electrode for supercapacitor applications. SEM images show spherical flakes like morphology. At a scan rate 10 mV/s, the as- synthesized V_2O_5 electrode achieved an exceptional specific capacitance of 640 F/g. This finding is significantly greater that most previously reported specific capacitances for V_2O_5/PANI. Showing the electro-deposition technique's efficiency in improving V_2O_5/PANI energy storage capacities. The high specific capacitance attained in this work can due to the V_2O_5/PANI nanoparticles distinctive shape and crystallinity, which were aided by the controlled process.

Key words: V_2O_5, PANI, energy storage, electro deposition

B 116

A green synthetic approach: Ternary NiCoFe layered double hydroxide as a sustainable electrocatalyst for water oxidation

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ABSTRACT

The development of highly effective and long-lasting sustainable electrocatalysts based on earth abundant elements is currently an emerging feature in green energy tecnology. The greenly manufactured ternary NiCoFe-LDH has been found to be an excellent electrocatalyst for the OER process. During the OER process, the ternary NiCoFe-LDH required the lowest necessary overpotential 230 mV (GC) and 250 mV (NF) at 10 mA cm^{-2} when compared to IrO_2 (370 mV). Moreover, ternary NiCoFe-LDH exhibits outstanding OER performance and stability for 150 h in alkaline medium with a potential loss of 2.5%. The solar-powered water oxidation at 1.56 V demonstrates outstanding performance of ternary NiCoFe-LDH for solar to hydrogen conversion. As a result, the greenly synthesised ternary NiCoFe-LDH was superior to the expensive electrocatalysts. As a consequence, low-cost industrial-scale H_2 generation using commercial solar cells might be feasible.

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Incorporation Of Sulfur Sites in NiFe-LDH/NF for Bifunctional Alkaline Water Electrolysis

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ABSTRACT

The growing need for global energy and concerns about greenhouse gases are directing the energy production from hydrogen energy. One of the promising methods to achieve hydrogen fuel is by using electrolyzers to split water and hydrogen. Nickel iron layered double hydroxide is one such electrocatalyst performing equivalent to that of conventional noble metal oxides (RuO_2, IrO_2) for oxygen evolution reaction (OER). However, their charge transfer property, electrochemical active sites towards the H* radicals discard the hydrogen evolution reaction. To emancipate such limitations, mixed anion treatment was carried out in NiFe-LDH with sulfur anions. The fabricated NiFe-S_x-$(OH)_{2-x}$ (x=5, 10, 15, 20 % in atom. %) electrodes were calibrated for water splitting in alkaline condition. The 10 percent sulfur incorporated NiFe-LDH (NiFe-OS10) electrode exhibits the water splitting performance with a minimal overpotential of 90 mV (η_{10}) for HER and 290 mV (η_{20}) for OER half cells in alkaline condition (1 M KOH). The overall cell potential required was 1.60 V @10 mA/cm^2 in the case of bifunctional water electrolysis. The anion mixture of sulphur in hydroxyl anions of NiFe-LDH, their influence in growth, morphology, charge transport and electrochemical interactions are discussed further in detail.

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B 118

Electrochemical Characterization of Hierarchical Porous Tungsten Carbide(WC) Electrodes in Various Electrolytes: Towards Optimized Supercapacitor Performance

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ABSTRACT

Tungsten carbide (WC) has emerged as a promising material for supercapacitor applications due to its unique blend of high electrical conductivity, exceptional mechanical properties, and chemical stability, making it an ideal candidate for advancing next-generation energy storage devices. This study introduces a method for synthesizing porous WC through a single-step mechanochemical process and subsequent heat treatment at 800°C in an argon atmosphere, resulting in WC indexed in the hexagonal phase as confirmed by X-ray diffraction (XRD). High-resolution scanning electron microscopy (HRSEM) and high-resolution transmission electron microscopy (HRTEM) were employed to investigate the surface morphology and topography, revealing the presence of porous nanoparticles with lattice fringes. Electrochemical performance assessments in both acidic and basic aqueous electrolytes. unveiled a charge storage mechanism involving a combination of capacitive and diffusive processes, with capacitive dominance. Consequently, the presented synthesis approach for tungsten carbide (WC) in this study offers a straightforward method for evaluating the performance of various analogous transition metal carbides in the context of supercapacitor applications.

Keywords: Carbide materials, Specific capacitance, Charge Storage mechanism, straightforward method.

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B 119

Hydrothermal Synthesis of Multifunctional Nickel Cobaltite Doped Vanadium Oxide Thin Films for Energy Conversion and Storage Devices

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ABSTRACT:

The multifunctional Nickel cobaltite doped vanadium oxide thin films are deposited hydrothermally on stainless steel substrate. For structural and morphological studies X-ray diffraction and Scanning Electron Microscopy analysis are done. The compositional and elemental mapping analysis are done using X-ray Photoelectron Spectroscopy and Electron diffraction X-ray spectroscopy. Electrochemical analysis is done for various application like supercapacitor, water splitting and urea oxidation reaction (UOR). The mesoporous Nickel cobaltite doped vanadium oxide thin films have exhibited the specific capacitance of 757 F/g at 0.001A/g current density and 509 Wh/Kg of energy density and 6.1kW/g of power density in 1M $LiClO_4$ electrolyte. The specific capacitance shows 93% retention at 2000 cycles. The internal resistance (Rs) of the electrode is only 4.23 Ω. Also, the film shows 1.33V of overpotential for hydrogen fuel generation Subsequently, 1.56 V is demanded for overall UOR catalysis with current density of 10 mA cm−2. This work offers useful information for designing a stable and efficient electrocatalyst for not only UOR but also electrochemical generation H_2 from waste water.

Keywords: Supercapacitor, vanadium oxide, nanoflakes, hydrothermal.

B 120

Hydrothermal synthesis of MnO_2 thin films for energy storage application

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ABSTRACT

Global research interest has been attracted to the increasing need for durable, portable energy storage systems with improved power and energy densities. In present work α-MnO2 thin films are deposited on stainless steel wired mesh substrate using hydrothermal method. Structural, morphological and electrochemical performance of prepared thin films is studied using different characterization techniques. The XRD studies confirms the tetragonal crystal structure of prepared MnO_2 thin films. The electrochemical behavior were studied using three electrode system in 1 M KOH electrolyte. The high electrochemical performance with maximum specific capacitance of 500 F g-1 at scan rate 5 mV s^{-1} and energy density of 75 Wh kg^{-1} at power density of 2.7 kW kg^{-1} has been obtained.

Keywords: α-MnO_2, Supercapacitor, Thin film

B 121

Ag_3PO_4/NiS_2 composite for hydrogen production under acidic condition

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ABSTRACT

Electrocatalytic watersplitting to produce H_2 plays an important role in developing the storage of renewable energy sources. The half-cell reaction (HER) suffers from sluggish kinetics to produce H_2. Despite, the noble metal based catalyst (eg. Pt) are too expensive and economically competitive. So, low cost catalyst have attracted many researches recent years, among which nickel based transition metal dichalcogenides are considered as promising catalyst. A well-known visible light activated semiconducting material Ag_3PO_4 acts as the host material, it has a suitable bandgap for fast transfer of electron-hole pair for producting the hydrogen. This study investigated the use of Ag_3PO_4/NiS_2 composite catalyst for HER activity synthesised by hydrothermal method by varying the weight percentage of NiS_2 as 1, 3, 5 on Ag_3PO_4. The characteristics of the prepared samples are examined using XRD, UV-DRS, SEM, and TEM. This combinational effect of Ag_3PO_4 and NiS_2 played a synergitic role on improving the catalytic activity. The findings for Ag_3PO_4/5 wt% NiS_2 demonstrate a low overpotential, Tafel slope, and value of electrochemical impedance spectroscopy. The results will be discussed.

Keywords: NiS_2, Ag_3PO_4, Composites, Electrochemical studies, Hydrogen evolution reaction

B 122

Cobalt- Copper Based Double Hydroxide as an Effective Electrode Material for Printed Supercapacitor Fabrication

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ABSTRACT

In this work we synthesized copper doped cobalt hydroxide nanoparticles using urea hydrolysis method and successfully employed for the fabrication of printed supercapacitor. The composite material shows very high specific surface area and excellent electrochemical properties. The optimized composition of PVA-KOH gel electrolyte was identified and successfully used for the fabrication of printed supercapacitor. The fabricated supercapacitor exhibited high areal capacitance of 12.27 mF cm^{-2} with 0.8101 µWh cm^{-2} areal energy density and 42.7 µW cm^{-2} areal power density. The supercapacitor showed excellent capacitance retention after several charge discharge cycles. Multiple capacitors were tested in series to show an overall sum of individual potentials and their applications were demonstrated with different electronic devices. Also, high capacitance retention was achieved even at different bending angles and there was no deterioration of the performance after several cycles, thus showing the mechanical stability of the capacitor. Therefore, it's applications range to flexible appliances.

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B 123

Hydrothermal Fabrication of a Dual-Phase 1T/2H MoS_2 Electrode Material for Utilization in Supercapacitor Applications

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ABSTRACT

To cease the usage of non-renewable energy, we investigate renewable sources and the difficulty relay on how to store these kinds of energy. Fortunately, the supercapacitors which play a crucial role in modern day energy storage devices are apt for this kind. In this study, Molybdenum disulphide (MoS_2) which is proposed as the electrode material for supercapacitors synthesized via facile hydrothermal method using ammonium molybdate tetrahydrate (AMTH) and thiourea as the precursors at 200ºC with different reaction time (24,36 and 48 hrs). The experimental parameters include varying reaction time and electrochemical studies of MoS_2. The crystallographic phase, morphology, chemical composition, specific capacitance, and cycle stability were characterized using X-ray diffraction, Field emission - Scanning electron microscope, Raman spectroscopy and Cyclic Voltammetry respectively. Both XRD and Raman studies reveals that the particles formed are of mixed phase (both 2H and 1T) phases. The morphology of the synthesized nanoparticles were alike nanoflowers. From FTIR, the respective functional groups and chemical bonds of molybdenum and sulphur were found. The impact of the reaction time contributes to the refinement of the MoS_2 morphology. Among these, the sample synthesized at 36 h exhibits the excellent specific capacitance of 1000 F/g at 1A/g.

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B 124

Heterostructure of Reduced Graphene Oxide Supported Tin (IV) Sulfide Nanopetals as an Anode Material for Sodium/Potassium-Ion Batteries

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ABSTRACT

Tin sulfide (SnS_2) materials have attracted broad attention in the field of electrochemical energy storage due to its layered structure with high specific capacity. Tin sulfide-reduced graphene oxide (SnS_2@rGO composite) material is investigated as an advanced anode material for sodium/potassium-ion batteries (SIBs and PIBs). In this work, a simple hydrothermal synthesis of ultrathin SnS_2 nanopetals covalently decorated on the surface of rGO is demonstrated as an anode material for SIBs and PIBs. The as prepared SnS_2@rGO displays an initial charge capacity of 749 (at 0.2 A g^{-1}) and 852 mAh g^{-1} (at 0.1 A g^{-1}) for SIBs and PIBs respectively. The SnS_2@rGO hybrid exhibited excellent cycle life which is attributed to the introduction of rGO in the composite as well as the in-built formed C-S bond. Moreover, the rGO matrix, firmly anchored with C–S bonds, envelops the outer SnS_2, effectively inhibiting direct contact between SnS_2 and the electrolyte. These combined effects contribute to impede the irreversible conversion of sulfur to sulfite, thus ensuring excellent structural stability throughout electrochemical cycling. The well-engineered structure not only guarantees the fast electrode reaction kinetics, but also ensures superior pseudo capacitance contribution during repeated cycles which is confirmed by kinetic studies. Thus, SnS_2@rGO is found to be a most promising electrode for sodium/potassium-ion batteries.

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B 125

Ag Decorated CoNi@CN Metal-Organic Framework As Cost-Effective Platinum-Free Efficient Counter Electrodes For Dye-Sensitized Solar Cells

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ABSTRACT

Developing counter electrodes (CEs) with improved catalytic activity has acquired much significance in DSSC applications, as the conventional Pt CEs are highly expensive due to their inadequacy. Concerning this issue, we have reported the efficient catalytic activity of Ag decorated nitrogen doped porous carbon-based metal organic framework (MOFs) (i.e, Ag decorated CoNi@CN) and used as CEs in DSSCs. The structural and vibrational properties were analyzed through X-ray diffraction and Raman spectral studies respectively. The morphology of the prepared MOFs were examined by TEM and SEM analysis. Then the electrochemical properties were studied through cyclic-voltammetry, Tafel polarization and impedance spectroscopy. With the advantages of large specific surface area and high porosity, the prepared MOF based CEs exhibit excellent catalytic activity and improved conductivity. Finally, the photoconversion efficiency (PCE) were evaluated for the fabricated DSSC with the prepared Ag decoratedCoNi@CN as CE. The obtained results shows that the prepared CEs are highly promising for achieving device efficiency.

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B 126

PV voltage Regulation Using Appropriate MPPT for Battery Charging Application

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ABSTRACT

Photovoltaic (PV) power yields varying DC power depending on the intensity of sunlight. However, by using the suitable maximum power points approaches the output of the PV power can be regulated by means of suitable converter. This paper presents the regulation of PV output voltage using fuzzy logic controller (FLC) on MATLAB Simulink through buck boost converter using battery based dynamics loads.

B 127

Electrocatalytic Water Splitting Performance of $SrTiO_3$/g-C_3N_4 Heterostructures Composite for Enhanced Hydrogen Evolution Reaction

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ABSTRACT

Water splitting is a field of research that holds great potential for the production of clean and sustainable energy. In this study, the $SrTiO_3$/g-C_3N_4 composite was designed to enhance the catalytic performance for HER applications. The $SrTiO_3$/g-C_3N_4 composite was prepared by a hydrothermal process involving the combination of strontium titanate ($SrTiO_3$) nanoparticles with graphitic carbon nitride (g-C_3N_4) sheets. The synergistic effect between $SrTiO_3$ and g-C_3N_4 in the composite plays a crucial role in its enhanced performance. This effect not only facilitates charge transfer but also promotes the utilization of solar energy. By combining the unique properties of $SrTiO_3$ and g-C_3N_4, the composite demonstrates improved HER activity, making it a potential catalyst for hydrogen evolution reactions in photoelectrochemical systems. The stability of the composite was investigated over extended reaction periods and utilizing this composite, hydrogen production can be achieved in a sustainable and efficient manner. This offers a promising pathway for the production of hydrogen, a clean and renewable energy source The composite was confirmed by XRD, SEM, FTIR, UV, and Raman Spectra of g-C_3N_4 on $SrTiO_3$.

Keywords: Graphite carbon nitride, Strontium titanate, Perovskite, Ferroelectric Material, Electrocatalysis Heterostructure.

B 128

Effective Hydrothermal Treatment of g-CN for CO_2 Reduction and Photocatalytic Applications

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ABSTRACT

An eco-friendly, inexpensive hydrothermal treatment technique was tried to raise graphitic-carbon nitride's (g-C_3N_4) photocatalytic efficiency. The g-C_3N_4 was hydrothermally treated in deionized water at different temperatures viz 90, 120,150, and 180 ˚C. X-ray diffractograms and FTIR spectra reveal the phase stability of the g-C_3N_4 after hydrothermal treatment by exhibiting the same diffraction planes and Fourier spectrum as pure g-C_3N_4. Optical absorbance spectra show blue shifts with increasing hydrothermal temperature. Pure g-C_3N_4 sample exhibits the band gap value as 2.7 eV and further increasing the temperature slight decrease in band gap value can be observed. SEM and TEM images clearly show the changes in surface morphology after hydrothermal treatment. Nyquist plots were used to study the charge transport mechanisms in all the samples. A degradation study was performed under visible light for 5 ppm,10 ppm, and 15 ppm of Rhodamine B dye. Among all samples, 180 ˚C samples show high efficiency (72%) for the dye degradation due to fast charge transfer and low recombination rate

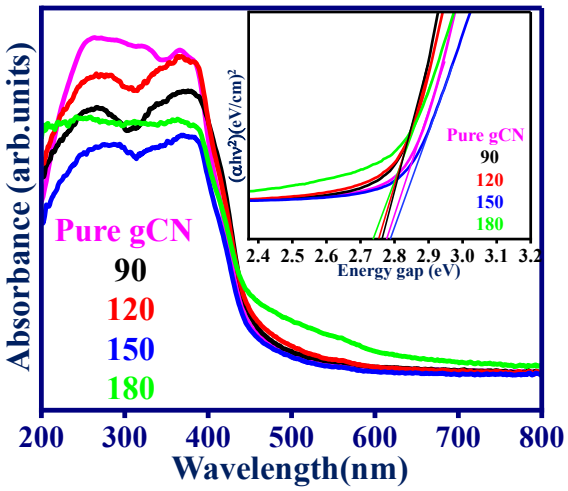

Fig.1-Absorbance Spectra of g-CN at various temperatures

B 129

Synthesis of $BiVO_4$/g-C_3N_4 and their Photocatalytic Water Splitting

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ABSTRACT

In a simple wet chemical approach, we had synthesised the Z-scheme type $BiVO_4$/g-C_3N_4 nanocomposite. Initially conducted X-ray diffraction technique had revealed the chemical and crystalline purity of the specimens. Further, morphology of the nanomaterials were well studied with the electron microscopes. Besides, we had studies the Raman spectroscopic analysis and X-ray photoelectron spectroscopic measurements of the nanocomposites. The optical absorption had revealed the enhanced absorption in the nanocomposite. When exposed to visible light, the BVO-CN photocatalysts demonstrated an overall catalytic water splitting activity of up to 177 μmol h−1 for H_2 production and 80.3 μmol h^{-1} for O_2 evolution in an application. For the increased photocatalytic activity, a potential Z-scheme mechanism is put forth and further supported by electron spin resonance spectroscopy. By creating a 2D nanoplates morphology, this study showed improved overall water splitting photocatalytic performance of $BiVO_4$/g-C_3N_4 photocatalyst and provided insight into the morphology design of Z-scheme semiconductor materials.

B 130

Ag doped SnS_2 Nanocomposites as Highly Efficient Counter Electrodes: A Hierarchical Nanostructures for Pt-Free Dye-Sensitized Solar Cell Application

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ABSTRACT

Recently, the layered SnS_2 has obtained more attention in the field of DSSC as a counter electrode (CE) material owing to its high catalytic activity. Despite this, the material with poor electrical conductivity will reduce the performance of the device during redox reactions. In this work, we proposed Ag-doped SnS_2 as a CE material. By varying the concentration of Ag, the aggregation of SnS_2 and the interface formation between materials has been studied. The studies that were conducted revealed a significant enhancement in the performance toward the reduction of electrolytes. The studies include XRD, SEM, TEM, BET, XPS, CV, EIS, Tafel, and I-V characteristics. The nanocomposites were prepared by a simple solvothermal method and morphological analysis shows the interface formation between the Ag and SnS_2, exhibited a high surface area which is helpful in providing more active sites for electrode-electrolyte interaction. The electrochemical measurements show low Epp values and lowest Rct values for the SA5 sample. With the obtained results we performed the I-V characteristics and sample SA5 exhibits the highest efficiency thus showing the excellent performance of the prepared counter electrode and should act as a replacement material for Pt CE in DSSC.

B 131

Development of Double-Doped Ceria and Barium Cerate Nanocomposite System as Electrolytes for It-SOFCs

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ABSTRACT

The present study focuses on developing a composite electrolyte material for Solid Oxide Fuel Cells (SOFCs) that operate at intermediate temperatures (400-600°C). In comparison to single perovskite materials, our investigation reveals a substantial enhancement in the ionic conductivity of the electrolyte when using a composite of perovskite and double-doped material. The chosen material for the IT-SOFC electrolyte, Double-doped ceria and barium cerate (SSRDC/BCO) nanocomposite, proves to be highly promising. The synthesis process involves creating the perovskite material BaCeO3 (BCO) using the combustion technique, with its structure verified through X-ray diffraction (XRD) and ionic conduction studies. Concurrently, double-doped ceria (optimized system ($Ce0_{.85}Sr_{0.075}Sm_{0.075}O_2$-d)) is synthesized through the Hydrothermal technique. The composite is formed with varying concentration ratios, namely 20-80, 30-70, 40-60, and 50-50, respectively. The confirmation of the composite structure is achieved through X-ray diffraction (XRD), and the data fitting is accomplished using Rietveld refinement with the Full-Prof suite. The electrical properties of gas-tight dense pellets comprising the composite material system are thoroughly explored using Impedance spectroscopy in the temperature range of 250-650°C. The results indicate a notable increase in conductivity, reaching up to 1-2 orders of magnitude in the case of the composite. Structural analysis of the composition is carried out using Field Emission Scanning Electron Microscopy (FESEM), revealing the formation of nano-sized particles. These findings collectively underscore the potential of the Double-doped ceria and barium cerate nanocomposite as an advanced electrolyte material for SOFCs operating at intermediate temperatures.

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B 132

Investigations of Physical and Electrochemical Properties of Tin Sulfoselenide (SnS_xSe_{x-1}) Synthesized Using Planetary Ball Milling

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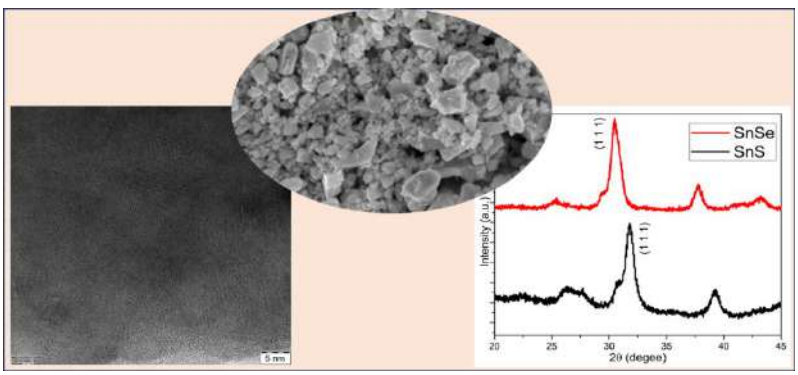
ABSTRACT

Tin sulfide (SnS) and tin selenide (SnSe) are among the most prominent binary compounds with their tunable direct bandgap and electrical properties, which make tin sulfoselenide (SnS_xSe_{1-x}) to be further explored in terms of bandgap and hence tuning optical properties. SnSSe powder was synthesized via high energy planetary ball milling method. The milled powder was characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), Raman spectroscopy, UV-Vis spectroscopy, photoluminescence, scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS). The electrochemical analysis of the SnS_xSe_{1-x} powder is done with the aid of cyclic voltammetry (CV) and Galvanostatic charging and discharging (GCD). XRD patterns revealed that the synthesized bulk powder exhibited single phase polycrystalline orthorhombic structure with a preferred orientation along (111) crystallographic plane. Micro structural properties of SnS_xSe_{1-x} compounds such as crystallite size, dislocation density, micro strain, number of crystallites per unit area, stacking fault probability and texture coefficient were calculated from the predominant (111) diffraction lines. The optical band gap value was calculated from reflection data. SnSSe thin film direct transition optical band gap found to be in the range of 1.08–1.25 eV. The electrochemical performance of SnS_xSe_{1-x} compounds are analysed using different electrochemical tools to find the specific capacitance of the materials and to check which composition is best suited for electrochemical sensors and energy conversion devices.



B 133

NiO/g-C_3N_4 Hybrid Materials for Sustainable Energy Storage

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ABSTRACT

Owing to the depletion of fossil fuels, there is a rising demand for efficient energy storage systemsto satisfy future energy demands. In this context, NiO has been regarded as a potential electrode material for next-generation supercapacitor devices because of its high theoretical capacitance [1]. However, the real-time application of NiO as an electrode material is obstructed by its limited cyclic stability. All carbonaceous materials possess EDLC behaviour where charge storage takes place as a result of the adsorption of ions at the electrode interface. On the contrary, the charge storage mechanism of metal oxides is based on the faradaic reactions. As a result, the latter outperforms the former in the case of charge storage but lacks conductivity and cyclic stability. Therefore combining carbon-based materials with pseudocapacitive materials is one of the greatest ways to increase the energy density of the supercapacitor without compromising its power density and cycle stability. Herein, we demonstrate NiO/g-C3N4 hybrid composite as a potential electrode material for supercapacitors. The porous nature of the electrode materials as revealed from the FESEM images facilitates faster ion transport and smooth interaction of electrode with electrolyte. Furthermore, the electrochemical performance of the developed electrode materials is analyzed bycyclic voltammetry and galvanostatic charge-discharge in a three-electrode system under 6M KOH electrolyte. NiO/g-C3N4 composite (1:1 ratio) exhibited higher specific capacitance (186 F/g) compared to pristine NiO (172 F/g) at a scan rate of 20mV/s. The excessive performance of hybrid composite can be attributed to the increased number of active sites. This study thus promotes the development of a cost-effective electrode material without compromising the device performance.

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B 134

Electrochemical Studies of Uio-66-NH_2 Prepared in the Presence of Different Modulators

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ABSTRACT

The UiO MOFs are three-dimensional porous materials, constructed by Zr^{4+} and dicarboxylic acid ligands. UiO MOFs have drawn extensive attraction lately due to the wide possible application in various fields such as membranes, featuring luminescence, magnetic properties, drug delivery, molecular sensing and detection, adsorption and separation, gas storage, catalysis, and so on [1] due to their incredible properties: very high surface area as well as high thermal stability, exceptional tunability and functionality, high adsorption capacity which is leading to efficient performance in activity and selectivity [2]. However, a new era of synthesizing high-quality UiO-66 using modulators provides exceptional control over the growth and improved reproducibility and crystallinity[3]. In this work, we discuss the effect of various kinds of modulators on the electrochemical properties of UiO-66-NH_2. We employed carboxylic acid modulators; acetic acid (AA), formic acid, (FA), and benzoic acid (BA), and also noncarboxylic acid modulators; water and HCl. The structural, morphological, and elemental studies of the sample were studied by XRD, FTIR, BET, and SEM. Electrochemical studies (LSV, CV, stability, and EIS) were performed in detail.

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B 135

Electrochemical Study of Novel Organic–Inorganic (PVA/PVP-ABO3) Nanocomposite Proton Conducting Membrane for HT-PEMFCs

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ABSTRACT

In the present study, organic-inorganic nanocomposite membranes constituted by (PVA-PVP) - ABO_3 ($BaCeO_3$/$BaZrO_3$-$SrCeO_3$/$SrZrO_3$) were synthesized for the first time, specifically designed as proton exchange membranes for high-temperature proton exchange membrane fuel cells (HT-PEMFC). Proton-conducting materials based on perovskite ceramic ABO_3 were meticulously prepared through the sol-gel combustion method. Utilizing the solution casting method, PVA-PVP-ceramic nanocomposite membranes incorporating $BaCeO_3$, $BaZrO_3$, $SrCeO_3$, and $SrZrO_3$ nanoparticles in various compositions were developed. The structural characteristics were verified through X-ray Diffraction (XRD) and FTIR, while thermal analysis was conducted using Thermogravimetric Analysis (TGA). Scanning Electron Microscopy (SEM) confirmed the uniform dispersion of ceramic particles within the polymer membrane. Impedance spectroscopy revealed the proton-conducting ability of the composite membranes, and the dynamics of proton ion conduction were elucidated through electric modulus spectrum analysis. The composite membrane exhibited commendable mechanical strength and thermal stability, maintaining its integrity up to 140°C. Notably, the poly(vinyl alcohol)-poly(vinyl pyrrolidone)-$BaCeO_3$ (PPBCO) composite membrane shown exceptional proton ion conductivity, reaching a maximum of 1.32 x 10^{-2} S/cm at 120°C compared to PVA, PVA-PVP, and other hybrid composites. This heightened conductivity was achieved through phosphoric acid doping. The phosphoric acid-doped composite membranes, comprising poly(vinyl alcohol)-poly(vinyl pyrrolidone)/barium cerate ($BaCeO_3$), exhibit substantial potential for efficiency in high-temperature proton exchange membrane fuel cell (HT-PEMFC) applications.

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B 136

2D Based Counter Electrode Emergent Materials in DSSC: Short Review

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ABSTRACT

Scientists should come forward with choices for replacing limited and hazardous fossil fuels due to the serious energy and environmental emergencies of our recent era. Scientists are motivated to create solar cells to transform natural sunlight into electricity because the sun provides a no-cost and plentiful source of renewable energy. The counter electrode (CE) is a key component of a dye-sensitized solar cell (DSSC) that serves as the redox process and it typically depends upon scarce Pt. To raise awareness of two-dimensional (2D) materials is imperative to replace expensive CEs with effective, affordable alternatives. Graphene, carbon nanotubes, polymers, and particularly transition metal dichalcogenides (TMDs), their hybrid systems are currently proposed as an innovative approach to electronic devices due to their unique features in recent years. There is a need for an obvious categorization of 2D materials-based counter electrodes as well as an in-depth discussion of fresh perspectives on electrode fabrication and optimization techniques due to the increasing number of studies and scientific publications on 2D counter electrodes that are being reported. A worldwide investigation on DSSCs counter electrodes to speed up the researchers' pursuits in this field is essentially defined by examining the latest and most reputable studies. 2D materials have been utilized as CEs in this short review that has mostly been graphene sheets, whether they are pristine, doped, or composite, and also TMDs-based CEs. Most prevalent characterization techniques and experimental procedures are examined in all topics along with an introduction to their greatest effective structures.

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B 137

Hierarchically Porous Niobium Carbide as a Novel Electrode Material for Supercapacitors

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ABSTRACT

Given the fast population increase and industrial development, environmental and energy constraints are deemed among the major concerns. Electrochemical energy storage devices such as supercapacitors, batteries, and fuel cells have superseded intermittent renewable energy sources in meeting the energy demands of society due to their cost-effectiveness, eco-friendly nature, stable cycling, and greater operating efficiency. Among them, supercapacitors owing to their greater charge-discharge rate, power density, capacitive retention, reliability, safety, and extended cycle life have gained prominence in recent years. However, the relatively low energy density of SCs precludes their applicability in certain fields. In this regard, transition metal carbide electrodes are considered potent due to their higher melting point, hydrophilic nature, good electrical conductivity, mechanical stability, structural stability, and chemical stability. In this regard, the present study mainly focuses on the fabrication of binder-free novel niobium carbide electrodes with a three-dimensional porous morphology via the vapor phase growth method. The physicochemical studies confirmed the uniform deposition of niobium carbide over the 3D porous structure. Further, the as-prepared electrodes demonstrated better electrochemical characteristics when tested for their efficiency using various analyses, such as CV, GCD, and EIS affirming the potential of niobium carbide as prominent negative electrodes in supercapacitors.

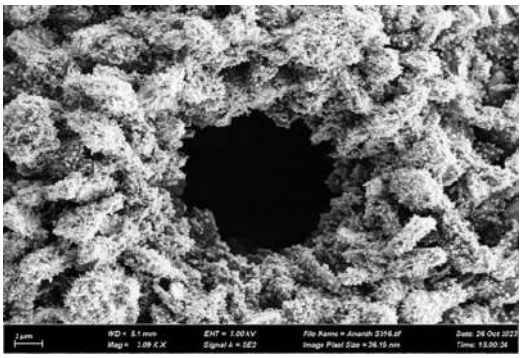

Figure 1: SEM micrograph of Niobium Carbide Electrode

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Dendrimer like Boron Nitride Grown on 3D Porous Metallic Framework as Electrodes for Supercapacitors

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ABSTRACT

Electrochemical energy storage systems such as batteries, supercapacitors, and fuel cells can effectively route to sustainable energy. Supercapacitors, in particular, are recommended due to their fast charge-discharge mechanism, improved power execution, energy density, and long life cycle. Carbonaceous compounds, polymers, and transition metal oxides used as potential electrode materials for supercapacitors have drawbacks such as lower energy density, cycling stability, structural stability, and so on. This necessitated the development of electroactive materials with a huge specific surface area, cyclic stability, and electrical conductivity for improving the performance of supercapacitors. In this regard, transition metal nitride electrodes belonging to a class of transition metal compounds are considered potent due to their outstanding chemical characteristics, catalytic activity, high electrical conductivity, wide potential window, wettability, mechanical stability, and high capacitance making them commercially viable. The present study investigates the fabrication of highly porous boron nitride-based supercapacitor electrodes via the vapor phase growth method, where the as-prepared electrodes demonstrated better electrochemical characteristics when numerous analyses were used to assess their efficacy such as CV, GCD, and EIS. Their improved performance can be ascribed to the greater charge-discharge withstanding capacity of the electroactive material and the binder-free electrode configuration facilitating greater ion through its strong active material interlinking network and consistent pore channels, making boron nitride an efficient electrode for supercapacitors.

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B 139

Local Structural & Charge Relaxation Study of Gd doped $La_2Ce_2O_7$ Pyrochlore System

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ABSTRACT

The pyrochlore-based system is gaining significant attention as a solid electrolyte in electrochemical energy devices, particularly solid oxide fuel cells (SOFC) due to its high proton-ion conductivity at the Low-temperature range (250-450°C). In this study, we investigate the $La_{2-x}Gd_xCe_2O_7$, pyrochlore system doped with strontium (Gd), where, x = 0, 0.02 and 0.04, 0.06, 0.08 and 0.1 with the aim of developing a proton-ion conductor as an electrolyte for Low-temperature SOFCs (LT-SOFCs). Structural information is collected from an X-ray diffraction tool and confirmed it through data analysis using the Rietveld Refinement technique. Raman spectroscopy reveals detailed insights into the dopant-induced local restructuring in the Lanthanum Cerate lattice. Ionic conductivity and activation energy data are extracted through AC impedance measurements. The ionic relaxation and ion hopping dynamics and its effect on ionic conductivity are revealed from the electric modulus study. M" relaxation peak and its distribution in relaxation time are analyzed using the Kohlrausch-Williams-Watts (KWW) fit. The presence of dopants induced structural deformations and oxygen vacancies in the LCO host lattice, leading to the disordering of vacancies and modifications in the stretching exponent 'β' and activation energy. Cooperative hopping dynamics through ion-vacancy interactions are found to be a notable influence on protonic conductivity. The optimized dopant composition of LGCO exhibits the highest conductivity peak. This suggests that apart from vacancy concentration and energy barriers for single-ion hopping, the cooperative dynamics of oxygen ions play a crucial role in determining the ionic conductivity values. Consequently, the LGCO system demonstrates potential for application as an electrolyte in Low Temperature-SOFCs.

Keywords: *Gd-doped $La_2Ce_2O_7$ pyrochlore; ionic conductivity, Charge relaxation; Ion-hopping dynamics.*

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Electrochemical Study of Superparamagnetic Manganese Ferrite for Supercapacitor Application

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ABSTRACT

Sustainable energy conversion and storage technologies are essential to modern society to meet the increasing energy demands. Among various energy storage technologies, supercapacitors have piqued the interest of scientists because to their high-power density, long cycle life, and fast charge/low discharge rates. They have a wide range of uses, including portable electronic devices, power backup, hybrid electric automobiles, and a variety of microdevices. Driven by the above-mentioned initiatives, extensive efforts are being undertaken to develop and improve the quality of the electrode material. Ferrites are one of the oxide spinels that excel in a variety of sectors due to their exceptional structural, optical, electrical and magnetic properties as well as their ability to exhibit different redox states and electrochemical stability. Among these, Manganese ferrite ($MnFe_2O_4$) has gained a lot of attention due to its environmental friendliness, multiple valences, large theoretical capacity (928 mAh/g), and affordable cost. Particularly interest in the application of $MnFe_2O_4$ in supercapacitors is due to their high pseudocapacitance, multi oxidation states of Fe and Mn ions which facilitates rich faradaic redox reaction, high power delivery, and high cycling stability. In fact, the use of $MnFe_2O_4$ in electrode material increases available active sites and also reduces the path lengths of OH-ion diffusion. The present work investigates the structural, magnetic and electrochemical properties of $MnFe_2O_4$. Single Phase Manganese ferrite was synthesized using sol-gel method and investigated as an electrode material for supercapacitors. The electrochemical properties of $MnFe_2O_4$ electrodes were studied in detail by assembling a three-electrode setup and carrying out cyclic voltammetry (CV), Chronopotentiometry (GCD) and AC impedance measurements. The impressive electrochemical performance makes $MnFe_2O_4$ electrodes a promising electrode material for high-performance supercapacitor applications. MnFe2O4 exhibits a higher specific capacitance of about 522 F/g (5 mV/s) in 3M KOH. This higher specific capacitance can be attributed to smaller crystallite size, more electroactive sites, high porosity and multiple valence states of Fe and Mn ions, as confirmed by XRD, FESEM and XPS analysis. Magnetic studies reveals that $MnFe_2O_4$ exhibit a superparamagnetic behaviour. The underlying physics for the unique magnetic and electrochemical properties of $MnFe_2O_4$ will be thoroughly discussed.

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Synthesis of g-C_3N_4/$NiFe_2O_4$/PANI Composite as a Supercapacitor with Improved Electrochemical Performance for Energy Storage applications

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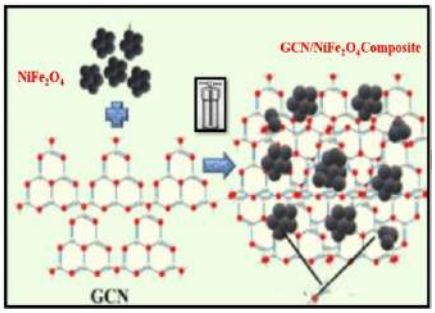
ABSTRACT

The unique dimensional (3D) porous structure of graphitic carbon nitride hybrid(g-C_3N_4), Nickel ferrite ($NiFe_2O_4$), and PANI composite was prepared by hydrothermal method followed by in situ polymerization. The electrochemical performance of g-C_3N_4/$NiFe_2O_4$/PANI was assessed as an electrode material for supercapacitor application by cyclic voltammetry (CV), Galvanostatic Charge-discharge (GCD) and Electrochemical impedance spectroscopic (EIS) techniques. Excellent chemical stability and cheap cost characterize g-C_3N_4, a material that facilitates electronic transmission in this direction by supporting vertical charge transfer during the charge-discharge process. In addition, $NiFe_2O_4$ has good theoretical capacitance, while PANI has excellent reversible redox reaction electrical conductivity and chemical stability. The specific capacitance of the g-C_3N_4/$NiFe_2O_4$/PANI composite was observed to be 770 Fg^{-1} by GCD studies, while it exhibited 75% retention of its initial capacitance even after 2000 GCD cycles. This study revealed that g-C_3N_4/$NiFe_2O_4$/PANI is a potential electrode material for supercapacitor application.



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B 142

Fabrication of Water Hyacinth-Derived Activated Carbon Hybrid Electrodes with Conducting Polymers for Enhanced Supercapacitor Performance

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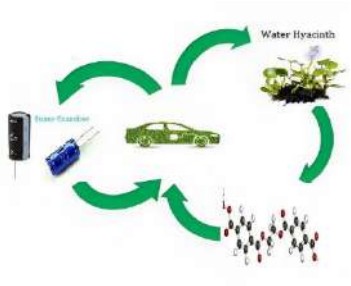
ABSTRACT

The escalating need for sustainable energy storage technologies has spurred interest in deriving electrode materials from renewable and eco-friendly sources. In this study, we present the fabrication of hybrid supercapacitor electrodes using carbon derived from water hyacinth (WH)an abundantly available aquatic weed. The WH serves as an excellent substrate for the deposition of conducting polymers: polyaniline (PANI), polypyrrole (PPy), and poly(3,4-ethylenedioxythiophene) (PEDOT). Each hybrid electrode was systematically synthesized via a simple *in-situ* polymerization method and subjected to rigorous electrochemical assessments. Preliminary results revealed that all conducting polymer hybrids showcased improved capacitive behavior compared to standalone WH. Notably, the WH/PPy hybrid electrode outperformed its counterparts, registering the highest specific capacitance. This enhancement can be attributed to the synergistic interaction between the porous structure of WH and the exceptional electronic conductivity of PPy. Our work elucidates the potential of utilizing water hyacinth as an eco-friendly precursor for advanced supercapacitor electrodes, with PPy emerging as the most promising conducting polymer for augmentation. This dual-fold approach, harnessing an environmental challenge for energy storage advancements, sets a precedent for future green energy research initiatives.



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B 143

Nanopower Matrix: Coreshell Nanoparticles Adorning Lithium MOF Battery for Enhanced Performance

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ABSTRACT

Lithium-Ion Metal Organic Framework (Li-MOF) has emerged as an important, yet highly challenging class of electrochemical energy storage material; we would like to use lithium-BTC and lithium-3 AMT as well as both together as a combination due to its dynamic applications such as electrochemical performance, capacity of storage, cycling stability and rate capabilities. The synthesis method, including solvothermal and hydrothermal techniques as employed to tailor the MOFs characteristics for optimal battery performance. This all will be an eco-friendly cause will use these MOFs with doping of Mn, Ni core-shell nanoparticles by sonication method developed by green synthesis process and synthesis of new cathode material. This research will be applicable to addressing challenges such as capacity degradation and safety concern associated with lithium-ion batteries and we would expect that it would unlock the full potential of lithium MOF based system and propel the evolution of next generation energy storage device.

Keywords: Li-BTC & Li-3AMT MOF, core-shell nanoparticles, eco-friendly battery, etc.

B 144

Structural And Electrical Properties of Novel Lanthanum Orthophosphate ($LaPO_4$) As Solid Electrolyte For Low Temperature Solid Oxide Fuel Cell

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ABSTRACT

Lanthanum orthophosphate is specially explored as prospective materials (1) for electrolytes of low temperature solid oxide fuel cell as facilitated mixed ion (oxygen and proton) conductivity at the temperature range (250 - 450 ° C) of SOFCs, (2) phosphor materials in the production of phosphor-based light emitting devices and few more as catalysis and biomedical applications, etc. In the present attempt, Lanthanum orthophosphate system is developed as electrolytes for LT-SOFCs. Pure phase LaPO4 was synthesized by using sol-gel synthesis method. Crystalline phase is achieved by heating the as-synthesis powder at 350 ° C for 5 hrs (optimized conditions). Structure of pure phase compound is confirmed by X-Ray diffraction (XRD) and it is found to be matched with single phases Monoclinic structure (JCPDS file-32-0493). To get more structural clarity, XRD data is simulated with Rietveld refinement using full prof suit open source. Obtained fitted parameter after Rietveld refinement ensure structural quality of developed sample. Raman spectroscopy study of the system performed to get more in-depth structural information of the system. Microstructure of the as-calcined $LaPO_4$ sample is revealed by Scanning Electron Microscopy (SEM). The ionic conductivity measured for the temperature range 250-650 ° C by using AC impedance spectroscopy to reveal its conductivity nature and prove its suitability for LT-SOFCs.

Keywords: Fuel cell, Phosphate, Lanthanum, Orthophosphate

B 145

Structural and Charge Relaxation Study of Gd, W co-doped $La_2Mo_2O_9$ System: Electrolyte for IT-SOFCs

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ABSTRACT

Gadolinium and tungsten co-substituted variants of lanthanum molybdate, characterized by the nominal formula $La_{2-x}Gd_xMo1.7\ W_{0.3}O_{9-d}$ (x=0.0, 0.1, 0.2, 0.3) and denoted as LMXG, were synthesized using the Pechini method. Structural analyses employing X-ray diffraction (XRD) and angle dispersive X-ray diffraction (AD-XRD) were conducted, and the obtained data were well-fitted utilizing Rietveld refinement with the Full-Prof suite. The XRD results revealed a cubic structure with a P 213 space group for both pure and co-doped LMX samples, confirming the co-dopant induced suppression of the order-disorder phase transition temperature of LMX. Further structural investigation through AD-XRD unveiled the monoclinic structure of pure LMX, characterized by the space group P 21. Raman spectroscopy provided detailed insights into the dopant-induced local restructuring within the Lanthanum molybdate lattice. Dielectric relaxation was examined through dielectric loss spectra, and AC impedance measurements were employed to extract data on ionic conductivity and activation energy. The outcomes indicated that co-doping enhances the oxy-ion conductivity compared to pure LMX. Notably, $La_{1.7}Gd_{0.3}Mo_{1.7}W_{0.3}O_9$ (LMXG3) exhibited a higher ionic conductivity of approximately 2 x 10^{-2} Scm^{-1} at 650°C, surpassing the conductivity of the pure LMX sample and other co-doped LMX variants. This investigation underscores the potential of the Gd and W co-doped LMX system as a solid electrolyte for intermediate-temperature solid oxide fuel cells (IT-SOFCs).

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B 146

N, S co-doped and boron doped Artocarpus heterophyllus wood derived Activated carbon for Supercapacitor Application

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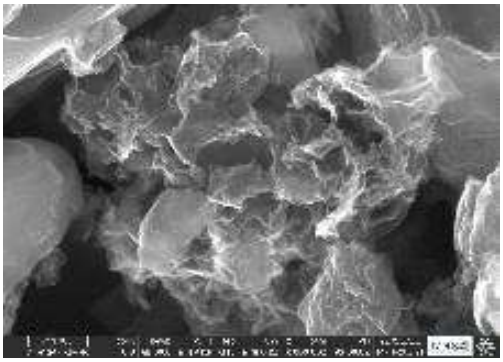
ABSTRACT

N,S co-doped porous carbons show appreciable prospects for various application in energy storage devices like Li-ion batteries and ultracapacitors due to its excellent surface wettability large electrical conductivity, better surface area, cost effectiveness and enormous pseudocapacitance. In this work, a prospective hierarchical N,S co-doped porous carbons synthesized by a sustainable method through one step carbonization and subsequent activation process by utilizing renewable Artocarpus heterophyllus wood as the primary source material with no templates and additional nitrogen source. The prepared Artocarpus heterophyllus wood derived porous carbons possess a huge specific surface area of 1094 m^2g^{-1} hierarchically ordered porous framework. Hence, a prospective electrode material for supercapacitor applications was successfully developed by a simple synthesis route with naturally available renewable resource Artocarpus heterophyllus wood.



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B 147

Dual-Capable Spinel Cobalt Oxide Nanoparticles for Electrocatalytic Oxygen Evolution and Contaminant Removal

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ABSTRACT

In this work, we focused on synthesis and electrocatalytic performance for the oxygen evolution reaction of cobalt oxide (Co_3O_4) nanoparticles, a promising metal oxide in electrocatalysis. As well as we studied its role in water treatment as a contaminant removal. Its tunable properties and nanoscale engineering potential for efficient Oxygen Evolution Reaction (OER) are highlighted, along with its capacity for adsorption and oxidation of contaminants. Fine cobalt oxide nanoparticles are produced by the sol-gel method followed by different sintering temperatures. To understand the impact of sintering temperature on surface morphology, size and shape of nanoparticles, FESEM and HRTEM characterizing tools are used. Thin film electrodes of Co_3O_4 are prepared by the doctor blade method and used to study linear swap voltammetry (LSV), and electrochemical impedance spectroscopy (EIS). The cobalt oxide electrode sintered at 600°C shows the highest catalytic activity with 258 mV overpotential at 10 mA cm-2current density and 17.33 mV sec-1 Tafel slope. It also shows excellent stability (10hrs) for OER in 1M NaOH. The role of these nanoparticles in water treatment is also focused. Experimental results demonstrate that lower sintering temperatures enhance electrocatalytic properties, contributing to the advancement of sustainable energy and water treatment technologies.

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B 148

Bimetallic Organic Framework (BOF) With Metal Node Engineering for Energy Storage Application

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ABSTRACT

Carbon cloth supported binder-free cobalt nickel based bimetallic organic framework (BOF) was grown by in-situ deposition of a template. The CoNi-MOF electrode employed as the positive electrode for supercapacitors (SCs) delivered well-pronounced conductivity, a high areal capacity (C_a) 2041 mC cm^{-2} at 2 mA cm^{-2} withstanding beyond 5000 continuous charge and discharge cycles. The outstanding electrochemical profile of CoNi-MOF electrode can be ascribed to the large surface area with ample redox sites, uniformly distributed layered architecture and multiple chemical states of the metals (Co and Ni). The asymmetric device assembled with (CoNi-MOF@CC// O, N, S@AC@CC) resulted in outstanding specific capacity of 125 Cg^{-1}, with high energy and power densities. On top of it the device has an appreciable stability by remaining intact even after 10,000 continuous charge and discharge cycles. This can shed light on fabricating flexible energy storage devices for portable electronics.

Keywords: *Bimetallic organic framework (BOF), metal node engineering, layered architecture, multiple chemical states, and flexible energy storage devices*

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B 149

Fabrication and Comparison of MOF-Derived Bunsenite of Various Solvents as Electrodes for Supercapacitor

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ABSTRACT

Efficient materials with high Specific capacity and long stability are highly desirable materials for supercapacitors. Here, Bunsenite(NiO) green crystalline was synthesized by the Hydrothermal method with various solvents like Water, ethanol, DMF, and ethylene glycol. The crystallographic morphology structure and phase purity of Nickel oxide (Nio) are investigated by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and Fourier transform Raman spectroscopy (FT-Raman). The electrochemical measurement of fabricated (Nio) was carried out by a series of Cyclic Voltammetry (CV), Galvanostatic charge-discharge (GCD), and Electrochemical impedance Spectroscopy (EIS).

Keywords: *Bunsenite, Hydrothermal, Supercapacitor, Solvent*

B 150

Synthesis and Electrochemical Characteristics of SnO_2 /GO Nanocompite as anode for Lithium-Ion Battery

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ABSTRACT

The study investigate the synthesis and characterization of Tin oxide (SnO_2) nanoparticles integrated with graphene oxide (GO). The SnO_2@GO composite exhibit high specific capacity ,a long term stability and excellent high rate capacity .The crystallographic structure is investigated by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and Fourier transform Raman spectroscopy (FT-Raman).The electrochemical performance of the prepared electrode was investigated by series of Cyclic Voltammetry (CV), Galvanostatic charge discharge (GCD) and Electochemical impedance Spectroscopy (EIS).

Keywords: *SnO_2, graphene oxide, electrode.*

B 151

A Facile Electrochemical Etching Route for Preparing $Ti_3C_2T_X$ MXene Using Low Concentration Electrolyte with Enhanced Electrochemical Performance

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ABSTRACT

The significant investigation currently being conducted focused around MXene-based super capacitors because of their remarkable flexibility and high electrochemical performance. Today's increasingly widespread use of super capacitors brings them to an extensive spectrum of challenging conditions. In this study we successfully synthesised the $Ti_3C_2T_X$ MXenes from Ti_3AlC_2 pristine electrode using a milder hydrochloric acid through electrochemical etching method. In this study, scalable $Ti_3C_2T_X$ MXenes are synthesized through intercalation of ions into Ti_3AlC_2 and etching of 'Al' layer from Ti_3AlC_2 to synthesise $Ti_3C_2T_X$ MXenes under significantly favourable conditions. The synthesised MXenes are characterised through XRD, XPS, SEM, and Raman analysis to confirm the synthesis of MXenes. High capacitance and good cycling stability can be achieved by this simple and scalable process for creating high- performance super capacitors. Our electrochemical approach broadens the spectrum of etching processes and subsequent MXene compositions that can be used to make a good super capacitor.

Keywords: *MAX phase, MXenes, etching, intercalation, XRD, XPS, SEM, Raman analysis, Capacitance, performance*.

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Synthesis and Characterization of Vanadium Pentoxide Composite with Graphitic Carbon Nitride Nanoparticles for Supercapacitor Applications.

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ABSTRACT

Supercapacitors are required-after energy storage technologies due to their increased power density, long-term cycle stability, and quick rate of operation. Vanadium pentoxides have drawn the great attention of electrochemists despite the fact that metal oxides are important components of energy storage systems because of its multi-valency, potential window, distinctive layer structure, low cost, and wide availability. Even though its poor electrical conductivity and ionic diffusivity, vanadium pentoxide generally has a low specific capacitance. However, to improve the sample doped or composite with carbon-based material graphitic carbon nitrate. The physiochemical behaviours of as synthesized material were examined by X-ray diffraction analysis, FT-IR spectroscopy, scanning electron microscopy, cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The Galvanostatic Charge-Discharge technique was used to determine the specific capacitance of V_2O_5/g-C_3N_4 nanoparticles.

Keywords: *V_2O_5, X-ray Diffraction, Cyclic Voltammetry, GCD, Electrochemical Impedance Spectroscopy and Scanning Electron Microscopy*.

B 153

Modulating Molecular Architecture: Tailoring Metal-Free Organic Polymers for Water Electrolysis

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ABSTRACT

The oxygen evolution reaction (OER) is of crucial importance in the quest to improve the efficiency of water electrolysis. It is essential to overcome the ongoing difficulties related to creating electrocatalysts that have a high current density, low overpotential, and long-lasting performance. An alternative electrocatalyst, devoid of metal, is proposed as a potential solution for efficient water electrolysis via the oxygen evolution reaction (OER) under alkaline conditions. The copolymer CMP1, including poly(triarylamine-thiazolo[5,4-d]thiazole), exhibits exceptional effectiveness and long-lasting performance, surpassing many existing catalysts utilized for comparison. This study highlights the challenges faced in OER electrocatalysis, the novel metal-free architecture of CMP1, its remarkable efficacy, and its potential impact.

B 154

Influence of Annealing Temperature on Structural and Electrochemical Properties of $MgFe_2O_4$ as Anode Material for Supercapacitors

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ABSTRACT

The world is facing a critical energy crisis caused by excessive consumption of fossil fuels and resulting environmental pollution. This is a challenge that needs to be addressed with urgency. Energy storage technology has become increasingly important in this context. Supercapacitors have been identified as a promising energy storage system due to their high specific capacitance, power density, and longer cycle life. However, their performance is limited, specifically in terms of low energy density and stability. Our research aims to overcome these limitations by focusing on increasing the specific capacitance of an electrode at the electrode-electrolyte interface. Spinel ferrites have emerged as a highly promising material for electrochemical analysis due to their multiple oxidation states of cation present in the material and their interesting surface redox activity at the interface. Our study focuses on the structural and electrochemical properties of Magnesium Ferrite as an anode material in neutral aqueous electrolytes. We synthesized the material by the sol-gel method and annealed it at different temperatures. Our X-ray analysis revealed a wider phase change in the material at higher temperatures. The electrochemical measurements demonstrated reversible and redox pseudo-capacitance, with the material annealed at 500ºC exhibiting the highest specific capacitance of 117 F/g at a current density of 0.5 A/g [1]. This material retains its capacitance of 58%. Our research holds tremendous potential for overcoming the limitations of supercapacitors and contributing to the development of more efficient and sustainable energy storage systems.

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B 155

Advancements in Proton-Conducting Solids: Materials, Properties, and Applications

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ABSTRACT

Proton conduction requires special host materials unlike electron conduction which is favorable in most of the materials. Proton, being the smallest known ion, is a promising candidate addressing concerns pertaining to energy conservation and enhanced CMOS compatibility. Devices which incorporates alkali metal ions (e.g. Li^+, Na^+, K^+, Ca^{2+} etc) are CMOS incompatible attributing to the contamination of fabrication tools. Proton-conducting solids have emerged as pivotal materials in the applications of hydrogen sensors, super-capacitors, water electrolyzer membranes, wearable devices, synaptic devices, smart windows, neuromorphic computing and many others. In this work, we discuss the diverse classes of materials exhibiting proton conductivity, including perovskites, metal-organic frameworks, and polymers, highlighting their structural features and proton transport mechanisms. Moreover, it explores into the critical factors affecting proton conduction, such as hydration, chemical composition, and temperature, elucidating their influence on the materials' performance. Fig. 1 demonstrates the temperature dependent proton conductivity of several materials such as $BaCeO_3$, $BaZrO_3$, MoO_3, Nafion, PEDOT:PSS, yttrium-stabilized zirconia (YSZ), graphene oxide, brownmillerite oxide, lanthanum molybdates(LAMOX), silicon dioxide, tungsten oxide. B. Dong et al. reported that Nafion shows highest proton conductivity of 1.5 S/cm for a 400nm diameter fiber at 30°C and 90% RH [1]. Moreover, N. Lu and co-workers demonstrated that hydrogen-intercalated brownmillerite oxide exhibits an unusually high proton conductivity of 0.028 S/cm to 0.33 S/cm in the temperature range of 40 °C and 140 °C [2]. However, other proton conductors have conductivity in the range 10^{-6}-10^{-2} S/cm which can be tuned by adjusting the fabrication methods, such as adding sintering assistance, doping and co-doping. The present report will pave a way to elucidate the choice of proper proton conducting material for a specific application.

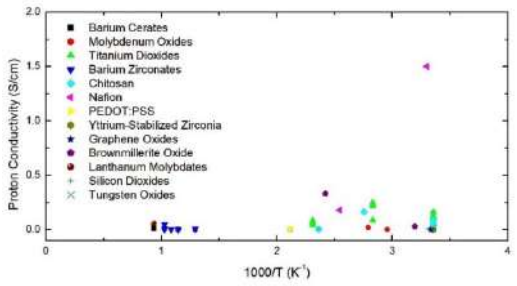

Fig. 1. emperature dependent proton conductivity in different solids showing Nafion has highest proton conductivity

B 156

Enhancing Aqueous Zinc Ion Battery Performance with a Modified $V_{10}O_{24}.12H_2O$ @Ti_3C_2 Cathode

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ABSTRACT

Aqueous zinc ion batteries (AZIBs) have emerged as promising candidates for energy storage systems due to their inherent safety, cost-effectiveness, and environmental friendliness. However, the development of zinc ion batteries is not yet successful as other commercialized batteries due to lack of an efficient cathode host. [1] This study presents the development and characterization of a novel cathode material for AZIBs, employing a modified vanadium oxide ($V_{10}O_{24}.12H_2O$@Ti_3C_2) cathode with MXene. The modified $V_{10}O_{24}.12H_2O$@Ti_3C_2 cathode material was synthesized via single step hydrothermal process by integrating Ti_3C_2 MXene, a two-dimensional transition metal carbide, into the $V_{10}O_{24}.12H_2O$ matrix. The pristine $V_{10}O_{24}.12H_2O$ and modified $V_{10}O_{24}.12H_2O$@Ti_3C_2 cathode were thoroughly characterized by XRD, FE-SEM, and BET surface area analysis.

The resulting composite material exhibited enhanced electrochemical properties, including improved specific capacity, cycling stability, and rate capability. The unique structural and chemical properties of Ti_3C_2 MXene, such as high electrical conductivity and large surface area, synergistically contributed to the overall performance enhancement of the cathode. The electrochemical behavior of the pristine $V_{10}O_{24}.12H_2O$ and modified $V_{10}O_{24}.12H_2O$@Ti_3C_2 cathode was systematically investigated through various techniques, including cyclic voltammetry, galvanostatic charge-discharge cycling, and impedance spectroscopy. The Ti_3C_2 MXene-modified cathode demonstrated superior electrochemical performance of 260 and 75 mAh/g at 0.1 and 2 A/g, respectively (219 mAh/g at 0.1 A/g for pristine $V_{10}O_{24}.12H_2O$ cathode), attributed to the synergistic effects of $V_{10}O_{24}.12H_2O$ and Ti_3C_2 MXene, leading to enhanced zinc ion diffusion kinetics and charge storage capacity.

Keywords: *Zinc ion battery, Aqueous electrolyte, Vanadium oxides, Mxene*

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B 157

Fabrication and Characterization of $BaCe_{0.75}Zr_{0.1}X_{0.15}O_{3-\Delta}$ (X= Y, In, Ga, Gd, Yb) Proton Conducting Electrolyte by EDTA- Citrate Complexing Method for IT-SOFC

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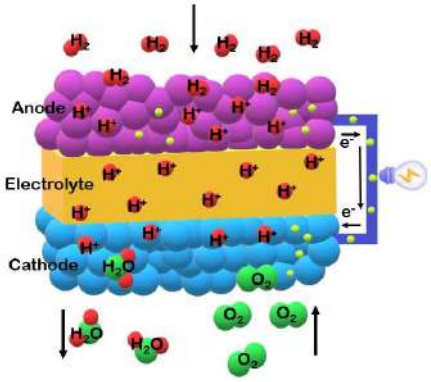
ABSTRACT

Barium cerate –zirconate is the most researched and promising proton-conducting electrolyte for the intermediate-temperature solid oxide fuel cell. The ionic conductivity is enhanced by the doping with the different aliovalent elements at the B-site of the barium cerate –zirconate electrolyte. $BaCe_{0.75}Zr_{0.1}X_{0.15}O_{3-\delta}$ (X= Y, In, Ga, Gd, Yb) are successfully synthesized by the EDTA- citrate complexing method at relatively low sintering temperature. The single phase of the orthorhombic perovskite structure is obtained and confirmed by the XRD pattern. The functional properties of microstructure, crystalline phase structure, densification, thermal behavior, chemical composition, and ionic conductivity are analyzed using different characterization techniques like X-ray diffraction, Field Emission-Secondary Electron Microscope, Thermogravimetric analysis, X-ray photoelectron spectroscopy and electrochemical impedance spectroscopy for this proton-conducting electrolyte materials.



Schematic diagram of the Proton conducting Solid oxide fuel cell

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B 158

Fabrication of Electrode Materials for Sustainable Energy Applications

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ABSTRACT

The fabrication of electrode materials plays a crucial role in advancing sustainable energy applications, particularly in the development of energy storage and conversion devices. We have fabricated porous carbon nanosheet and nanostructured rhodium (Rh) thin film-based electrode materials for supercapacitor and water splitting applications, respectively. The electrode materials were characterized by FESEM, XPS, Raman, XRD and N_2 adsorption-desorption analysis. The constructed supercapacitor showed an operating potential window of 1.1 V in 1 M KCl neutral electrolyte solution. At 2.25 A/g the calculated specific energy was ~ 39.04 Wh/kg, along with a high specific power of ~ 1237.5 W/kg. The porous carbon material was able to retain specific energy of ~ 22.92 Wh/kg and specific power of ~ 41,250 W/kg at a high current density of 75 A/g. The porous carbon was used for making a coin cell prototype supercapacitor device and tested with a light emitting diode (LED). The Rh thin film electrode exhibited outstanding electrocatalytic activity for oxygen evolution reaction (OER). The effect of the supporting electrolytes on OER activity and the crystal planes of RhTF electrodes were analyzed using electroanalytical techniques and computational simulation methods. Tafel slope (TS) analysis revealed that electron transfer kinetics was slower for the NaOH compared to the KOH.

Keywords: Porous carbon, Rhodium, Electrocatalyst, supercapacitor, Oxygen evolution reaction.

B 159

Hard Carbon synthesized from Teak (Tectona grandis) wood as prospective Electrode for Supercapacitor

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ABSTRACT

The efficient material with high Specific capacity and long stability are highly desirable material for supercapacitor. Here in, hard carbon were synthesized from teak wood. The teak wood-derived hard carbon with high crystallinity cellulose present in wood has lead to high porosity, which is employed as electrode to improve electrochemical characteristics of Supercapacitor .Hard carbon derived from wood exhibits large surface area and gives good conductivity for supercapacitor. The crystallographic morphology structure and phase purity of hard carbon is investigated by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and Fourier transform Raman spectroscopy (FT-Raman). Thus highly porous hard carbon is synthesized and characterization techniques are performed and electrochemical properties is investigated for better performance.

Keywords: Hard Carbon, Electrode, Supercapacitor

B 160

Li-ion Capacitors and Recycling Li-ion batteries

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ABSTRACT

Recycling lithium-ion batteries (LIBs) are gaining attention in the recent past since the short lifetime of ~3 years in electronic devices and ~5-10 years in EVs could generate a mammoth volume of spent LIBs, with 2 million metric tonnes expected by 2030, which encourages the development of effective recycling technologies. With environmental concerns, spent LIBs has triggered massive interest in emerging various crystal structures of metal oxides and different kinds of carbon materials that provide the opportunities to replace commercial materials beyond the energy storage and conversion applications cost-effectively. Finally, the requirement for the workhorse anode, graphite, is also demanding. The discovery of graphene, also driving a graphite demand, further upsurges the global graphite market, paving the search for new battery-grade graphite sources. The existing spent LIBs industrial recycling technologies overlook that graphite should be recycled to meet the global demand, creating an opportunity for reuse in the LIB manufacturing process and reducing the burden of resource dependency. The recovered graphite anode renders excellent performance in Li-ion capacitors with activated carbon as the counter electrode. The performance has been compared with commercial graphite, hard carbon, synthetic graphites, semi-crystalline carbon, etc.

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Enhancing magnesium ion conduction in PVB based polymer electrolyte with ionic liquid forsolid – state battery applications

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ABSTRACT

Incorporating ionic liquids into polymer electrolytes offers a promising strategy for enhancing ionic conductivity and performance in solid-state batteries. This study investigates the effects of doping a PVB: $MgCl_2.6H_2O$ electrolyte system with 1-Ethyl-3-methylimidazolium methyl sulfate. The synthesized polymer electrolyte films were characterized using XRD, FeSEM, FT-IR, DSC, UV-Vis, conductivity, impedance, and transference number measurements. The results demonstrate a significant increase in ionic conductivity with temperature and dopant concentration, reaching 2.47 x 10^{-3} S/cm at ambient temperature for the optimized composition. Transference number measurements confirm dominant ionic conduction. The composite electrolyte exhibits improved structural, thermal, and optical properties suggesting the potential of this ionic liquid-doped with PVB: $MgCl_26H_2O$ polymer electrolyte for solid state battery applications.

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Carbon Anchored ZnCoS as Potential Electrocatalyst for Hydrogen Evolution Reaction

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ABSTRACT

Clean and sustainable energy production is a great concern in modern world since the growth in population has drastically increased. In the current scenario, we need to develop alternative energy harvesting technologies to match the growing energy demand. The production of hydrogen through electrochemical water splitting is considered as an effective and viable way to rectify the issue owing to its high energy density. Electrochemical water splitting involves two half reaction namely hydrogen evolution reaction (HER) in the cathode counterpart and oxygen evolution (OER) in the anode counterpart. The production of hydrogen through water splitting can be further enhanced by the use of electro catalysts which possess high active sites and conductivity. Transition metal chalcogenides are viable alternatives for hydrogen evolution reaction considering the desirable overpotential and the abundance compared to the conventional costly catalysts such as Pt/C. Recently, Cobalt Sulphide (CoS) has emerged as a potential material for energy storage and conversion applications as a results of the active sites and its intrinsic conductivity. Here we have developed CoS with different Zn Doping ratios and clubbed it with the carbon counterpart for enhanced surface area and conductivity as well. The synergistic effect of Zn as a catalytic promoter along with the additional surface area delivered by the carbon further enhanced the HER performance. We have varied the carbon amount in order to assess the optimal ratio for the maximum performance.

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Advancements in Multilayer Anodes for Enhanced Performance in Lithium-Ion Batteries

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ABSTRACT

The pursuit of high-performance lithium-ion batteries has intensified, driven by the burgeoning demand for efficient power sources in various technological applications. Multilayer anodes have emerged as a promising avenue to mitigate challenges associated with volume expansion and contraction during charge/discharge cycles, particularly in high-capacity materials like silicon. Several transformations have been undergone by lithium based rechargeable batteries since they ere first proposed in the early 1960's. Initially, metallic Li was used as the anode, but serious safety hazards were posed because of dendritic Li growth during cycling. Therefore, other anode materials, graphitized carbon is the most used anode material in commercial lithium – ion batteries. However, its theoretical capacity is very less. Therefore, some metal anodes with high theoretic capacity, such as Si, Sn, Sb, Al, have been studied extensively.

Si has attracted much attention because the highest specific capacity for any anodes studied to date. However, the metals that can act as active materials exhibit drastic volume expansion/contraction during Li+ insertion/ extraction. Theoretical capacity is significantly reduced after the first few charge/discharge cycles due to the loss of mechanical integrity. Several ways to overcome the volume exchange problem include decreasing the size of the structures to nano-size, using composites with active/active or active/inactive matrices, or using thin films of alloys[1].

Extensive investigation has been conducted on metal-based alloys as an anode material for lithium ion batteries to enhance the specific capacity. The multi-layered structure design is advantageous because of its ease of fabrication, as compared to nano-wires and 3D nano-particles. Present study discuss about the multilayer thin films which has been used as a anode material for rechargeable thin film batteries.

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B 164

Synthesis of Zr_2C MXene by using waste plastic as a source of carbon

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ABSTRACT

The expansion of both globalization and industry has brought up two major problems: pollution and the scarcity of cleaner fuel. The research community has been captivated by the exceptional properties of MXene as a 2D material, such as its high surface area, conductivity, and layered structure. Among these properties, the catalytic activity of MXenes has garnered particular interest and investigation within the realm of materials science. However, regrettably, limited research has been conducted on the catalytic activity of Zr_2C MXene. The synthesis of MXenes involves the synthesis of the MAX phase, followed by selective etching of the A layer from the MAX phase. The synthesis of MAX phases plays a key role in tuning the properties of MXenes. In the present study, we propose a novel route to prepare the Zr_2AlC MAX phase as a precursor for Zr_2C MXene. We have prepared the Zr_2AlC MAX phase by utilizing waste plastic as a sustainable carbon source, ZrO_2 as a zirconium source, Al as an aluminum source, and Mg as a reducing agent. A specially designed stainless-steel autoclave was used to prepare the MAX phase at lower temperatures, i.e., 800 °C. The experimental parameters, such as temperature, time, and composition, were varied to prepare the Zr_2AlC MAX phase. Furthermore, Zr_2C MXene is prepared through the etching process of the Zr_2AlC MAX phase. X-ray diffraction (XRD) was primarily utilized to confirm the successful formation of the desired MAX phase and MXene. This study aims to evaluate the suitability of Zr_2C as an electrode material. We have investigated Zr_2C enduring stability in electrochemical environments and explored their applicability in energy storage devices. This novel approach aims to integrate waste plastic as a carbon source for advanced material synthesis at lower temperatures.

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MXenes: A Green Solution for Cleaner Fuel Production

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ABSTRACT

To address the energy crisis and environmental problems caused by the excessive combustion of fossil fuels, the scientific community is urgently focusing on green energy generation from sustainable and renewable resources. One promising option among several is the use of hydrogen as a fuel source, which might help solve these problems. Hydrogen fuel has the greatest energy density and produces no greenhouse gases, which are two of its main advantages over competing fuels. An environmentally friendly method of hydrogen evolution is electrochemical water splitting that has recently gained a lot of interest from both academics and businesses. In an electrochemical cell, the two half-reactions that are essential for electrochemical water splitting are the oxygen evolution reaction (OER) at the anode and the hydrogen evolution reaction (HER) at the cathode. The efficiency of this process is highly dependent on the electrocatalyst material. Both HER and OER processes often use noble metals and metal oxides as electrocatalysts. It has been difficult to commercialise the technique due to the high cost and rarity of certain precious metals. These days, MXenes are all the rage as a novel family of 2D materials that show a lot of promise for electrochemical water splitting. 2D MXenes are carbides and/or nitrides of early transition metals, where n is an integer, X is carbon and/or nitrogen, T_x is the surface termination group, and M is an early transition metal. The bulk version of MXenes, called MAX phases, is selectively etched during synthesis (where A pertains to a group of 13 or 14 elements). Till now, around 30 MXenes have been documented via experiments, and another 100 are expected theoretically, with processing advances yet to come. Energy storage and conversion, nano-sensors, healthcare applications, and electromagnetic interference shielding (EMI) are just a few of the many areas where MXenes have shown great promise. In the present talk different MXenes synthesized in our laboratory and their electrochemical properties will be presented for their applications.

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Understanding the Effect of Size Variation of Bio Compatible Prussian Blue as Cathode Material in Supercapacitor Application

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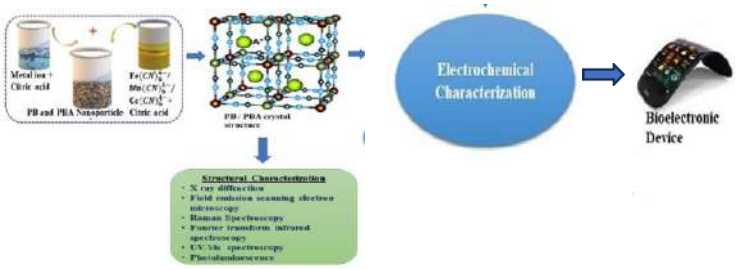
ABSTRACT

Supercapacitor has attracted increasing attention as efficient and biocompatible cathode material due to its higher charge capacity, high energy and power density and prolonged durability. Prussian Blue (PB) and its analogues (PBAs) are biocompatible as well as a highly porous open framework with tuneable chemical compositions are found to be a potential electrode material for energy storage and are being utilized in various metallic nanostructures form for several electrochemical applications. In this proposal, my objective is to examine the potentiality and biocompatibility of PB and PBA nanostructures to obtain the most suitable and compatible electrode material for implantable bioelectronics devices. Pure PB nanostructures have already been synthesized b simple reflux method. Samples have been characterized by XRD, FESEM, TG-DTA analysis, FTIR spectroscopy, UV-Vis spectroscopy, and cyclic voltammeters (CV, GCD, EIS). Structure studies reveal that the prepared nanostructures are phase pure of cubic shape, while IR studies show the existence of defect states and variation of water molecules within the nanostructure. UV-Vis spectroscopy studies provided further necessary insights regarding the defect structures and related electronic properties. As PB and PBAs are highly influential on electrochemical behaviour, hence a model has been developed to explain the specific capacity- 89.53F/g and 146 F/g at 2 mV/sec of virgin PB nano cubes of sizes approximately 60nm and 230 nm. In this context, it may be stated that environmentally friendly and low-cost cathode material was prepared for supercapacitor application.



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B 167

Preparation and Characterization of Poly (vinyl alcohol) – Chitosan Composite Membrane for DMAFC Application

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ABSTRACT

This study is based on preparation of Poly (vinyl alcohol) (PVA)-based anion exchange membranes for Direct Methanol Alkaline Fuel Cells (DMAFCs). PVA, which is a nontoxic, synthetic polymer is a suitable material for polymer electrolyte membranes due to its hydrophilicity, film forming capacity and methanol barrier property. Chitosan (CS) is a natural polymer that is abundant in nature and has properties of biodegradability and non-toxicity. Due to the presence of amine groups and hydroxyl groups in CS, it is easy to modify and provide high hydrophilicity, chemical, mechanical and thermal stability. PVA-CS composite membranes offer advantages due to improvement in properties relative to the properties of the single components.

In this work, polymer electrolyte membranes were prepared using PVA and CS by solution casting technique. Aloe vera (AV) has been added to improve ionic conductivity. Tartaric acid (TA) has been used as crosslinking agent. The effects of type of crosslinking and concentration of crosslinking agent on membrane stability were investigated. Various characterisation techniques like TGA, SEM, XRD, FTIR, water uptake, swelling ratio and AC Impedance Spectroscopy were used to study thermal stability, structural properties, hydrolytic stability and ionic conductivity of the prepared membranes. It is found that mechanical and thermal properties of PVA-CS composite membranes can be enhanced by adding TA as crosslinking agent.

Keywords: *Poly (vinyl alcohol), chitosan, aloe vera, tartaric acid, anion exchange membrane*.

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B 168

Implementing bimetallic metal organic framework for high performance asymmetric supercapacitors

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ABSTRACT

Metal organic frameworks (MOFs) are used in various fields like gas absorption, catalysis, energy storage, and conversion as well as in the field of luminescence. As compared to Metal organic frameworks, Bimetallic metal organic frameworks show enhanced and synergistic effects and thus can be used widely for the development of commercial energy storage devices, especially supercapacitors. In this work the synergistic effect of cobalt and aluminum bimetallic MOF is studied as electrode material for supercapacitors by electrodeposition method. This Co-Al MOF exhibits a specific capacitance of 1014.08 Fg-1 at a current density of 40 Ag^{-1} in 1 M KOH in three electrode system. The asymmetric device of Co-Al MOF as the positive electrode and carbon cloth as a negative electrode is also manufactured which exhibits high specific capacitance of 124.26 Fg^{-1} at a current density of 0.25 Ag^{-1}. Apart from a good specific capacitance, Co-Al bimetallic MOF as a device also exhibits a great cycling stability of 93 % capacitance retention even after 12000 cycles. We have such a good specific capacitance in 1 M KOH alkaline electrolytes for both 2 electrodes as well as three electrode systems which is remarkable in the field of supercapacitors. The observed results shows that this work can be used further to make an asymmetric hybrid supercapacitor in the future.

Keywords: *Supercapacitors, Metal organic framework, Energy storage, Asymmetric device, electrodeposition*

B 169

Electrodeposition of $NiCo_2O_4$ for Supercapacitor Application

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ABSTRACT

$NiCo_2O_4$ thin films were directly grown on stainless steel mesh via a facile electrodeposition method. The structural properties revealed the formation of cubic $NiCo_2O_4$. The capacitive performance of the as-obtained $NiCo_2O_4$ electrode was evaluated by cyclic voltammetry (CV) measurements.

B 170

Turmeric Leaves-Derived Biomass Waste Carbon: A Sustainable Frontierfor Supercapacitor Applications

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ABSTRACT

"The escalating energy consumption and deteriorating environmental conditions have spurred the quest for readily recyclable materials. In this context, India, as the world's foremost producer, consumer, and exporter of turmeric, playing a significant role in global cultivation and production (accounting for almost 75% in 2022-23), presents a unique opportunity. This study explores the electrochemical performance of biomass waste-derived carbon sourced from turmeric leaves (Curcuma longa L.) for supercapacitor applications. The growing demand for sustainable energy storage systems has driven research into alternative materials, and biomass-derived carbons emerge as promising contenders due to their abundance, cost-effectiveness, and eco-friendly nature. Turmeric leaves, abundantly available as agricultural waste, offer a promising avenue for carbon material production. The approximate composition of dried turmeric leaves converted into carbon per 100 g was 43.3 g carbohydrate, 6.0 g crude protein, 0.5 g crude fat, 9.4 g crude ash, 34.5 g total fiber, and 6.3 g moisture, facilitating conversion through the pyrolysis process. The resulting material showcases remarkable fluffiness, with a yield reaching [43%], achieved without any chemical additives, making it a sustainable synthesis. Furthermore, the material exhibits remarkable electrochemical performance, demonstrating a specific capacitance of 171.56 Fg-1 at a current density of 0.5 Ag-1 in 1M H2SO4, an energy density of 23.83 Wh kg^{-1}, and a power density of 249.99 W kg^{-1} for three- electrode systems. The cyclic stability of 100% over 2244 cycles reflects the material's potential scalability in industrial and commercial settings, suggesting promising prospects for bulk production and commercial utilization. In summary, this investigation underscores the potential of turmeric leaves-derived biomass waste carbon for supercapacitor applications, offering an environmentally friendly and sustainable solution.

Keywords: Supercapacitor, Biomass, Turmeric leaves, Activated Carbon, Energy Storage.

B 171

A Study on the Effect of Graphitic Carbon Nitride on the Electrochemical Properties of Zinc-Iron Binary Hydroxide Nanosheets for Pseudo capacitor Electrode Applications

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ABSTRACT

Two-dimensional nanostructured metal hydroxides have received great interest of scientific researchers on account of their potential to be used as electrode materials for energy storage devices. Enhanced electrochemical properties exhibited by binary, ternary, and quaternary metal hydroxides triggered wide research of these material groups for supercapacitor electrode applications. In this work, the possibility of achieving synergistic effect of different metal hydroxides through the formation of binary hydroxides and their nanocomposite with carbonaceous material has been investigated. The ability of metals in binary hydroxide to complement each other in different properties has also been analyzed. Zinc-iron binary hydroxide nanosheets and zinc-iron binary hydroxide / graphitic carbon nitride nanocomposites were synthesized through a hydrothermal method. The details on crystalline phases, chemical bonds, and morphology of the samples were acquired from X-ray diffractograms, FTIR spectra, and HRTEM micrographs. The electrochemical behavior of the prepared samples were inferred by analyzing their cyclic voltammograms and chronopotentiograms and Nyquist plots. A two-electrode electrochemical system was employed to analyze the practicability of the electrode material. Zinc-iron binary hydroxide displayed a specific capacitance value of 142F/g at 1A/g which was then enhanced to 466F/g through the addition of graphitic carbon nitride. Thus the carbonaceous material has found to be having a constructive influence on the binary metal hydroxide.

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B 172

Prospective and Electrochemical Analysis of LMR-NMC as Cathode Materials for Lithium-ion Battery Applications

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ABSTRACT

Lithium ion battery is a most promising new generations energy storage device by converting chemical energy into electrical energy which has conquered the market in the field of advanced portable electronic device such as mobile phones, laptops and digital cameras, etc. The lithium ion batteries need more update for electrical vehicle applications in terms of high power density, high energy density and long cycle life of performance and safety concerns. For high energy density, Mn-based cathode materials and LMR-NMC cathode materials are very important cathode materials in next generation lithium ion batteries. The synthesis of LMR-NMC cathode materials prepared by solution combustion methods. The structural, morphological and electrochemical properties of all as prepared sample have been investigated by various characterizations techniques, namely, powder X-ray diffraction (XRD), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Cyclic Voltammetry (CV), Galvanostatic Charge & Discharge (GCD) and electrochemical impedance spectrum analysis.

Keywords: *LMR-NMC, CV, GCD, EIS.*

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Synergistic Effect of Molybdenum Oxide and MoS_2 Hybrid Electrocatalyst for Hydrogen Evolution

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ABSTRACT

The ultimate goal of hydrogen economy is to develop a catalyst that is both efficient and economical. Harnessing the abundant resources of earth to produce hydrogen from water ideally requires a minimal external energy[1]. Several techniques are being explored to fabricate metal oxide, metal sulfide, and metal nitride based electrocatalysts with modified microstructures and dimensions to enhance the water-splitting process[2]. Among these, MoO_3 nanostructures with an indirect bandgap (ranging 2.7 – 3.1 eV) are proven as reliable water-splitting electrodes, exhibiting high stability in aqueous solutions under acidic conditions[3]. However, a more effective approach for increasing the activity of hydrogen evolution reaction (HER) involves a hybrid catalyst that combines two different functional components. In this context, MoO_3/MoS_2 heterostructures were synthesized using a facile hydrothermal method followed by a liquid exfoliation. The structural and microstructural properties are analysed using X-ray diffraction, high-resolution scanning electron microscope, and high-resolution transmission electron microscopy. The tuning of bandgap of the composite materials was examined through UV-Visible diffuse reflectance spectroscope. The electrochemical analysis were used to explore the overpotential, tafel slope, and the quantity of hydrogen released during the water-splitting process.

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B 174

Comparative Study on The Electrochemical Performance of Trimanganese Tetraoxide (Mn_3O_4) Under Different Synthesis Technique

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ABSTRACT

Trimanganese Tetroxide (Mn_3O_4) nanomaterial like Nano cube, nano sphere and nano square structures were respectively prepared employing co-precipitation, Sol-gel and hydrothermal technique. The obtained samples were characterized comprehensively. The XRD examination verified that Mn3O4 formed the tetragonal structure and that it had a spinel structure. The as-synthesised samples' agglomerated nanocube, nanosphere, and nanosquare formation were seen using HRSEM examination. The structural behaviour of the samples was validated by the SAED pattern and high resolution HRTEM image. Through EDX spectra, the produced samples' elemental composition was verified. The type IV isotherm and mesoporous structure of the prepared samples were confirmed by the BET analysis. All of the samples' electrochemical behaviour was analysed based on the electrochemical characterization. The hydrothermal approach has the highest specific capacitance of the three, measuring 0.5 A/g.. Also the highest capacity retention was shown in hydrothermal sample due to its lower Rs and Rct values obtained from EIS.

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Synthesis and Electrochemical properties of Graphene oxide for Supercapacitor Application

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ABSTRACT

This research article presents a comprehensive electrochemical characterization of Graphene Oxide (GO) synthesized using a modified Hummers method. Graphene Oxide, a derivative of graphene, has gained significant attention in various fields due to its unique properties, including excellent electrical conductivity, large surface area, and chemical functionalities. The electrochemical characterization involves a thorough investigation of the synthesized GO's structural, morphological, and electrochemical properties. Techniques such as cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge-discharge analysis are employed to assess the electrochemical behaviour of the material. the cyclic voltammetry for as prepared graphene oxide is performed with the scan rate of $5mVs^{-1}$ to $100mVs^{-1}$ for two kinds of electrolytes KCl and KOH. The calculated values of specific capacitance is found to be higher for lower values of scan rates and is decreasing as the scan rate is increased which is a typical response of pseudo capacitive behaviour. The study explores the impact of the different electrolytes on the electrochemical performance of GO, focusing on factors such as capacitance, charge/discharge kinetics. The findings of this research contribute to the understanding of the relationship between the synthesis method type pf electrolyte and the electrochemical properties of graphene oxide. Insights gained from this study may have implications for the development of graphene-based materials for energy storage devices, sensors, and other electrochemical applications.

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B 176

Study Of Structural, Thermal and Electrical Properties of Sodium Based Metal Oxide-Polymer Composite Electrolyte for Battery Application

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ABSTRACT

Hybrid polymer-ceramic electrolytes with high ceramic loading are a promising solution to achieve high safety and optimal mechanical properties in all-solid-state rechargeable batteries[1]. NZTO is a potential sodium solid electrolyte of all-solid-state batteries. Na ion conductivity and electrochemical performance of layered $Nak_{1..5}$ Zn $S_{0.5}$ $B_{0.5}$ -doped electrolytes with Polymer was prepared using a solution casting method using distilled water as a solvent and subjected to various studies like by Fourier transform infrared (FTIR), differential scanning calorimetry (DSC), AC impedance spectroscopy and (TGA). The FTIR analysis reveals complexation behaviour of the electrolyte. DSC analysis has been used to find the glass transition temperature (Tg) of the prepared polymer electrolytes. AC impedance analysis has been used to study the electrical characterization of the prepared polymer electrolytes. The temperature-dependent ionic conductivity obeys the Arrhenius behaviour. The highest conductivity has been achieved $4.0*10^{-5}$ S cm $^{-1}$ at room temperature . It was found that doping enhances ionic conductivity and gives low activation energy confirmed by complex impedance spectroscopy (CIS). The impedance spectroscopy technique performed in the frequency range between 100 Hz to 8 MHz at different temperatures and obtain highest conductivity $4.0 * 10^{-5}$ S/cm .

Keywords: PVA; ionic conductivity; FTIR; composite thin film polymer electrolyte

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Enhanced Bifunctional Electrochemical Performance by Controlling Crystallinity at the Interface of MoS_2 and Nitrogen Doped Carbon

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ABSTRACT

A high atomic percentage of nitrogen atoms integration into a graphitic carbon matrix is very challenging and at the same time intensely significant because of the fact that this integration strengthens the competency of carbonaceous materials. Further, the hierarchy of nanostructure comprising this type of graphitic nitrogen-doped carbon matrix and transition metal dichalcogenides along with opulent M–N–C interfacial bonds is highly beneficial in electrochemical energy applications. In this work, using an interfacial polymerization, a facial hydrothermal rote and subsequent annealing process, a core@shell hierarchy of ultrathin MoS_2 integrated over nitrogen doped graphitic carbon (NC) is reported. The well optimized NC@MoS_2 hierarchy exhibits tremendous electrocatalytic activity exhibiting low onset overpotential and Tafel slope for hydrogen evolution along with remarkable chronoamperometric stability in acidic electrolyte. Further, unique architecture of NC@MoS_2 with high porosity and specific surface area maximizes combined effect of NC matrix and MoS_2 as well as synergistic effects to get high specific capacitance along with excellent cyclic retention in alkaline electrolyte compared to its individual components. The source of these peerless electrochemical activity is mainly the interfacial Mo–N–C bonds which is discussed and explored further in detail.

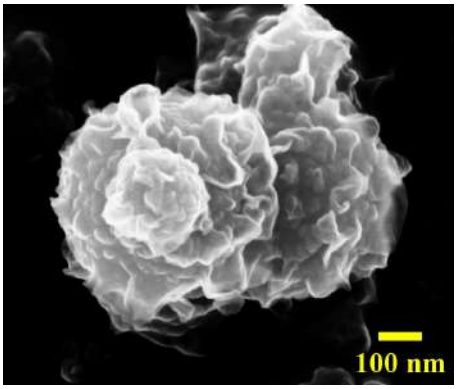

Figure: Well Optimized NC@MoS_2 Hierarchy

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A New Method to Design a High-Entropy Oxide in Conjunction with Rgo to Improve the Performance of Lithium-Ion Battery Anodes

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ABSTRACT

This research aims to address the inherent limitations in the cycling endurance of conversion-type anodes used in rechargeable lithium-ion batteries (LIBs) by employing innovative high entropy materials and advanced fabrication techniques. Specifically, the study explores the utilization of a novel entropically stabilized glycerate form (HEG) that incorporates first-row transition metals (Fe, Co, Ni, Mn, Cr) as a promising LIB anode. This HEG-based anode exhibits an impressive reversible capacity exceeding 500 mAh/g at a rate of 0.1 A/g sustained over 270 cycles. Moreover, the study introduces a groundbreaking method to rapidly convert HEG into a spinel-phase high entropy oxide (HEO) using CO_2 laser treatment. This transformation enables the development of a binder-free anode comprising laser-induced reduced graphene oxide (rGO) and HEO ($(Fe_{0.45}Co_{0.14}Ni_{0.2}Cr_{0.13}Mn_{0.08})_3O_4$) composites. The resulting composite, termed HEO@rGO, demonstrates a significant specific capacity of approximately 794 mAh/g at 0.1 A/g after 100 cycles and maintains a specific capacity of around 530 mAh/g at 0.5 A/g after 200 cycles. These achievements notably surpass the performance levels reported in previous studies on high entropy materials. Furthermore, detailed analyses of the charge storage mechanism reveal the persistent presence of the spinel structure within HEO, along with a partial transition toward a rock salt configuration. The fluctuating cycling stability profile observed in the study correlates with variations in charge transfer resistance and lithium diffusion throughout the cycling process. In essence, this study pioneers the use of high entropy materials in LIB anodes, demonstrating exceptional cycling endurance and capacity, while shedding light on the underlying mechanisms governing their performance, which involve structural transformations and lithium diffusion dynamics.

Keywords: High entropy glycerate, High entropy oxide, Laser scribe, High entropy materials, lithium storage.

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B 179

Inexpensive Transition Metal-Based Materials for Hydrogen-Based Society

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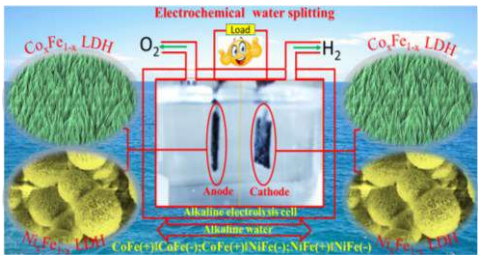
ABSTRACT

The successful development of a hydrogen-based society requires advancements in technology and the rational design of H_2 production, storage, delivery, and usage. The demand for H_2 production is rapidly increasing and receiving more attention since it can be used as a feedstock and energy carrier for various applications such as in the transportation, chemical industry and power sectors. Water electrolysis by using sustainable electricity is a promising route to split water into green H_2 and O_2 gases. The green H_2 production and consumption do not cause air pollution. Over the past few decades, Pt, Ir- and Ru-based materials have been widely used in industrial proton-exchange membrane water electrolyzers. Nevertheless, these materials are not suitable for largescale H_2 production due to their cost and scarcity.[1] Alternatively, non-precious-metal-based materials have shown promising catalytic activity towards OER, and thus attracted great research interest, particularly the first-row transition metals such as Mn, Fe, Co, Ni and Zn-based materials.[1] Over the past decade, a wide range of metal catalysts for OER and HER have been reported, which are synthesized in various forms such as oxides, (oxy)hydroxides, sulphides, phosphides, selenides, carbides, nitrides, and tellurides. In this presentation, some of the recently developed low-cost transition metal-based materials for green H_2 production will be discussed. For example, the Ni/Co/Fe-based layered double hydroxides and core@shell heterostructured Co-phosphide@Fe-phosphide materials synthesized by a simple hydrothermal method and subsequent heating process requires lowest cell potential of 1.59 and 1.53 V at a current density of 10 mA cm^{-2}, respectively. The metal organic framework-derived Fe–Co–O/Co@NC-mNS/NF (+/−) electrolyzer needs a low cell potential of 1.58 V to derive same current density. All these studies are remarkable in enhancing the overall performance of alkaline electrolyzers.[2,3]



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B 180

Electrochemically Deposited Layer Double Hydroxide Electrode Material Suitable for Energy Storing and High-Performance Supercapacitor

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ABSTRACT

Electrochemical performance of supercapacitors, including specific capacitance and cycling stability, is highly dependent on electrode material. Researchers have focused on layered double hydroxides (LDHs), due to their large electrochemically active surface and also possess the characteristics required for high-performance supercapacitors and thus considered one of the most potential electrode materials SCs. However, the problem of capacitance retention is still a major issue that should be explored more thus this work focuses on design and synthesis of layer-by-layer deposition of CoNi-CoMg-CoNi electrode to form sandwich-like structure on substrate. We here introduced a novel approach of multi-layering hydroxides using electrochemical deposition process with variation of deposition time of middle layer i.e, CoMg. The obtained products were labelled as Co/($Ni_1Mg_1Ni_1$), Co/($Ni_1Mg_{1.5}Ni_1$), Co/($Ni_1Mg_2Ni_1$), & Co/($Ni_1Mg_{2.5}Ni_1$) according to the variation in deposition time. Surprisingly, Co/($Ni_1Mg_{1.5}Ni_1$) electrode where discharging time of the middle layer is 355.25 seconds exhibits a specific capacitance of 1421 Fg^{-1} at a current density of 2 Ag^{-1} in 2 M KOH showing remarkable capacitance retention of 90%. Again, to verify practical use of as prepared electrode material [Co/($Ni_1Mg_{1.5}Ni_1$)] a two electrode asymmetric device was fabricated in 2 M KOH. The fabricated device shows high energy density of 83.25 $Whkg^{-1}$ with power density of 749.52 Wkg^{-1} at 0.25A/g current density. Not only this high capacitance retention of 90% after 9000 cycle in 2M KOH was achieved. Thus, our study demonstrates the practical application of as prepared electrode material as supercapacitor to come up with the major issue of hydroxide that is capacitance retention while reserving high capacitance and high energy density.

Keyword: *Supercapacitor, Layer double hydroxide, Electrodeposition, Sandwich like structure*

B 181

Scalable Microbial Fuel Cells: Carbon Veil and SS Mesh as Electrodes

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ABSTRACT

Scalability of microbial fuel cells (MFCs) on a large scale depends on the cost of electrodes. To address this challenge, the potential of stainless steel (SS) mesh and carbon veil (CV) as electrodes for MFCs due to their affordability was investigated here. The study aimed to assess the suitability of both materials as anode and cathode viz Carbon Veil-Carbon Veil, Carbon Veil-Activated Carbon Modified Carbon Veil, Carbon Veil-SS mesh, and Carbon Veil-Activated carbon modified SS mesh, with a focus on optimizing the anodic area (5,10 and 20-times cathodic area), which was found to significantly impact system performance. Electrochemical characterization of these electrodes in glucose medium revealed highest anodic peak current for CV (1.2 A/m^2), indicating its suitability as anode material. Performance studies showed that the Carbon Veil-Activated carbon modified SS mesh system gave the highest current and power density with values 0.7 W/m^3 and 0.06 A/m^2, respectively. Furthermore, an increase in anodic area enhanced MFC performance, with the maximum power density observed at an anode/cathode area of 20, corresponding to 1.2 W/m^3. When the MFC system was fed with real-time kitchen wastewater (KWW), a maximum power density of 0.83 W/m^3 was achieved, confirming its suitability for real-time wastewater treatment. The COD removal efficiency of system in different cycles of run were 89.4±6.6 %. Overall, this study highlights the potential of utilizing low-cost electrodes, such as SS mesh and carbon veil, to enhance the scalability and practicality of MFCs for real-time application.

Keywords: *microbial fuel cell, anode, carbon veil, scalability, power density.*

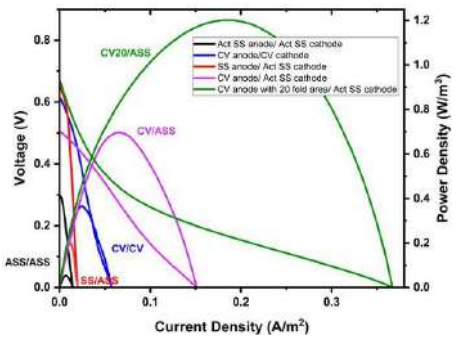

Figure Comparison of MFC performance for various electrode combinations

B 182

Unleash the Remarkable Potential of Co-Doped NiO Flakes Flower as Exceptional Electrode Materials for Supercapacitors Application

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ABSTRACT

The need for sustainable and environmentally friendly energy storage solutions has increased due to concerns about global energy sustainability and environmental impact. One promising technology is the supercapacitor, which can help overcome the challenges associated with traditional energy systems. This study focuses on the synthesis and characterization of cobalt-doped nickel oxide (Co-NiO) nanomaterials as potential electrode materials for high-performance supercapacitors. The $Co_xNi_{1-x}O$ nanomaterials were synthesized using a simple hydrothermal method and demonstrated a unique flake flower morphology. The Scherrer formula, as confirmed by X-ray diffraction (XRD), indicates a decrease in the size of crystallites upon cobalt doping. Scanning electron microscopy shows a morphology resembling flower-like flakes, while Ultraviolet-Visible (UV) spectroscopy is utilized to determine the bandgap of the electrodes. Incorporating cobalt doping caused notable alterations in the structure and electrochemical traits of the material. The pure form of nickel oxide (NiO) had a specific capacitance of 541 Fg^{-1} at $1Ag^{-1}$. However, the $Co_xNi_{1-x}O$ nanocomposite with a doping concentration of x=0.05 displayed a remarkable specific capacitance of 992 Fg^{-1} at $1Ag^{-1}$. The proposed method for doping holds the potential to enable the creation of exceptional supercapacitor systems with remarkable performance.

Keywords: NiO, hydrothermal, doping, flake flowers, supercapacitor.

B 183

Exploring the Potential of MnO_2/g-C_3N_4 Composite Cathodes for Stable Operation in Aqueous Zinc-Ion Batteries

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ABSTRACT

This novel research article investigates the potential of a composite material consisting of MnO_2 and g-C_3N_4 for application in aqueous zinc-ion batteries. This study explores the advantages of g-C_3N_4 sheets over commonly used materials in the design of a hybrid composite for enhanced electrochemical performance. Aqueous zinc-ion batteries have garnered significant attention due to their high safety compared to conventional lithium-ion batteries[1]. This research aims to address the electrochemical properties of the zinc anode and cathode materials, with a focus on stability and performance. This article presents the development of a g-C_3N_4-coated MnO_2 nanorod cathode, demonstrating its potential for stable operation in aqueous zinc-ion batteries. Furthermore, this study delves into the concept of integrating MnO_2 nanorods into g-C_3N_4, highlighting the potential of this composite for improved battery performance. This research contributes to the growing body of knowledge on advanced materials for energy storage applications, particularly in the context of aqueous zinc-ion batteries. These findings hold promise for the development of high-performance cathode materials, offering potential benefits in terms of stability, safety, and electrochemical properties. This study underscores the significance of composite materials in advancing the field of energy storage and lays the groundwork for further exploration of MnO_2/g-C_3N_4 composites in aqueous zinc-ion battery technologies[2].

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B 184

Rational design of NiO/Co_3O_4@rGO hybrid composite as battery type electrode material for the enhancement of electrochemical properties of Supercapatteries

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ABSTRACT

A supercapattery is a cutting-edge energy storage technology that combines the high energy density of a battery with the remarkable rate capability and power density of a supercapacitor. The improved performance is largely due to the successful assembly of NiO/Co_3O_4@rGO composite arrays using a hydrothermal method for supercapattery. At the same time, rGO serves as a conductive scaffold, facilitating efficient electron transport throughout the electrode material. NiO/Co_3O_4@rGO electrode material exhibits good electrochemical performance in a three-electrode assembly, achieving a maximum specific capacity of 711 C g^{-1} at an operating current density of 1 A g^{-1}. Due to their synergistic effect, a high-performance supercapattery device (NiO/Co_3O_4@rGO//α-Fe_2O_3/rGO)with impressive energy storage capabilities, efficient charge-discharge cycles, and extended cycle life is fabricated for the first time. The fabricated device exhibits exceptional energy storage performance with a remarkable power density of 795.3 W kg^{-1} and an ultrahigh energy density of 76.2 Wh kg^{-1}. After 10,000 consecutive continuous cycles of charge and discharge, the fabricated asymmetric supercapattery device exhibits outstanding performance, delivering 99 percent columbic efficiency.

Keywords: *Hybrid energy devices, Synergistic effect, Supercapattery device, Energy storage materials, Electrochemical performance, Transition metal composition, Specific energy and power.*

B 185

Engineering Porous Carbon Nanofibers from Sacrificial Polymers for High-Performance Supercapacitors

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ABSTRACT

The pursuit of high-performance electrode materials for supercapacitors has intensified due to their role in enabling efficient energy storage and rapid charge-discharge cycles. Carbon nanomaterials, especially electrospun carbon nanofibers (CNFs), have great potential as electrode material for supercapacitors due to their freestanding nature, high aspect ratio, high surface area with tunable porosity, and good electrical conductivities. The surface area is a significant factor that determines the electrochemical performance of supercapacitors. One of the prominent strategies to enhance the surface area of CNFs is the addition of a sacrificial polymer in the electrospinning precursor solution that decomposes during pyrolysis, leaving behind a porous structure. In this work, we have studied polyvinylpyrrolidone (PVP) and polymethyl methacrylate (PMMA) as sacrificial polymers in polyacrylonitrile (PAN)-based carbon nanofibers (CNFs). A systematic study was conducted comparing the morphology, pore structure, and performance of the PMMA and PVP blend CNFs with varying weight ratios. It was found that the weight ratio of 70:30 (PAN: sacrificial polymer) gave the highest performance for both the sacrificial polymers, PMMA and PVP, which is attributed to the micro-mesoporous structure and enhanced specific surface area. Moreover, using the composite of PMMA and PVP with PAN demonstrated the highest surface area and specific capacitance. In a symmetric supercapacitor cell with 1M H_2SO_4 electrolyte, an excellent electrochemical performance of 209 F g^{-1} at 5 mV s^{-1} was achieved.

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Role Of Fe Concentration in Oxygen Evolution Reaction of Strontium Ferrite Nanoparticles

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ABSTRACT

The impact of Fe concentration on structural changes and its role in water splitting in strontium ferrite nanoparticles synthesized by Co-Precipitation method is explored in this study. These synthesized materials are characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Linear swap voltammetry (LSV) and Electrochemical impedance spectroscopy (EIS) which reveals the phase of the material, morphological study, changes in overpotential and charge transfer mechanism respectively. The outcomes of this study furnish crucial insights into the interrelationship between iron concentration and the catalytic activity of strontium ferrite, laying the groundwork for the development of efficient and economically viable catalysts for OER, thus contributing to the advancement of renewable energy technologies. These materials shows high catalytic activity with 460 mV overpotential at 10 mA cm-2 current density and 95 mV sec-1 Tafel slope. It also shows excellent stability (10hrs) for OER in 1M NaOH.

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Electrolyte Based on Almond Gum

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ABSTRACT

Lithium-ion batteries are a crucial component of modern society, as they are the predominant technology utilized in portable electronic devices, including smartphones, tablets, and laptops, which have become an indispensable part of our lives. Research on new energy materials that meet the special needs of electronic devices is of interest to researchers. Electrolytes are of significant importance as fundamental components ofbatteries. Liquid electrolytes have been conventionally employed in most conventional batteries. However, it is worth highlighting that liquid electrolytes exhibit certain challenges, including but not limited to leakage, limited electrochemical stability, and flammability. Consequently, to address these limitations, synthetic solid-state electrolytes have emerged as potential solutions; however, they have some environmental issues.Biopolymers are functionally equivalent to synthetic polymers and are eco-friendly and biocompatible. In this study, a solid-state electrolyte based on a biopolymer obtained from almond trees was used as the polymer host, and different concentrations of lithium chloride were incorporated as ionic salts for the development of solid-state electrolytes for lithium-ion batteries. The prepared biopolymer was examined using characterization techniques, and the results showed enhanced structural and ion transport properties. The ionic conductivity increased from 1.38×10^{-8} S/cm to 1.03×10^{-4} S/cm.

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Indium Oxide Decorated Graphitic Carbon Nitride/ Multi-walled Carbon Nanotubes Ternary Composite for Supercapacitor Applications

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ABSTRACT

The increasing global energy demand facilitated the development of various renewable and clean energy systems and energy storage applications. The impressive attributes of supercapacitors position them as a promising up-and-comer within the realm of electrochemical energy storage applications. Herein, we report the synthesis of indium Oxide decorated graphitic carbon nitride/ multi-walled carbon nanotubes (g-C_3N_4/CNT/In_2O_3) ternary composite by a one-pot solvothermal method as a promising electrode material for supercapacitors. Graphitic carbon nitride, a structural analogous of graphite with aromatic tri-s-triazine units, possesses the advantages of carbon-based materials and also the characteristics of N-doped materials. However, its susceptibility to restacking, due to robust π-π interactions, leads to the recombination of g-C_3N_4 layers and restricts the accessible active surface area, consequently reducing its electrochemical performance. The pseudo-capacitive behavior of In_2O_3 enhances the specific capacitance of the system and serves as a spacer, mitigating the aggregation of g-C_3N_4 layers. The addition of MWCNTs enhances the conductivity and cycling stability of the composite by establishing a network structure that links the g-C_3N_4 layers together. The structural and morphological properties of the composite were analyzed by various analytical techniques. The electrochemical studies of g-C_3N_4/CNT/In_2O_3 ternary composite showcased a remarkable specific capacitance of 1081.4 F g^{-1} with a capacitance retention of 94.5 % after 2000 cycles at 2 A g^{-1}. The ease of synthesis and the superior electrochemical performance of g-C_3N_4/CNT/In_2O_3 ternary nanocomposite showcased it as a potential candidate for supercapacitor applications.

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B 189

Electrocatalytic Hydrogen Evolution Reaction of Ultra-High Dielectric Constant Ceramic 0.5($BaTiO_3$-$BiMnO_3$) Nanomaterials

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ABSTRACT

Electrocatalytic water-splitting reaction and the generation of hydrogen fuel is highly important in energy storage applications owing to depletion of fossil fuels with pollution. Low cost, superior activity, and non-noble metal-based durable electrocatalysts are highly crucial for commercial application. Chemically produced $BiMnO_3$ modified $BaTiO_3$ (0.5$BaTiO_3$-0.5$BiMnO_3$) ceramic nanomaterials exhibit high dielectric constant with electrocatalytic hydrogen evolution reaction (HER) activity. The modification of $BaTiO_3$ and sintered at high temperature leads to the creation of oxygen vacancies which reflected from the powder X-ray diffraction and X-ray photoelectron spectroscopy study. The dielectric measurement demonstrates relaxor nature with 8.1 × 10^8 dielectric constant value at the Tc (450°C) for 1 kHz frequency. The powdered materials are loaded on nickel foam substrate and used for electrocatalytic HER investigation in a three-electrode system under alkaline conditions. The calculated overpotential is 223 mV at 30 mA cm^{-2} current density and the related Tafel slope value is 152 mV dec^{-1}. In the chronoamperometry analysis, the catalyst material shows long-term durability nature that indicates robust nature, which is promising for the designing of reliable electrocatalysts in water-splitting reactions.

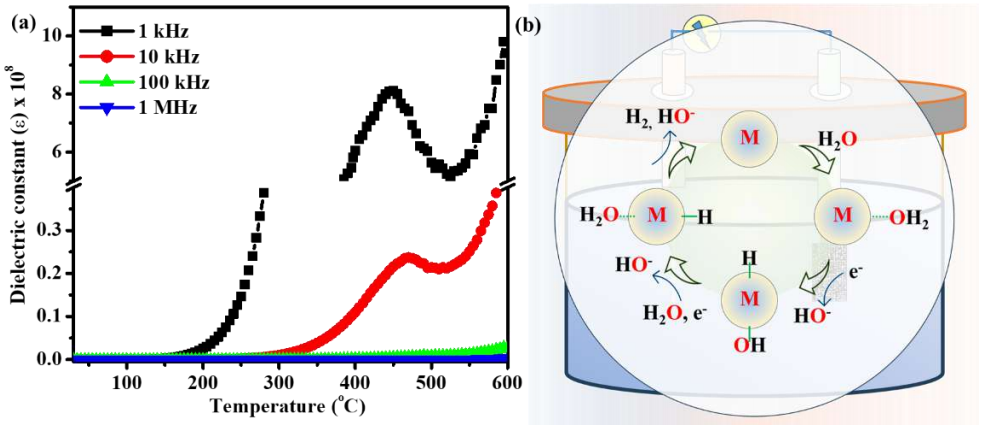

Figure 1. (a) Dielectric constant vs. temperature plot, and (b) electrocatalytic HER mechanism of 0.5($BaTiO_3$-$BiMnO_3$) Nanomaterials

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Electrochemical and Optoelectronic Properties of Magnetron Sputtered Deposited TiN:C films

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ABSTRACT

Electrochemical capacitors (ECs) with high power capabilities and stable cycling can effectively improve the state of the art in power delivery and energy storage. Titanium nitride (TiN), and C-doped Titanium nitride (TiN:C) films (~150 nm total thickness) were deposited using a dc-magnetron sputtering system. A highly intense peak at 36.65º was observed confirming the presence of the TiN phase in the TiN films with a d-spacing of 2.45 Å and crystallite size of 16.34 nm. In XRD of TiN:C a highly intense peak at 2 theta value of 38.3º was observed due to (013) Bragg plane with decreased d-spacing of 2.15 Å and crystallite size of 16.07 nm. The photoluminescence spectra of TiN: C thin films indicate the broadening of emission wavelength in the visible region with a maximum emissive peak around 360 nm. The X-ray photoelectron spectroscopy (XPS) confirmed Ti (2p), C (1s), and N (1s) core orbitals are at 455.12 eV, 283.23 eV, and 394.15 eV on the surface of TiN and TiN:C thin films. With various electrolytes and high-rate cycling conditions, the TiN:C thin film electrodes exhibited excellent cycling stability with negligible capacitance fading after 1,000 cycles and a great rate capability, allowing the (dis)charge rate to extend from 0.2 to 20 V s^{-1} and retaining nearly 80% of the capacitance in a three-electrode system.

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Electrochemical Synthesis of Green Ammonia and Green Urea at Room Temperature: A Lab-to-Land Initiative

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ABSTRACT

There are several types of fertilizers that mostly contain macronutrients like phosphorus, potassium, and nitrogen. Due to its role as the primary limiting factor for plant development, the manufacturing of nitrogen-based fertilizers (such as ammonia, nitrate, and urea) has consistently presented a substantial worldwide obstacle. In order to address the issue of world hunger in the next thirty years, there will be a sustained increase in the utilization of nitrogen-based fertilizers. The impact on energy and the environment will be substantial, as almost all nitrogen-based fertilizers are produced from ammonia and nitric acid, both of which have considerable energy and carbon footprints. To achieve the production of ammonia, urea, and nitric acid without relying on fossil fuels, it is imperative to develop novel technical solutions[1-3].

In our laboratory, we have designed and developed electrocatalytic methods to produce green ammonia, green urea, and nitric acid under ambient conditions using electrocatalysts. All these processes are protected with appropriate IPR. We have completed the field trial of the green ammonia synthesis and initiated the technology transfer and process of licensing for pilot scale production of green ammonia with a multinational company.[4-6]

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High Specific Capacity α-Ni(OH)$_2$/Ni-MOF Supercabattery

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ABSTRACT

Supercabatteries combine features of both batteries and capacitors to deliver high power and energy densities. Among various classes of materials, Metal Organic Frameworks (MOF) hold great promise as supercabattery material, due to their high surface area and tunable structural properties. In this work, Ni-MOF with 1,4 benzenedicarboxylic acid as organic linker was synthesized at various temperatures, resulting in formation of different phases of Ni (such as α-Ni(OH)$_2$) along with Ni-MOF. These different phases affect the specific capacity to a greater extent. A specific capacity of 567.6 C/g at a current density of 1 A/g and 246.6 C/g at 20 A/g was obtained for Ni-MOF synthesized at 150 ºC (Ni-MOF 150). A supercabattery was assembled with Ni-MOF 150 and reduced graphene oxide (rGO) as two electrode device and its efficiency was investigated.

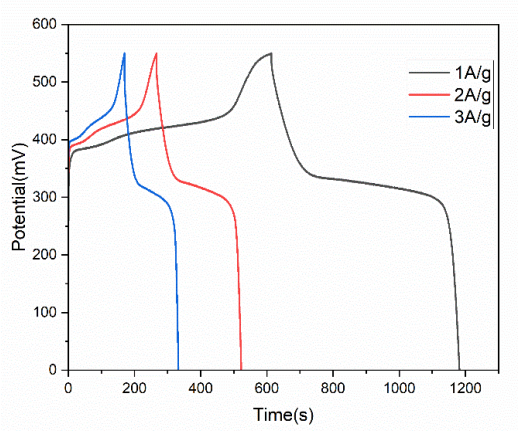

Figure 1. GCD curve of Ni-MOF 150 for lower current densities

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A Study of Aqueous Electrolytes for Carbon Electrode In Supercapacitors

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ABSTRACT

Supercapacitors are playing a very important role in energy storage systems due to its high-power density and quick charge discharge processes. Supercapacitors are made up of various kinds of electrode and electrolyte materials. The electrochemical performance of supercapacitors are based on the concentration of electrolyte used. Selection of a proper electrolyte with suitable concentration helps to enhance the capacitive behaviour for an active material. Here, different aqueous electrolytes like KCl, NaCl, Na_2SO_4, KOH and NaOH of different molarity are used to study the capacitive behaviour using carbon screen printed electrodes. The electrochemical characteristics is calculated by using cyclic voltammetry at a scan rate of 100 mV/s. Among these electrolytes 2M KOH shows a high capacitance value of 17.50 mF.

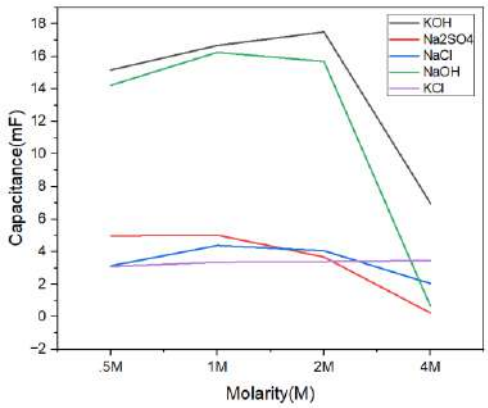

Figure 1: Capacitance Vs molarity of KOH , Na_2SO_4, NaCl, NaOH and KCl

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B 194

CoNi@CN Metal-Organic Framework as Cost-Effective Platinum-Free Efficient Counter Electrodes for Dye-Sensitized Solar Cells

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ABSTRACT

Developing counter electrodes (CEs) with improved catalytic activity has acquired much significance in Dye-sensitized solar cells (DSSCs), as conventional Pt CEs are highly expensive due to their inadequacy. In this work, we synthesized Cobalt (Co)-based Metal-Organic Framework (MOF) as a self-sacrificing template to prepare Nickel (Ni)-modified Co wrapped nitrogen porous carbon (CoNi@CN). The molar ratio of Co and Ni is varied for optimizing the electrocatalytic activity in the CE. The structural and vibrational properties were analyzed through X-ray diffraction and Raman spectral studies respectively. The spherical morphology of the prepared MOFs were examined by SEM and TEM analysis. CoNi@CN-III possesses a large specific surface area, high porosity and abundant active sites of MOFs. Further, the prepared CoNi@CN-III enhance the catalytic activity by 13% which is confirmed by cyclic voltammetry (CV) analysis. From the Tafel analysis, J_0 and J_{lim} is calculated as 0.6665 and 1.2432 mA/cm^2 respectively. Consequently, the fabricated DSSC device (CoNi@CN-III) has achieved a power conversion efficiency of 7.60% which is higher than that of Pt CE (6.69%). The prepared (CoNi@CN-III) device has been a promising substitute for Pt-based CE in DSSCs.

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Breaking Lithium Barriers: A Sustainable Sodium-Ion Battery Anode Prototype

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ABSTRACT

Recent advances in lithium-ion battery (LIB) technology have significantly enhanced daily energy production and storage for a wide range of applications.[1] Despite their extensive use in electronic gadgets and zero-emission automobiles, there are increasing concerns about burden balancing for renewable energy and smart grids, as well as the long-term sustainability of lithium sources due to lack of supply and projected price hikes. The ability of lithium-ion batteries (LIBs) to meet the growing demand for small- to large-scale energy storage applications remains unknown.[2] To address these challenges, current research focuses on alternative energy storage systems. Because of the widespread availability of sodium and its similar chemistry to LIBs, sodium-ion batteries (SIBs) are regarded as the most ideal source of energy storage. Thus, SIBs are attractive options for the next generation of energy storage solutions. [3]Current developments in SIB technology have been made possible by the use of certain carbon-based materials, MXenes and transition metal oxides (TMOs) (or sulphides), as anodes.[4][5] However, both carbonaceous and TMO materials have disadvantages due to their elevated irreversible capacity and inadequate capacity retention. This study presents a successful demonstration of using a combination of carbonaceous materials and transition metal oxides as anodes for sodium-ion batteries (SIBs), which is the first instance of such synergy. The developed sodium-ion battery prototype featuring a green-synthesized anode material with a specific capacity of 315 mAh/g, energy density of 297.7 Wh/Kg, and power density of 94.5 W/Kg demonstrates promising performance. The research addresses concerns over limited lithium resources, emphasizing the importance of sustainable and cost-effective alternatives.

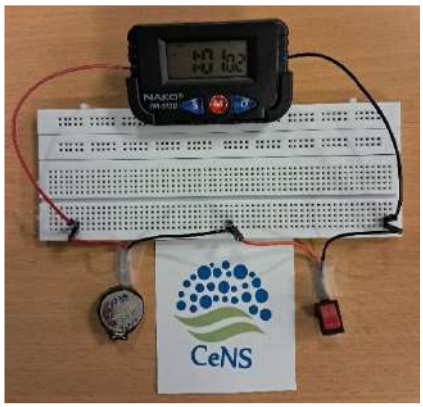

Figure: Fabricated SIB Powering LCD Display

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Tailoring Ternary NiMnFe Layered Double Hydroxides for High Performance Supercapacitor Application

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ABSTRACT

The growing trend towards renewable energy has created a demand for energy storage for later utilization. In this regard, Supercapacitors have gained undivided attention among the scientific community as energy storage devices due to their prodigious power density, magnificent cycling stability and cost-effectiveness. Transition metal-based Layered Double Hydroxides (LDHs) has been regarded as a desired contender for supercapacitor electrode due to their high theoretical capacitance, two-dimensional structure, composition tunability, hydrophilicity and high redox surface area [1]. However, the low conductivity and agglomeration limit the electrochemical performance of LDHs [2]. To address these issues, NiMnFe LDH is grown on Ni foam by one-pot hydrothermal method to reduce agglomeration [3] and to increase surface area. The synthesized samples were characterized by their phase, morphology, and functional groups. The electrochemical measurement such as CV, GCD and EIS was performed in aqueous 3M KOH electrolyte to understand the charge storage mechanism of the electrode materials. The prepared sample exhibited a battery-type supercapacitor behavior with a high specific capacity of 1936 C/g at 1 A/g in three-electrode electrochemical studies.

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B 197

Li^+ Ion Conduction Mechanism of Flaxseed gum Based Solid Biopolymer Electrolyte forPrimary Battery Application

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ABSTRACT

The development of all-solid electrochemical devices like solid-state batteries, supercapacitors and fuel cells requires the utilization of polymeric ion conducting electrolytes. One such biodegradable polymer electrolyte has been reported and its effect of doping various wt.% of Lithium carbonate (Li_2CO_3) into SPEbased on flaxseed gum (FG) on structural, thermal, morphological, transport, electrochemical stability window, and cell properties have been investigated for potential application in proton batteries. FG/ Li_2CO_3 SPEs were prepared via the solution casting technique. The properties of FG/ Li_2CO_3 SPE were characterized via X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS) and open circuit voltage (OCV) analysis. X-ray diffraction (XRD) analysis was used to identify the crystalline or amorphous nature,diffraction peaks, and their corresponding angles of the SPEs. The interactions between the polymer (FG) and Li_2CO_3 were observed with the changes in FT-IR peaks. The ionic conductivity is observed to increasegradually from 10^{-7} to 10^{-5} S/cm when the concentration of Li_2CO_3 increases, which has been identified using EIS analysis. The TNM result was obtained from the DC polarisation technique, and that confirmedthe conducting species of the highest conducting FG/ Li_2CO_3 SPE are mainly due to ions. The changes in structural morphology of FG/ Li_2CO_3 SPEs have been determined from SEM morphology. Using the highest ionic conducting SPE, the proton battery has been constructed, and the OCV has been reported. As a result,it can be concluded that the highest conducting FG/ Li_2CO_3 SPE has demonstrated an optimistic performance and has the potential to be utilized in proton batteries.

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Facile Synthesis of Copper-Doped $Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ Nanocomposite as An Anode Material for Sodium-Ion Capacitors

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ABSTRACT

Sodium-ion capacitors (SICs) have been seen as potential energy storage devices because of their high power/energy density, cycle stability, and cost-efficiency. But they are also restricted by the mismatched reaction kinetics between the battery-type anode and capacitor-type cathode. In this work, the solid-state route followed by calcination has been used to prepare layered P2-$Na_{0.67}Ni_{0.33-x}Cu_xMn_{0.67}O_2$ (x=0.07) nanopowder. Further, Thermogravimetric analysis (TGA), X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy, and Field emission scanning electron microscopy (FESEM) analyses were used to characterize this nanopowder. Cyclic voltammetry, Electrochemical impedance spectroscopy, and Galvanostatic charge-discharge investigations in aqueous 1 M Na_2SO_4 + 0.5 M KOH solution were used to investigate the electrochemical behavior of the prepared layered P2-$Na_{0.67}Ni_{0.33-x}Cu_xMn_{0.67}O_2$ nanopowder-based electrodes. At a constant current density of 2 A g^{-1}, the layered P2-$Na_{0.67}Ni_{0.33-x}Cu_xMn_{0.67}O_2$ acquired a high specific capacitance. The good electrochemical performance of $Na_{0.67}Ni_{0.33-x}Cu_xMn_{0.67}O_2$ is attributed to the partial replacement of Cu ions for Ni ions, which results in a reduction in lattice parameter and improved structural stability during the Na^+ ion intercalation/deintercalation reaction process. Furthermore, the $Na_{0.67}Ni_{0.33-x}Cu_xMn_{0.67}O_2$ has a superior cycling stability, retaining better capacity retention even after 1500 continuous charge-discharge cycles at a constant current density of 2 A g^{-1}.

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Fabrication of Bio-Based Supercapacitors using Agar-Gel Polymer Electrolyte

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ABSTRACT

Supercapacitors stand out as sustainable and high-performance energy storage solutions, revolutionizing industries with their compact size and eco-friendly nature. Yet they grapple with electrolyte leakage issues. Gel electrolytes offer a promising remedy. Here we fabricate a bio- derived electrolyte-based supercapacitor. Agar-based gel electrolyte is obtained by stirring 40ml 5wt% of PVA solution, 1.2 g of agar powder, and 16ml 1M H_2SO_4 using a magnetic stirrer for about 2hrs. A gel-like colloid is formed which is kept undisturbed. 1M H_2SO_4 was added to enhance conductivity. The performance is analyzed via cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. For comparing the performance, the standard gel-based H_2SO_4 electrolyte is formed by stirring 40ml of 1M H_2SO_4 with 4g PVA powder in a magnetic stirrer for 1 hr. Then it's electrochemical performance is evaluated using the same type of electrode. The results show that the bio-based electrolyte yields impressive capacitance values, with the gel-type formulation ensuring leak-free performance.

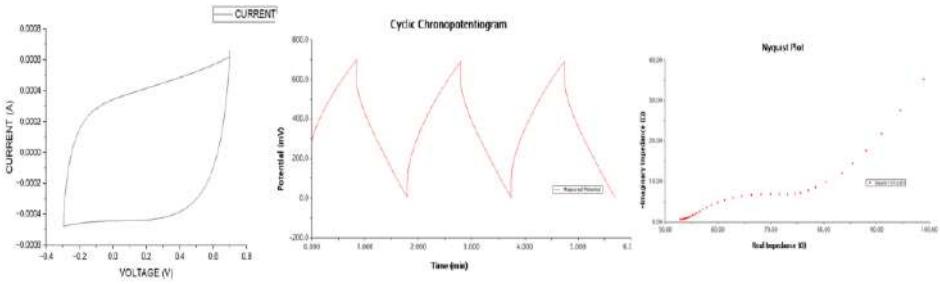

Fig 1: Evaluation of electrochemical performance a) Cyclic voltammetry at 5mV/s b) Cyclic Chromopotentiogram at 0.1 A/g c) Nyquist plot

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B 200

Highly efficient CuO-Co_3O_4 Heterostructure for Enhanced HER and OER Activity

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ABSTRACT

In this study, we report the successful synthesis of a novel CuO-CO_3O_4 heterostructure with enhanced catalytic activity for both the Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER). The heterostructure was synthesized through a facile hydrothermal method, involving a carefully optimized combination of chemical precursors and controlled heat treatment. The resulting material was thoroughly characterized using various analytical techniques, including X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), High resolution transmission electron microscopy (TEM), UV-vis spectroscopy, Raman spectroscopy, and X-ray photoelectron spectroscopy. The XRD, RAMAN, and SAED pattern analysis confirmed the formation of a well-defined CuO-CO_3O_4 heterostructure phase, and microscopic imaging techniques revealed the nanosheets decorated on nanorods morphology of the synthesized particles. The electrocatalytic activity of the CuO-CO3O4 heterostructure was systematically investigated for both HER and OER in alkaline conditions in 1M of KOH. The heterostructure exhibited remarkable electrocatalytic performance, surpassing catalysts in their bare form. It has been observed that the overpotential of heterostructure is 231 mV vs RHE and 0.380 mV vs RHE at 50 mA/Cm^2 current density for HER and OER respectively; Moreover, the prepared heterostructure attained the current density of 400 mA/cm^2 and 190 mA/cm^2 for HER and OER respectively. There has been significant enhancement in the the Tafel slop, C_{dl}, and ECSA which valued at 98 mV/dec, 670 µFcm^{-2}, and 16.75 cm^2 respectively. In conclusion, our study presents an efficient synthesis route for CuO-CO_3O_4 heterostructures and the superior electrocatalytic performance for both HER and OER positions these heterostructures as promising candidates for advanced water splitting applications.

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B 201

Multifaceted Insights into Au Coatings Electrodeposited from a ChCl-EG Based Deep Eutectic Solvent (DES) Bath: Unravelling the Effect of Surfactant Polarity and Current Density on The Morphology, Mechanical Properties, And Anti-Tarnishing Efficacy

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ABSTRACT

In the present work, the effect of surface polarity of cationic [cetyl trimethylammonium bromide (CTAB)], anionic [sodium dodecyl sulfate (SDS)], and non-ionic [polyvinylpyrrolidone (PVP)] surfactants on the structural, mechanical and anti-tarnishing efficacy of Au coatings electrodeposited from a choline chloride-ethylene glycol (ChCl-EG) based bath is investigated. X-ray diffraction studies and first-principles calculations reveal that both cationic and anionic surfactants tend to get adsorbed on facets other than (111), effectively facilitating the growth of Au along the (111) planes during electrodeposition. Electrochemical characterizations of the bath are carried out to analyze the critical role played by various surfactants during the reduction of gold from the electrolytic bath. The influence of the polarity of the surfactants, as well as the applied current density on the micromorphology, surface topography and mechanical properties of the coatings, is also assessed. In the presence of CTAB, the electrodeposited Au layer has a smooth surface with almost a globular morphology. However, in the presence of SDS, the morphology of the Au coating changes from globular to sharp-edged facets. In the presence of PVP, the Au coating has an irregular faceted type morphology. The changes in the surface topography of the coatings are studied using atomic force microscopy (AFM). The findings of the electrochemical impedance spectroscopy (EIS) studies and static immersion tests reveal that in the presence of cationic and anionic surfactants, the Au coatings have better resistance to tarnishing in a sulphide environment. Therefore, a strategy for developing tarnishing-resistant Au coatings via electrodeposition involves the control of surface morphology, which is well facilitated by using proper surfactants.

Keywords: *First-principles study; ChCl-EG; Deep Eutectic Solvents; Au Coatings; Anti-Tarnishing Coatings; Surfactant Polarity*

B 202

The Impact of Cl^- On Electro Chemical Properties of PPy Coated on SiO2 Encapsulated Carbon Nanosheets Based Anode Material for High Stable and Faster Li ion storage

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ABSTRACT

A simple sol-gel technique combined with pyrolysis process was used to prepare Polypyrrole (PPy) coated porous carbon nanosheets-SiO_2 composite (PPy/CNS- SiO_2) as anode material. Owing to its high capacity, abundant reserves, environmental friendliness, and low working potential, SiO_2 is considered among the foremost promising anode material for Li-ion battery (LIB). However, the huge volume changes in SiO_2 during charge and discharge process leads to pulverization, which ruptures the solid electrolyte interface film resulting in short cycle life and rapid capacity decay. Herein, we mainly dedicate the attention on low cost with high specific capacity and good rate capability anode materials for construction better battery performance. The 2D architecture of porous carbon nanosheets would offer a sufficient space to buffer a large volume expansion of SiO_2 that maintained mechanical integrity of the overall electrode during the lithiation/delithiation process. In addition, the conducting polymer coated on the surface of CNS- SiO_2 composites efficiently suppresses the volume expansion and rapid capacity fading caused by serious pulverization and low electronic conductivity of SiO_2. The presence of Cl^- on the structural, electronic properties of CNS- SiO_2 effectively improve the electrochemical stability and the Li^- ion transport performance. Cl^- contribute to increase Li^+ diffusion by reducing the migration energy and improve the conductivity by reducing the bandgap of the electrode material which helps to enhance the rate capability. As an anode, this material show a remarkable specific reversible capacity of 1380.5 $mAhg^{-1}$ at 50 mAg^{-1} current density and a 100% capacity retention and high Columbic efficiency after 300 charge–discharge cycles. Overall, our synthesized electrode material appears to be high performance LIB anode compare to commercial graphite which makes it's a superior anode material for next-generation, high-power, long-life and affordable Li-ion battery.

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Nanostructured Urchin-Like $NiCo_2O_4$ Catalyzed with Surface Oxidized $LiBH_4$ System for Hydrogen Storage Applications

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ABSTRACT

The mesoporous $NiCo_2O_4$ nanostructure was synthesized by facile hydrothermal method and mixed with surface oxidized $LiBH_4$ system by wet-impregnation method, followed by heat treatment. The calculated BET (Brunauer-Emmett-Teller) surface area of $NiCo_2O_4$ and $LiBH_4$+75% $NiCo_2O_4$ systems are 124.05 and 136.62 m^2/g, respectively. The possible hydrogen storage properties were investigated for surface oxidized $LiBH_4/NiCo_2O_4$ systems for the first time. Typically, the hydrogenated $LiBH_4$+25% $NiCo_2O_4$, $LiBH_4$+50% $NiCo_2O_4$ and $LiBH_4$+75% $NiCo_2O_4$ systems desorbed 2.85 wt.%, 3.78 wt.% and 3.91 wt.% of hydrogen respectively, in the dehydrogenation temperature range of RT to 275 °C. Further, the $LiBH_4$+75% $NiCo_2O_4$ system exhibits better kinetics than others, which released ~ 5.8 wt. % of hydrogen during isothermal dehydrogenation at 250 °C in 60 minutes. The hydrogen binding energy was calculated as 0.28, 0.27 and 0.26 eV for $LiBH_4$+25% $NiCo_2O_4$, $LiBH_4$+50% $NiCo_2O_4$ and $LiBH_4$+75% $NiCo_2O_4$ systems, respectively. Moreover, the calculated activation energy of $LiBH_4$+25% $NiCo_2O_4$, $LiBH_4$+50% $NiCo_2O_4$ and $LiBH_4$+75% $NiCo_2O_4$ systems are 17.99, 17.03 and 16.92 kJ/mol, respectively. These results showed that hydrogen sorption properties are significantly increased by the influence of mesoporous structure and low activation energy of $LiBH_4$+75% $NiCo_2O_4$ system.

Keywords: *Hydrogen storage; $LiBH_4$; $NiCo_2O_4$; surface oxidation; activation energy; binding energy.*

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B 204

High-efficient and Cost-effective Electrochemical Symmetric Supercapacitors fabricated using Phytochemical-derived Selective Silver Nanocrystal-on-Cobalt Oxide Nanocomposite

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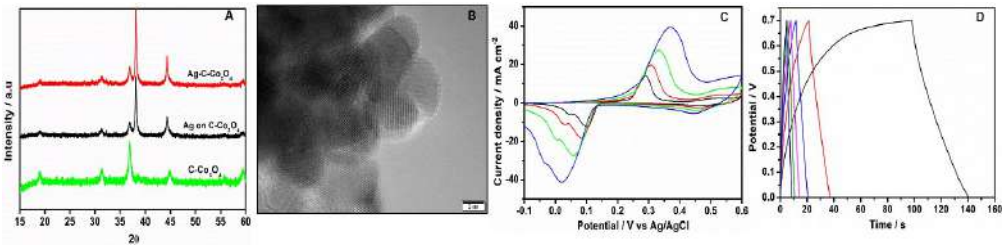
ABSTRACT

An electrochemical symmetric supercapacitor has been developed employing a silver nanocrystal-over-cobalt oxide nanocomposite synthesized by directed deposition of silver nanocrystals critically over cobalt oxide with the use of exclusively eco-friendly phytochemical reagents alone. One-pot synthesis of the silver nanocrystal-on-cobalt oxide nanocomposite (nanoAg-Co_3O_4 composite) was achieved by stepwise addition of aqueous solutions of cobalt and silver ions to the phytochemical extract, and the mixture was treated for 24 h at 95 C. The nanoAg-Co_3O_4 composite was drop-casted on carbon fibre paper (CFP) to fabricate the supercapacitor electrode, and it exhibited a pseudo-reversible redox peak in cyclic voltammetry in the region of 0 – 0.4 V vs Ag/AgCl. The electrode exhibited a specific capacitance of 400 F g^{-1} at 0.5 A g^{-1} current density in galvanostatic charge-discharge (GCD) analysis over the potential window of 0.65 V and the coulombic efficiency was 90%. The retention rate of the specific capacitance was 77% over the range of 0.5 A g^{-1} to 4 A g^{-1}. Free-standing symmetric supercapacitor fabricated with nanoAg-Co_3O_4 coated CFP electrode exhibited a specific capacitance of 240 F g^{-1} at 2 A g^{-1} current density with a potential window of 0.7 V. The symmetric supercapacitor exhibited a maximum energy density of 16.4 Wh kg^{-1}, and the maximum power density was as high as 8.4 kW kg^{-1} with an energy density of 8.6 Wh kg^{-1}.



(A) Powder XRD profiles and (B) HRTEM images of nanoAg-on-Co_3O_4 nanocomposite. (C) CVs and (D) GCD curves of nanoAg-on-Co_3O_4 nanocomposite as working electrode recorded in aq. 6 M KOH.

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Investigation on Flaxseed Gum-PVA based Solid Biopolymer Electrolyte for Primary Battery Application

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ABSTRACT

Ionically conducting polymer electrolytes received significant attention in a wide variety of energy storage devices particularly batteries, supercapacitors and fuel cells. Flaxseed gum with PVA based biopolymer electrolyte has been reported and its effect of doping various wt% of ammonium Iodide (NH_4I) on structural, morphological, transport,and cell properties hasbeen investigated for application in proton conducting batteries. FG/PVA-NH_4I SPEs were prepared via the solution casting technique. The properties of FG/PVA-NH_4I SPE were characterized via X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS) and open circuit voltage (OCV) analysis. The XRD analysis reveals remarkable enhancement in the amorphous nature with the incorporation of NH_4I.The complexation between FG, PVA and NH_4I was proven using FTIR analysis with the formation of OH bond. The impact of NH_4I in FG/PVA matrix was investigated mainly via electrochemical impedance spectroscopy (EIS). The TNM analysis was done by DC polarisation technique, and that confirmed the conducting species are mainly ions in the highest conducting SPE. The changes in structural morphology of the SPEs have been determined from SEM morphology. Using the highest ionic conducting SPE, the proton battery has been constructed, and the OCV has been reported. This study explores the influence of an ionic dopant NH_4I, when incorporated into the FG matrix, the ionic conductivity is increased to 5.29×10^{-4} S/cm. This improves the functionality of the battery and further boosts its stability.

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Structural, Vibrational and Electrochemical Studies of Bulk And Nano SnSb for Supercapacitor Application

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ABSTRACT

The great power density of electrochemical capacitors, also known as supercapacitors, makes them extremely helpful for maintaining pulse power as compared to batteries. Supercapacitors are crucial components for meeting the growing demand for energy and resolving energy crises because of their high-power density, exceptional cycle stability, fast charge-discharge interval, and environmental friendliness. In this work, co-precipitation and vacuum melting reactions were used to prepare bulk and nano SnSb. For both bulk and nano SnSb. The PXRD, UV–vis spectroscopy, Raman spectroscopy, SEM, and TEM micrographs also X-ray photoelectron spectroscopy are deeply scrutinized to vindicate the structural, optical, vibrational, and morphological and oxidation state of the as-synthesized bulk and nano SnSb. Bandgap values of both bulk and nano SnSb are 0.64 and 0.77 eV determined by the Kubelka- Munk relation. For analysing electrochemical properties three electrode system is deployed and the highest specific capacitance of 257.31 F/g and 504.46 F/g is recorded for bulk and nano SnSb. Due to good electrochemical property, nano SnSb is chosen for further device fabrication by Swagelok assembly asymmetric type. It has recorded the highest power density of 4000 W/Kg and energy density of 7.8 Wh/Kg.

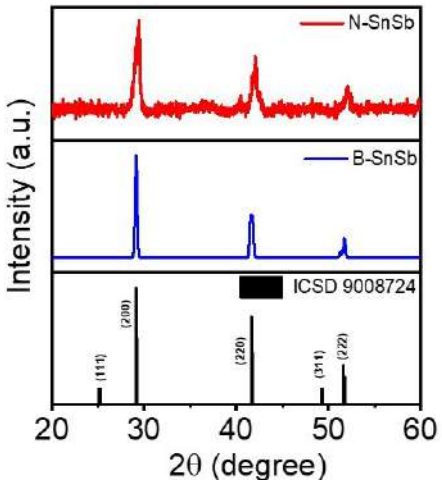

Figure 1: XRD pattern of bulk and nano SnSb

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Boron Supported 2D Nanostructured Bimetallic Oxide ($NiMoO_4$) as Electrocatalyst for Improved Electrocatalytic Seawater Oxidation Performance

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ABSTRACT

Design and development of effective electrocatalysts containing non-precious materials for oxygen evolution reaction (OER) in seawater splitting remains a significant challenge for large-scale industrial hydrogen production. Non-precious bimetallic oxide constructed catalyst demonstrations utmost promising candidate to obtain boosting electrochemical water oxidation performance. Herein, we present a Boron induced transition bimetallic oxide nanostructure electrocatalyst as $NiMoO_4$ vertically standing nanosheets over the nickel foam substrate (B-$NiMoO_4$/NF) for electrochemical water oxidation process in alkaline fresh/simulated seawater conditions. $NiMoO_4$ nanostructure on NF substrate has been successfully obtained using a straightforward two-step hydrothermal reaction route and thermal annealing processes. The surface morphology with elemental characteristics of the resultant B-$NiMoO_4$/NF sample exposes highly homogenous vertical standing nanosheets assembled on NF surface. The electrochemical water oxidation performance of as-prepared electrodes demonstrates as the function of diverse boron reaction times (3, 6 and 9 hours) in fresh and simulated seawater electrolyte conditions will discuss.

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V_2O_5 Nanoribbons for improved Cyclic Stability in Aqueous K^+- ions Based Supercapacitor

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ABSTRACT

Highly desirable electrochemical energy storage devices include supercapacitors (SCs) due to their high-power density, infinite lifetime, and fast charge-discharge rate. Due to its layered structure, facile oxidation state, reversibility and high abundance, V_2O_5 has garnered researcher attention among other transition metal oxides. Due to its high surface-to-volume ratio, nanostructure V_2O_5 shows better electrochemical properties than bulk V_2O_5. Triblock copolymer surfactant Pluronic p123 assisted ultralong V_2O_5 nanoribbons (VNRs) were made in one step hydrothermally. The high length of VNRs shortens the diffusion path of electrolyte ions, reducing volume expansion during intercalation and de-intercalation and producing excellent electrochemical results. Over 2000 cycles, VNRs retain 39% of their initial capacitance with highest specific capacitance of 140 Fg^{-1} at 5 mVs^{-1}.

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Facile Synthesis and Higher Supercapacitor Performance of Ag_2Se Nanomaterials

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ABSTRACT

The Ag_2Se supercapacitor electrode material has been synthesized by a facile hydrothermal method taking octylamine as solvent and silver nitrate and selenium powder as precursor. The octylamine acts as a suitable medium for the nucleation and growth of Ag_2Se nanomaterial. The synthesized Ag_2Se was characterised by XRD, UV and fluorescence spectroscopy to study the crystallinity and band gap of the nanomaterial. From the XRD spectrum, sharp and distinguished peaks are obtained which suggested the crystallinity of the material. The electrochemical performance of Ag_2Se was executed taking 1M of Na_2SO_4 AND KOH to reveal the supercapacitor characteristics of the synthesized material. The highly high capacitance of the Ag_2Se nanomaterial was determined using the CV and CD plot. Thus, the electrochemistry of the Ag_2Se nanomaterial proved that, it can be used as a high energy and power density electrode material for high performance super capacitor.

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Synthesis Of Electrocatalysts for Urea Oxidation Reaction

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ABSTRACT

The use of energy in the biomedical field has gained considerable interest with the goal to harvest energy for healthcare through portable devices that can be powered by wearable biofuel cells, which can provide continuous information to those wearing them.[1] Particular attention has been given to fuel cells that can generate energy from urea present in the human body, the average human adult urine that can be produced in one day can contain about 2-2.5 wt% of urea.[2] Urea itself has a higher energy density than liquid hydrogen, making a potential energy carrier. Considering the UOR (Urea Oxidation Reaction) produces water, nitrogen and carbon dioxide which has it's issues with alkaline media, membranes are required as they are compatible with CO_2 and improve cell performance.[3] Another important reaction to consider is the ORR (Oxygen Reduction Reaction) which occurs in many energy storage devices and produces hydroxide anions in alkaline media and has a slow kinetic rate. Platinum catalyst as well as enzymes are regularly the most common in the scenario of these reactions,[4] but are very scarce and high cost to design, so many propositions seek to use low-cost non-precious catalyst for these reactions as they are also more stable in the alkaline media. Here we propose the design of Ni based electrodes that have a higher affinity to urea oxidation used on a template of carbon ink over a membrane to function as a portable urea biofuel cell that is wearable on the skin to take advantage of the urea present in human sweat.

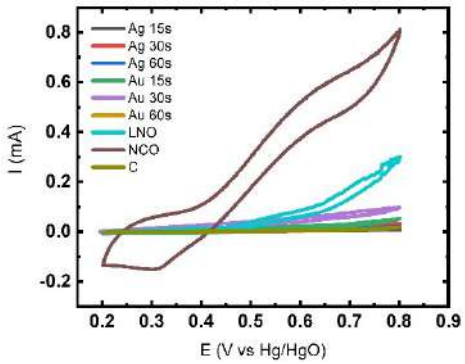

Fig.1. Cyclic voltammograms for urea oxidation reaction with different electrocatalysts.

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CoMn@CN Metal-Organic Framework as Cost-Effective Platinum-Free Efficient Counter Electrodes for Dye-Sensitized Solar Cells

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ABSTRACT

In DSSC applications, the development of counter electrodes (CEs) with increased catalytic activity has taken on great importance because typical Pt CEs are insufficient and therefore very expensive. In relation to this matter, we have documented the effective catalytic activity of metal organic frameworks (MOFs) based on porous carbon and doped with nitrogen (CoMn@CN), which are employed as CEs in DSSCs. Vibrational and structural characteristics were examined using Raman spectral analysis and X-ray diffraction, respectively. Through TEM and SEM research, the produced MOFs' morphology was investigated. Next, Tafel polarisation, impedance spectroscopy, and cyclic-voltammetry were used to investigate the electrochemical characteristics. The produced MOF-based CEs have enhanced conductivity and outstanding catalytic activity due to their high porosity and large specific surface area. Finally, the photoconversion efficiency (PCE) were evaluated for the fabricated DSSC with the prepared CoMn@CN as CE. The obtained results shows that the prepared CEs are highly promising for achieving device efficiency.

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B 212

Optimizing the Thermal Energy Storage Performance through Nanostructured Phase Change Materials for medium temperature applications

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ABSTRACT

The current generation of electricity from renewable resources is insufficient to attain the present worldwide need for energy. The main purpose is to bring more than one updated technique that could build the space in energy distribution. One of the most widely used materials is phase change materials (PCM). Recently energy storage research has been improved PCM is a natural phase transition material, which can be combined with energy storage total systems to conserve renewable energy. Due to their low thermal conductivity, the practical application of organic PCM is limited to thermal energy storage. To overcome this drawback, in this study, D-mannitol PCM and various proportions of nanoparticles (silicon carbide) were used as matrix and heat conduction enhancers of phase change materials (PCMs), respectively. The objective of this research is to look at the thermal characteristics of D-Mannitol as a PCM for the thermal energy storage system. D –Mannitol PCM absorbs heat, which causes it to transform from solid to liquid, and this heat is stored as the latent heat of fusion. Differential Scanning Calorimetry (DSC) measurements were used to determine the melting point and enthalpy of fusion of D-Mannitol - PCM. The melting started at 164°C and reached the peak at 174°C, with a fusion enthalpy of 326.8 J g-1 for 10°C min-1. The thermal conductivity of PCM is investigated by a laser flash test. The structural and morphological characteristics of nanocomposite PCM were investigated by a High-resolution transmission electron microscope (HRTEM) and X-Ray Diffraction (XRD). The thermal conductivity Nano PCM of is increased from 0.7 to 1.9 W/m·K . D Mannitol nano PCM is the best choice for medium temperature applications.

Keywords: *Thermal Energy storage, Phase change material (PCM), Silicon Carbide, DSC, XRD, HRTEM*

B 213

Zinc Ferrite Nanoparticles as Electrode Material for Supercapacitor

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ABSTRACT

Global energy crisis due to limited fossil fuels, along with rising pollution has necessitated utilization of renewable energy, in line with United Nations' Sustainable Development Goals of affordable and clean energy to be met by 2030. Intermittent nature of renewable energy supply has made use of storage mechanisms like batteries and supercapacitors, essential. The pursuit of high-performance and sustainable energy storage solutions has led to an intensified exploration of alternative electrode materials for supercapacitors. This work deals with development of supercapacitors using low band gap electrode material and investigates the electrochemical potential of zinc ferrite ($ZnFe_2O_4$) as a candidate for supercapacitor applications. Zinc ferrite, is a spinel-type mixed metal oxide, known for its cost-effectiveness, abundance, and environmental friendliness, offers a compelling alternative to traditional electrode materials. In this regard, zinc ferrite ($ZnFe_2O_4$) nanoparticles has been synthesized by facile chemical precipitation method. The structural and morphological characterisation by X-ray diffraction and scanning electron microscopy revealed formation of nano-crystalline spinel ferrite particles with uniform morphology. The XRD representation confirmed the spinel structure of the zinc ferrite nanoparticles. The electrochemical performance of as prepared samples was investigated by Cyclic voltammetry, Galvanostatic charge discharge (GCD) and Electrochemical impedance spectroscopy (EIS) in three electrode configurations. CV results shows the typical pseudocapacitive like behaviour. Furthermore, the results revealed good specific capacitance, cycling stability, and capacitance retention percentage in Alkaline electrolyte. Our studies suggest the use of zinc ferrite as low-cost stable oxide of earth abundant metals as a viable electrode material for practical application in the development of supercapacitors.

Keywords: Zinc Ferrite, Spinel structure, Pseudocapacitive, Supercapacitor.

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B 214

Nano-Flake Morphology of Carbonized Aluminum Doped Betel Green Leaves and its Dye Exctract for Energy Conversion and Storage Applications

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ABSTRACT

Naturally occurring betel leaves are employed in many medical applications since the extracted dye has unique physical properties are suitable to use in solar cell and super capacitor. By integrating them together into photo-supercapacitor (PSC) devices, which can store immediately converted energy gives way world's energy demand can be met. The XRD, FTIR, and FESEM methods evidence to design the carbonization of betel leaf extract, which can change structural phase, chemical interaction, and morphology respectively. In particular, leaf extract samples with porous and aluminium doped nano-flake morphology with high surface areas can accommodate more charge carriers. As a result, these have uses in energy storage. Similarly, the high absorbance of the extracted dye at 357 nm indicates its employment as a dye sensitizer in DSSCs, which results in a decreased PCE of about 0.1% because of the charge recombination mechanism. Electrochemical energy storage via the EDLC mechanism is clearly demonstrated by the CV and GCD analysis. Through the electrochemical storage of photo-converted energy, this strategy offers a simple and sustainable method of harnessing solar energy that could eventually lead to successful improvements in this field.

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B 215

High-Performance α-Fe_2O_3 Nano Cubes as a negative and NiO as a positive electrode material for Supercapacitor

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ABSTRACT

In the quest for sustainable energy storage solutions, the exploration of electrode materials for supercapacitors holds significant promise. This study investigates the sustainability aspects of utilizing hematite (Fe_2O_3) as a negative electrode material and nickel oxide (NiO) as a positive electrode material for supercapacitors. Abundant Availability, high theoretical specific capacitance and low cost of transition metal oxides such as iron oxides' makes them attractive as electrode materials. Hematite, abundant in nature and characterized by its low cost and environmental friendliness, is evaluated for its potential as a sustainable negative electrode. In order to achieve improved performance, high conductivity, shorter ion-diffusion path, faster ion accessibility, and rational morphology of electrode material is highly desirable. We have successfully achieved high specific capacitance and better retention by synthesizing a mesoporous α-Fe_2O_3 nano cubes. The as-prepared and annealed α-Fe_2O_3 nano cubes show high reversible redox activity along with good thermodynamic stability. The half-cell anode using these nanostructure gives rise to a high specific capacitance and ~90% of the capacitance can be retained at even after 1000 redox cycles, suggesting good cyclic stability. The performance of these Nanoporous α-Fe_2O_3 nano cubes is much superior to reports on iron oxide-based supercapacitors. Because of their unique nanostructure, large specific capacitance and wide operating potential, a novel NiO//Fe_2O_3 asymmetric supercapacitor (ASC) was assembled by using NiO Nanoflower (NFs) as positive electrode and α-Fe_2O_3 Nanocubes as negative electrode, respectively. A two electrode α-Fe_2O_3//NiO device was fabricated which showed excellent power and energy density of ~627 W/kg and ~23.32 Wh/Kg respectively based on the total mass of both the electrodes. The present work underscores the significance of advanced sustainable solutions in the development of efficient 3D Nanoporous α-Fe_2O_3 energy storage systems, paving the way for a more sustainable future.

Keywords: *Transition metal oxides (TMOs); α-Fe_2O_3; 3D Mesoporous Networks; Supercapacitor.*

B 216

Vapor Phase CVD of Robust Vertical MoS_2 Nanosheet Occupied with MoO_2 on Molybdenum Foil as a Binder-Free Lithium-ion Battery Anodes

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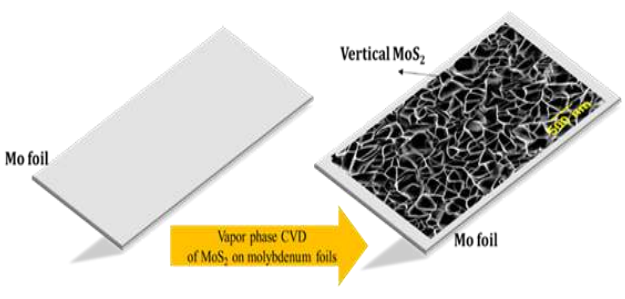
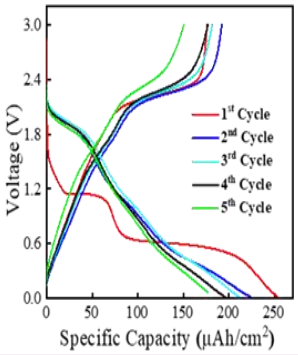
ABSTRACT

Self-supported molybdenum disulfide (MoS_2) nanostructures directly grown on current collectors are promising anode materials for Lithium-ion batteries (LIBs). Here, we report vapor phase chemical vapor deposition (CVD) of self-integrated vertical MoO_2/MoS_2 nanosheets directly on molybdenum foil, as a potential approach towards the fabrication of binder-free anode for LIBs. The partial conversion of deposited MoO_2 crystals to MoS_2 layers results in the formation of MoO_2/MoS_2 hybrid structure, which enhances the electrochemical performance of MoS_2 anode material. The MoS_2 nanosheets without additional conductive or binder agents attached directly to the current collector offered extremely efficient transfer of ions and electrons. This can be attributed to the high electrical conductivity of MoO_2 and extremely exposed active sites of MoS_2. The scanning electron microscopy, Raman spectroscopy, and X-ray diffraction results provided evidence for the stepwise conversion of MoO_2 to MoS_2. Furthermore, the electrochemical studies performed on MoO_2/MoS_2 hybrid material on molybdenum foil revealed an areal capacity of 253 μAh/cm^2 along with detailed cyclic voltammeter and electrochemical impedance spectroscopy (EIS) studies, demonstrating the hybrid structures potential as a promising anode material for Li-ion micro batteries. Our findings show that the entire capacity of the LIBs can be configured by engineering the anode material and the MoO_2/MoS_2 as an anode material can be a good choice in overcoming the limitations of single anode materials.





B 217

High-Performing Au doped PtCo Nanoparticles for Oxygen Reduction Reaction

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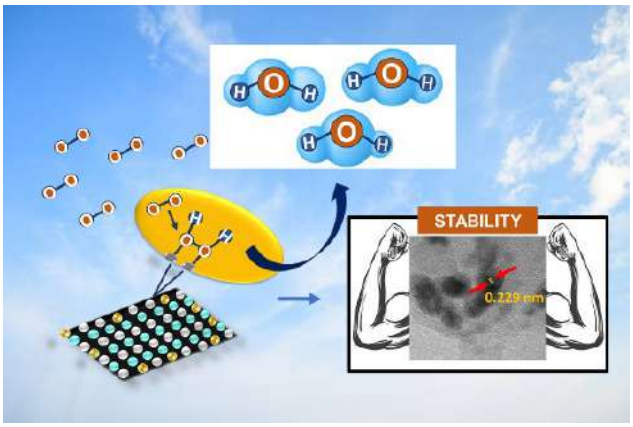
ABSTRACT

To achieve fuel cell commercialization, the performance enhancement and cost reduction of catalysts are still the main challenges. To improve the catalytic activity and durability for oxygen reduction reaction (ORR), we prepare Au−PtCoparticles entrapped in a porous carbon by simple refluxing procedure [1]. The optimal Au−PtCo particles in catalyzing ORR has initial specific and mass activities 6 times higher than the commercial catalyst of Pt/C. Such a larger activity is higher than most of the Pt-based catalysts reported in the literature. Intensified durability testing induces little degradation of the catalytic activity, particularly the Au-doped one, after potential cycling of the catalyst for thousands of cycles under harsh electrochemical conditions involving an acidic medium and a high potential range of 0.66−1.3 V. This is in big contrast with the higher degradation shown by most previous catalysts. The excellent activity and durability are attributed to synergistic effects of the confining support of the porous carbon, and the homogeneous incorporation of a trace amount of Au[2]. The new catalyst of Au−PtCo/C represents a new strategy for performance enhancement and cost reduction and thus promotes practical applications of proton-exchange membrane fuel cells.



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C 001

Wearable Technology for OSA Detection: Microphone-Based Snoring Analysis

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ABSTRACT

Snoring, a recurring habit often disregarded within the Indian community, can signal a grave underlying issue—Obstructive Sleep Apnea (OSA). OSA is a severe sleep disorder characterized by recurrent interruptions in breathing for more than 10 seconds during sleep, typically due to partial or complete airway obstructions. Neglecting OSA can lead to a range of significant health risks, including increased likelihood of occupational accidents, motor vehicle accidents, heightened susceptibility to severe depression, cardiac and cerebrovascular diseases, and reduced life expectancy. The main objective of the study is to detect snoring while at sleep and also to classify it as normal snoring and OSA snoring. Arduino nano 33 BLE sense is used to capture the snore signal, it houses a built-in MP34DT05 sensor. The sensor has a signal-to-noise ratio of 64dB and sensitivity of -26dBFS ±3dB. This captures the sound signal of the individual, it is further processed to extract the Mel-filter bank energy features, Mel Frequency Cepstral Coefficients and Spectrogram features. The features are further used to build a model and the same is trained using edge impulse to classify the signal. The dataset is divided into training, testing, and validation sets, with 80% of the data allocated to training, 20% to testing, and an additional 20% within the training data set aside for validation purposes. The results indicate that the spectrogram-based approach achieved an accuracy rate of 96.9%, while the other two methods yielded accuracy rates of 93.8%. This autonomous system can facilitate the detection of Obstructive Sleep Apnea (OSA) through the analysis of snoring patterns, subsequently alerting the subject to implement preemptive measures for remediation. Timely intervention and rectification can enable the subject to attain an undisturbed and restful night's sleep, thereby augmenting their overall quality of life.

C 002

Flexible Capacitance Pressure Sensor for E-Skin Application

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ABSTRACT

Flexible pressure sensors are a booming business in the current period due to their promise in applications such as robotics, prosthetic hands, electronic skin, human-machine interactions, and so on. Capacitance pressure sensors (CPS) have various advantages over conventional transduction systems. In general, a capacitance pressure sensor is made up of a dielectric layer sandwiched between two conducting electrodes. In recent years, researchers have been looking towards wearable sensors with high sensitivity and a wide operating range. The researchers uncovered numerous approaches to improve the dielectric properties of CPS as a result of their examination into the flexible capacitance pressure sensor. It is feasible to build capacitance pressure sensors with high capacitance by inserting fillers into the insulating polymer matrix, which increases its dielectric permittivity. Here, a polymer nanocomposite is used as the dielectric layer to create a capacitance pressure sensor with exceptional sensitivity. To make the polymer nanocomposite, the high dielectric material ZnO and the conductive filler carbon black are equally spread throughout the polymer matrix. This dielectric layer is sandwiched between silver conductive electrodes. The conductive silver electrodes are obtained by screen printing technique. The sensor has a sensitivity of 2.56293 N^{-1}. It has a wide working range of 0-75 N and a quick response/recovery time of 36 ms/29 ms. The sensor is a potential candidate for real-time monitoring of human activities. So, they can be used in the field of wearable electronics and robotics.

C 003

Efficient Detection of Nitric Oxide using rGO/TMCPP Nanocomposite-Based Chemiresistive Sensor

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ABSTRACT

In this innovative research, we present a meticulous exploration of the synthesis and utilization of a cutting-edge chemiresistive sensor tailored for the remarkably discerning detection of nitric oxide (NO) gas. Our novel approach is focused on a development of the sansors based on the composite material ingeniously crafted from reduced graphene oxide (rGO) and 5,10,15,20-tetra-kis(4-methoxycarbonylphenyl)-21,23H-porphyrin (TMCPP). This sensor emerges as an exceptionally promising candidate in the realm of NO gas sensing, owing to its unparalleled repeatability and selectivity exclusively geared towards NO. The synthesis of graphene oxide (GO) involved a meticulous refinement process employing an enhanced variant of Hummer's method, culminating in the thermal reduction of GO into the highly responsive rGO. The resulting rGO/TMCPP composite material was methodically cast onto an indium tin oxide (ITO)-coated electrode using a precision-driven drop-casting technique. The material's physical and chemical attributes were rigorously scrutinized through an extensive array of characterization methodologies, offering profound insights into its fundamental properties. Remarkably, the rGO/TMCPP sensor exhibited rapid response and recovery times, falling within an impressive timeframe ranging from 59 to 110 seconds. Furthermore, the developed sensor showcased an exceptional proclivity for corrosive NO, exhibiting unparalleled selectivity alongside outstanding repeatability, reproducibility, sensitivity, and linearity. Specifically, the sensor demonstrated a wide detection range, spanning from 50 parts per million (ppm) to 500 ppm for higher concentrations, and from 2.5 ppm to 25 ppm for concentrations below the stringent limits set forth by the Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL). These innovative findings underscore the unparalleled potential of the rGO/TMCPP composite as an immensely effective chemiresistive sensor meticulously tailored for NO detection. Its applicability extends across a myriad of industrial and environmental monitoring domains, signifying a monumental leap forward in the realm of gas sensing technologies.

Keywords: *sensor, graphene oxide, reduced graphene oxide, porphyrin, response - recovery time, selectivity, and NO gas.*

C 004

Acridine Based Porous Organic Polymer as a Fluorescent Probe for the Detection of Nitro aromatics

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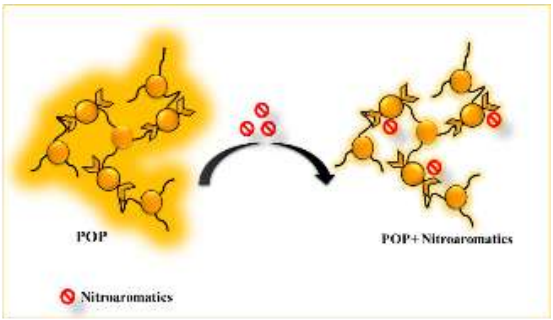
ABSTRACT

Organic materials with tenacious porosity and appropriate functionality remain a major task among the researchers. Porous organic polymers (POPs) are a key subclass of these materials, which are fabricated from small organic molecule-based building units through covalent linkages. These polymers possess wide surface area, high porosity, low density and a flexible chemical structure, as well as excellent physico-chemical stability. A variety of POPs have been reported, including Covalent Organic Frameworks (COFs), Conjugated Microporous Polymers (CMPs), Polymers of Intrinsic Micropore Size (PIMs) etc. These polymers are being explored as potential platforms for a range of applications, including gas storage and separation, catalysis, energy applications, organic electronic devices and more. Recently, POP materials have shown a progress in sensing fields including explosive sensing, humidity sensing, pH sensing, bio-sensing, gas sensing, metal ion sensing, etc. Owing to several global terrorist incidents in the last few decades along with the toxicity, detection of nitro explosives has gained tremendous research thrust. Nitro explosives have electron-withdrawing nitro groups and therefore they are electron deficient compounds and could easily interact with electron-rich fluorescent sensory materials. So keeping this in mind we fabricated a triazine based acridine cored fluorescent polymer material which could find application as fluorescent sensor for the detection of nitro aromatics.



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C 005

Silver-Based Supramolecular Hydrogel for the Development of Smartphone-Enabled Alkaline Phosphatase Sensor

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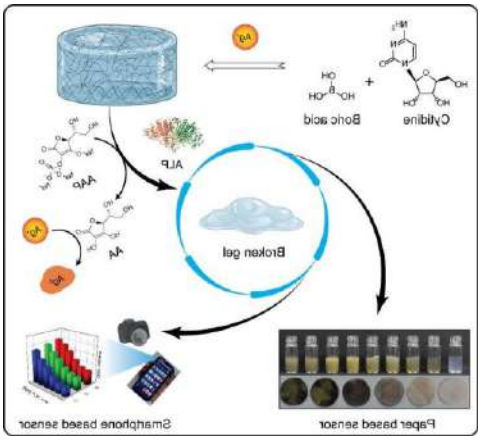
ABSTRACT

Alkaline phosphatase (ALP) is an important bio-marker responsible for various conditions related to hepatobiliary, osteopenia, pregnancy, and certain cancers. Our development of an easy-to-use paper-basedsensor for ALP provides a point-of-care diagnostic device. A silver-coordinated cytidine hydrogel is a potential candidate to show responses under different concentrations of ALP. We prepared and characterized a three-component hydrogel system comprising cytidine, boric acid, and silver nitrate. The gelation occurs rapidly within a minute at room temperature and atmospheric pressure, which makes the system more convenient to use. Reduction of Ag^{+} by the in situ generated ascorbic acid by ALP allows the development of colorimetric sensor based on the gel-coated paper, enabling quantification of ALP concentration. This portable sensor works efficiently on a smartphone color-scanning app, which makes it easier for point-of-care detection. RGB values obtained from scanning indicates the ALP concentration in the range of 1-100 nM, which is independent of mobile cameras. Further, the hydrogel was lyophilized to obtain cryogel which enables naked-eye colorimetric detection of ALP with a detection limit of 0.23 nM (0.016 U/L). The sensing strategy works well in spiked human serum in solution and paper-based sensor. Overall, the cytidine-based gel system presents an effective point-of-care diagnostic system for the detection of ALP with high sensitivity.



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C 006

Polydiaminobenzoic Acid Based Electrochemical Sensor for the Picomolar Detection of Preeclampsia Biomarker

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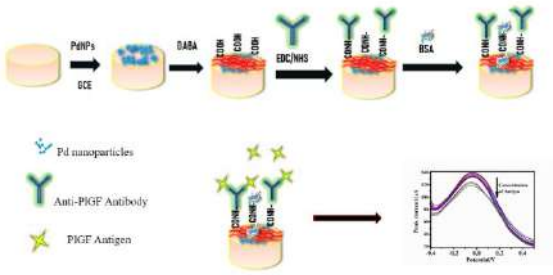
ABSTRACT

Placental Growth factor (PlGF) serves as a valuable biomarker for identifying pregnancy-related hypertension disorder, Preeclampsia. In this study, we have concentrated on the development of a label-free immunosensor, which enables the electrochemical identification of the PlGF antigen for diagnosing Preeclampsia. The sensor was crafted using simple electrochemical techniques, involving the deposition of Palladium nanoparticles onto the glassy carbon followed by the electropolymerization of diaminobenzoic acid (DABA) onto the PdNPs/GCE. Covalent immobilization of the antibody (aPlGF) onto the pDABA/PdNPs/GCE was carried out using amide bond formation. The interaction between the antibody and antigen was quantified using differential pulse voltammetry. The immunosensor exhibited a dynamic range from 10 to 250 pM with a limit of detection of 2.86 pM. We applied the developed sensor towards artificial blood and urine samples through spike recovery analysis.



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C 007

Investigation on Hydrothermal Synthesis of $LaFeO_3$ Based Fast Response Humidity Sensor for Real-Time Breath Monitoring and Non-Contact Sensing

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ABSTRACT

The use of flexible humidity sensors has greatly increased in recent years due to various public health concerns. A global trade and research design focuses on non-contact sensors for monitoring humidity effects in a variety of fields, such as healthcare, robotics, and human-machine interfaces. We are focusing on one of the prime humidity sensing materials, $LaFeO_3$ for the detection of non-contact resistive sensing and real time breath monitoring. Firstly, $LaFeO_3$ was synthesized by a one-step hydrothermal method without any urea concentration (LFO1). The XRD and FESEM image of the synthesized material confirms the proper phase formation of the material having a crystalline size of 28 nm and rhombohedral structure. To compare the morphology and sensor response, $LaFeO_3$ was synthesized again using the hydrothermal method with urea concentration (LFO2). A reduction in the crystalline size of 19 nm results from urea treatment, as well as the appearance of nano-perforated structures as determined by XRD analysis and FESEM. The sensing properties of the synthesized sensing materials were studied at different humidity percentage from 11% to 90% at 25 °C. LFO2 sensing material provides an accessible response time of 9 seconds and a recovery time of 16 seconds. With this fast response time and good sensitivity, the developed sensor is further used in the monitoring of respiration-controlling systems for patients having asthma, cough, skin moisture, and in addition to this, cold sweat diagnosis for heart patients.

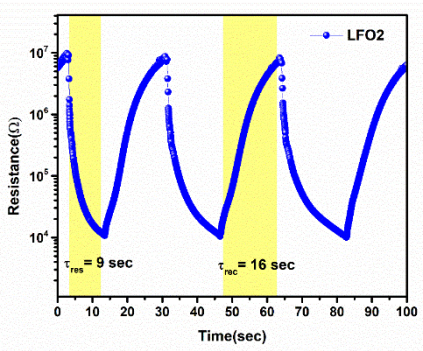

Fig-1 Humidity response and recovery curve of $LaFeO_3$ (LFO2)

C 008

A First Principle Study on Co-doped WS_2 Monolayer as a Promising Gas Sensor for Industrial Pollutants.

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ABSTRACT

Tungsten disulphide (WS_2) has received a lot of interest for its usage in a variety of fields due to its acceptable bandgap and adjustable features. In this paper, Density functional theory (DFT) has been used to thoroughly examine the structures and electronic characteristics of pure WS_2 and Co-WS_2, as well as the adsorption characteristics of various gas molecules (NO, NO_2, NH_3, BCl_3, and SO_2). The physical and chemical interactions before and after gas adsorption can be assessed by determining the adsorption distance, adsorption energy, charge transfer, electron localisation function (ELF), electron difference density (EDD), recovery time, work function, also by comparing the band structure, the density of states (DOS) and the projected density of states (PDOS). Our results showed that Co-WS_2 has better conductivity and enormous charge transfer than pure WS_2. Additionally, as compared to pure WS_2, the Co-WS_2 exhibits stronger adsorption for the gas molecules NO_2, BCl_3, and SO_2. Subsequently, for pure WS_2, there is no electron localization overlap, but for Co-WS_2, there is electron localization overlap for certain gas molecules, which highlights the physisorption as well as the chemisorption character of gas molecules. We came to the conclusion that Co-WS_2 is the right approach for gas-sensing applications.

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C 009

Development of LSPR-Based Glucose Sensor Using Short-Term Period Thiol-Functionalized Gold Nanobipyramids

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ABSTRACT

Glucose is essential for human health because it serves the primary function of providing energy for the body's cells. The low glucose level can cause hypoglycemia with dizziness, confusion, weakness, sweating, trembling, and even loss of consciousness. On the other hand, a high glucose level can increase the risk of developing type 2 diabetes, a long-term disorder that interferes with the body's control of blood sugar levels. This may result in numerous consequences, such as nerve damage, renal disease, and cardiovascular disease. Therefore, it is crucial to detect and keep track of glucose to ensure that it stays within the usual range. An alternative glucose detection method is proposed using a Localized Surface Plasmon Resonance (LSPR), called a plasmonic sensor, to improve several areas from conventional methods, such as invasive, needing an expert for the result analysis and needing long-time detection. The gold nanobipyramids (GNBPs) are chosen as a sensing material due to their advantage, such as being inert, slow to react with other chemicals, conducting electricity well, and safe as catalysts. Also, they produce higher electric field enhancement, increasing sensitivity and selectivity compared to other structures. The GNBPs are synthesized using the seed-mediated growth method (SMGM), divided into seeding and growth processes. Then, GNBPs are functionalized by thiol groups for a short period, i.e., 3 hours, to improve the sensor performance. The short-period thiol-functionalized GNBPs (t-GNBPs) with a length of 117.99 ± 10.37 nm, a width of 43.64 ± 4.13 nm, and an aspect ratio of 2.72 ± 0.34 are tested in the glucose medium with a 10^0 – 10^6 µM concentration. The result shows that a plasmonic sensor using short-period t-GNBPs for glucose detection performs a high sensitivity factor of 40.116 nm/RIU for t- SPR and 13.080 nm/RIU for l-SPR and high linearity through R^2 over 0.9; an excellent selectivity towards three different analytes; good stability with a low error value of 0.58 ± 0.0008 a.u for the t-SPR peak and 0.74 ± 0.000033 a.u for the l-SPR peak; and good repeatability with a low CoR value of 0.00544 and 0.00886 for the t-SPR and l-SPR peak, respectively. In addition, the limit of detection for this system is 1 µM. This result shows that short-period t-GNBPs perform a better sensing parameter than long-period t-GNBPs. Hence, the plasmonic sensor using short-period t-GNBPs to detect glucose is successfully developed with promising performance for practical application.

Keywords: *functionalization, glucose detection, plasmonic sensor, thiol*

C 010

Investigation of Semiconductor Sensor Material Synthesized Via Simple Combustion Technique to Detect Hazardous Gases

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ABSTRACT

The simple combustion process was followed to synthesize Zn doped Ni-Mn ferrite $Ni_{0.6-x}Mn_{0.4}Zn_xFe_2O_4$ (x=0.1, 0.5), these ferrites were characterized by XRD which revealed phase purity with broad peaks and crystallite size of a few nanometers obtained using Scherrer's formula. The crystallite size was found to be in the range of 10-20nm. The XRD peaks were well matched with standard PDF 2 data having ICDD card number: 00-069-0164. The microstructural properties of the synthesized compound were analyzed by SEM and TEM microscopy revealing the agglomeration of particles, shape, and uneven distribution. The lattice interplanar spacing was calculated from TEM images using Image J software. The interplanar distance 'd' obtained from XRD calculations was very well matched with TEM data. The SAED images revealed the semi-crystalline nature of the sample. The histogram plot gave the variation in particle size. BET analysis report gave information on the physical adsorption of gas molecules on the surface which ultimately measured the specific surface area of the sample. Semiconducting properties were confirmed using two probe resistivity studies from RT – 500°C. A decrease was observed in resistivity with an increase in temperature thus proving the semiconducting behviour of the samples. The band gap was also determined from UV -DRS spectrophotometer. A gas sensing study was performed on reducing and oxidizing test gases using 100 ppm of gas at RT. The LPG showed a percent response of 70% and 59% while Cl_2 showed a very less % response of 13 % and 3%. It was also found that the ferrite under study has a faster response and quick recovery for reducing gas as against oxidizing gas.

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C 011

Green Innovative Microstrip Patch Antenna Design for Reduced Radiation From Mobile Phones

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ABSTRACT

The development of sustainable technology is crucial for the long-term well-being of our planet. One area where sustainable technology can be applied is in the design and development of microstrip patch antennas for next-generation applications. In this paper, it is aimed to design and develop a prototype microstrip patch antenna that is sustainable and also helps to reduce the SAR value. This reduces the impact of mobile phone radiation on human health and the environment as well. Specific absorption rate, which stands for the radio frequency energy rate, is used to calculate the amount of radio frequency radiation a head has exposed to. To achieve these objectives, COMSOL simulation and design tools to optimize the antenna's performance is done. The Federal Communications Commission in the US set a SAR level for phones of 1.6 W/Kg, and India uses the same standard. Thus, phones with a rating of less than 1.6 W/kg are seen to be decent. In the proposed antenna design, the sar value is found to be 0.0432 $X10^{-5}$ W/Kg. The Microstrip patch antenna is designed with the slot to operate at 2.45 GHz frequency. The rectangular patch receiving device is made of glass epoxy with a thickness (h) of 1.6 mm, a width (W) of 4 mm, a length (L) of 50 mm, and slot dimensions (W) of 21.5 mm, 2 mm, and 15 mm below the origin, as illustrated in figure 5.2. The antenna is then powered by insert feeding.

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C 012

Non-enzymatic Electrochemical Sensor based on MOF-5/Graphene Composite for Glucose Detection

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ABSTRACT

Diabetes is a widespread chronic illness that affects individuals globally, necessitating the continuous monitoring of glucose levels. The increasing prevalence of diabetes mellitus cases worldwide has driven the development of more reliable and precise glucose sensors. However, traditional enzymatic glucose sensors suffer from various limitations, such as challenges in implementing enzymes, cost-related issues, and stability issues. In recent years, significant advancements have been made in the development of enzyme-free glucose sensors. Metal-Organic Frameworks (MOFs) provide an attractive platform for creating enzyme-free glucose sensors due to their highly organized structure, large specific surface area, exposed active sites, and structural adjustability. Nevertheless, the poor conductivity of MOFs limits their application as electrochemical sensors, and this limitation can be overcome by incorporating metals, metal oxides, or carbon-based materials. In this context, a composite material was prepared using MOF-5, which consists of zinc ions and benzene dicarboxylic acid (BDC) ligands, along with graphene nanosheets. This prepared composite was employed as a non-enzymatic electrochemical sensor for the detection of glucose. The MOF-5/graphene composite exhibits exceptional electrocatalytic activity for glucose oxidation, high sensitivity, a low detection limit, and good selectivity. It holds the potential to be used as a non-enzymatic electrochemical glucose sensor.

Keywords: *Biosensors, Metal organic frameworks, Diabetes, Graphene, 2D materials*

C 013

Multiplexed Detection of Biomolecules using Label-Free Surface Enhanced Raman Scattering (SERS) Plasmonic Platforms from Bi embedded in ZnO-TiO_2 films.

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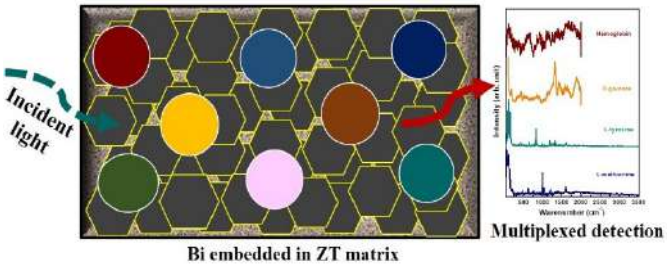
ABSTRACT

Ecandrewsite structured Zinc-Titanate [$Zn(TiO_3)$] were synthesized and developed into films (ZT matrix) using wet chemical route from the precursor mixture of ZnO and TiO_2 nanoparticles (Nps). Bismuth (Bi) Nps were DC sputtered and embedded inside the ZT by vacuum annealing (Bi-ZT). GI-XRD and Raman revealed the structural formation of Bi in ZT, majorly in hexagonal phase. An orientation change in growth as seen can contribute to the increase in number density of available free electrons. An absorption, more prominent in the UV-Vis region is observed with an absorption tail extending towards the NIR, with the wide energy band gap calculated to 3.54 nm in case of Bi-ZT. The AFM revealed a continuous particle distribution with an rms roughness of 1.87 nm. XPS gave the chemical state of existence, giving the influence of oxidation in the bilayer films developed. The standard dye molecules Methylene Blue (MB) and Rhodamine 6G (RH6G) were tested on the films for SERS in prior to bioanalytes. The multiplexed label-free SERS detection of bio molecules of wide spectral range from various amino acids to vitamins and glucose to hemoglobin, were studied using 785 nm Raman laser. Bi existing in the metallic phase inside ZT dielectric matrix, contributes to both electromagnetic and chemical enhancement mechanisms as seen from the SERS results. The results reveal the potential of the fabricated films as an alternative and green SERS platform for diverse applications in healthcare.



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C 014

Room-Temperature Flexible Ethanol Sensor Based on Novel La-Modified $ZnFe_2O_4$ Gel with Low Limit of Detection

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ABSTRACT

The objective of creating low temperature gas sensors has stimulated research into creating new incredible materials with large surface for quick response and low limit of detection. In this investigation, for the low temperature ethanol sensing, we created a unique Lanthanum doped zinc ferrite based gel, using a hydrothermal approach. The morphological and structural investigation of synthesized gel was done using XRD, FESEM along with EDS and UV spectroscopy. The sensing experiments findings indicate a good response (R_o/R_g = 20) at 25 ºC temperature in the presence of 50 ppm ethanol with a very low limit of detection (LOD=0.2 ppm). In-situ FTIR was used to confirm the room temperature conversion of ethanol into acetaldehyde through oxidation. Additionally, the developed sensor has an incredibly quick response time of 19 seconds and recovery time of 8 seconds. The sensor not only gives better response and recovery, but also provides long term stability with time as well under different bending conditions. This research may open up novel avenues for developing low-temperature ethanol sensors for reliable and efficient monitoring of the rising concern regarding the indoor atmosphere.

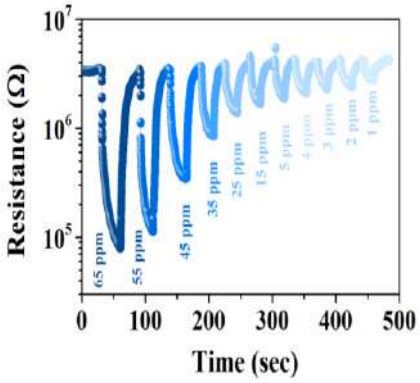

Fig.1. Sensing response of La-doped $ZnFe_2O_4$ based sensor at different ethanol concentrations.

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C 015

Dynamic Motion Analysis for Parkinson's Disease Detection Using Wearable Smart Watch

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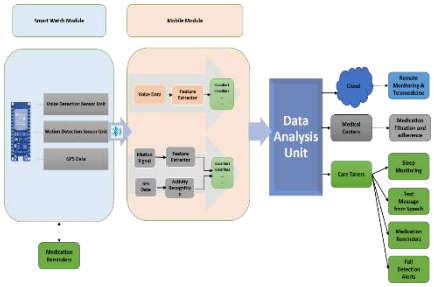
ABSTRACT

Parkinson's disease (PD) stands as the second most prevalent neurodegenerative disorder. In India, determining the precise number of PD patients proves challenging due to a lack of awareness about PD symptoms among the geriatric population and a significant gap between the number of PD patients and the availability of trained neurologists. This research presents a holistic approach to Parkinson's disease detection by integrating Motion Analysis Models with a Parkinson's Smart Watch Device. Utilizing advanced machine learning techniques, our study explores the synergy between motion estimation models and wearable technology for comprehensive motion analysis. The smartwatch, equipped with MEMS inertial sensors, monitors and captures detailed motion data. This system offers a nuanced understanding of motor patterns, contributing to accurate and early detection of Parkinson's disease. Using the ESP32 microcontroller with integrated IMU sensors, we can develop a cost-effective solution for real-time motion estimation in Parkinson's patients, aiding in remote monitoring and providing valuable data for healthcare practitioners. By combining the strengths of machine learning models and wearable devices, our approach provides a more comprehensive and effective solution for Parkinson's disease detection and monitoring.

Keywords: *Wearable devices, Parkinson's disease, motion estimation, smart watch, ESP32.*

BLOCK DIAGRAM



C 016

Hydrothermal Growth of $MoSe_2$ Nanoflower for Room Temperature Operated High-Performance Ammonia Sensor and Its Industrial Application

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ABSTRACT

Increasing technological, industrial and agricultural development give rise to the emission of various harmful gases, thus elevating the pollution level. Among various gases, ammonia is the one which is mostly used and produced in various industrial and agricultural activities, thus making susceptible and selective ammonia sensors is of great interest. In this study, we fabricated an ammonia sensor using Molybdenum diselenide. $MoSe_2$ nanoflowers were synthesized by using a one-step hydrothermal method without using any precipitating agent. The structure, morphology and composition of the obtained nanoflowers were investigated using characterizations such as XRD, FESEM with EDS, and UV-visible spectroscopy. The developed sensor shows an excellent response of (R_o/R_g = 524) for ammonia gas at 400 ppm with a fast response and recovery time of 12 sec and 22 sec respectively, at room temperature of 25˚C. The fabricated ammonia sensor exhibits long-term stability with low limit of detection (LOD). The developed ammonia sensor also displays remarkable selectivity, making it a highly effective material for industrial applications.

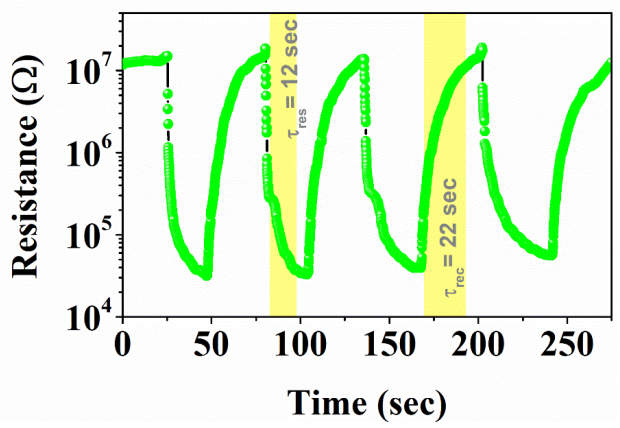

Fig.1. Sensor's response and recovery time plot at 400 ppm.

C017

Glyco-Functionalized Graphene Oxide Based Binary Composite for E. Coli Adsorption and Sensing

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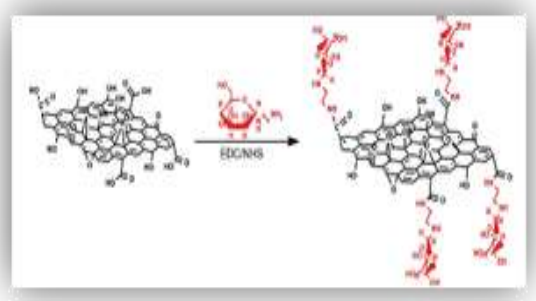
ABSTRACT

Carbon allotropes, such as fullerenes, carbon nanotubes, and most recently, the incredible material graphene, are delineated as some of the most pre-eminent materials of the twenty first century[1]. Among the diverse forms of carbon, graphene often reveals unique properties, mainly due to its high thermal and electrical conductivity, elasticity, toughness, lightness, and resistance. The early diagnosis of diseases plays a vital role in healthcare for the extension of human life, for which the Graphene oxide (GO), the oxidized form of graphene laced with oxygen containing groups is a promising material[2]. GO-based biosensors have helped in the early diagnosis of diseases by detecting and monitoring relevant biomarkers[3], providing a better understanding of various physiological and pathological processes. Owing to their versatility, biocompatibility, small size, large surface area, and potential to interact with biological cells and tissues, GO–based biosensors have generated tremendous interest, resulting in significant advances and promising application prospects, and rendering alluring physicochemical and biological properties for biomedicine[4]. In the current work, we are presenting a binary glyco-functionalized graphene oxide-based composite for E. coli sensing and adsorption. We have developed the system using D-Mannose, the sugar monomer of the aldohexose series of carbohydrates, and the C-2 epimer of glucose. The synergetic effect of specific mannose recognition and the interaction of bacteria with graphene oxide layers has made the system a suitable material for the sensing studies of bacteria.



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C 018

Silver Dendrites Nanostructures: Formation Mechanism, Properties and Applications

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ABSTRACT

A "Dendrites" refers to tree-like structure, branched or growth of crystalline structure. Their unique structure contains a high surface area along with narrow gaps and as well as the sharp edges which makes the morphology quite interesting providing enhanced plasmonic hot spots at the edges [1]. This inspires its application for surface enhanced Raman scattering (SERS) where localized plasmonic field is used to enhance the Raman single providing the opportunity to detect upto single molecule [2]. In the current study, we report the metal assisted growth of Ag nano-dendrites structures along with several structural and optical characterizations such as XRD, SEM, TEM etc [3]. The paper also focuses on the strong understanding and mechanism for fabrication of silver dendrites. The additional objective of the paper is to dig deeper into physics to find out why only certain materials form dendrite structures.

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C 019

Tailoring SPR Penetration Depth towards Whole-Cell Biosensing

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ABSTRACT

Surface plasmon resonance belongs to one of the gold standard surface sensing methods having the advantages of highly sensitive, direct, label- free detection up to pg/ml detection ability. The technique is broadly used to identify the interaction between the biomolecules via changing the refractive index of the sensing as target molecule interacts with it [1]. Although SPR is a very useful method, it suffers from the low penetration depth (up to 200 nm) hence limits its application by microbe sensing [2]. A conventional solution for the same is use of long range SPR (LRSPR), which is basically achieved through sandwiching a thin film of the low index polymer material between the prism and metal layer which leading the slow decay of light which causes higher penetration depth but due to high index material, the experimental execution makes bit difficult [3]. In the present study, we report a successful approach for designing and fabrication of nearly guided wave SPR (NGWSPR) based chip for increasing the penetration depth of SPR electric field up-to 2 micrometers. This helped to apply SPR for the large molecule sensing such as pathogens, bacteria etc. This makes the study applicable for whole cell biosensor and hence for clinical diagnosis and health care industry.

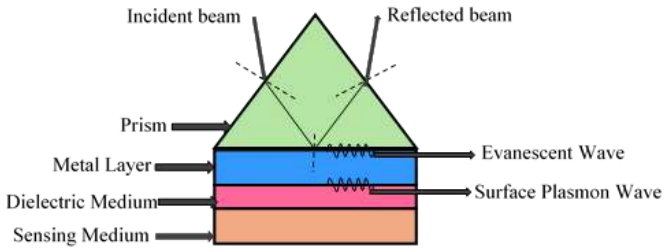

Fig. 1. Schematic Diagram of NGWSPR (The dotted line should be normal to the prism surface)

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C 020

Wearable Sensor-Based Fall Detection Using Machine Learning with Sisfall Dataset

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ABSTRACT

Accidental falls can lead to severe injuries and, in some cases, even fatalities, particularly in situations where immediate assistance is not readily available. Fall Detection Systems (FDSs) play a critical role in identifying falls and swiftly triggering the necessary help. In this study, we introduce an innovative FDS that leverages wearable sensors—specifically accelerometers and gyroscopes—in combination with Machine Learning (ML) techniques for signal processing and fall detection. Our approach involves the extraction of various features from signal segments, followed by classification as either falls or routine daily activities. The classification model utilizes the Support Vector Classification (SVC) algorithm which classifies the data based on the Activities of daily living (ADL), the model is trained on a meticulously annotated dataset that distinguishes between human activities, including falls and regular daily routines. To evaluate the effectiveness of our method, we employed the model on the publicly accessible Sisfall fall dataset. Our findings are then compared with those of prior studies that employed the same dataset.

Keywords: *Fall Detection Systems, Wearable sensors, Accelerometers, ADL, Machine Learning.*

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C 021

Efficient Room Temperature Detection of DMMP Using CdS Thin Film Based QCM Sensor

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ABSTRACT

Dangers of exposure to chemical warfare agents (CWAs) are severe, including immediate harm to individuals, long-term health effects, and environmental damage. Dimethyl methylphosphonate (DMMP) detection assumes importance since it is a simulant for Sarin which had been utilized for attacks on Japanese subway in 1995. In the present study, nanocrystalline Cadmium Sulphide (CdS) nanocrystalline thin films have been deposited onto Quartz Crystal Microbalance (QCM) substrates for detection of DMMP gas at room temperature. CdS nanocrystalline thin films have been synthesized, using a chemical synthesis method coupled with spin-coating technique. The performance of the CdS film on QCM sensing platform has been evaluated by exposing it to a concentration of 100 ppm DMMP gas. Remarkably, the synthesized sensing film exhibited a sensing response of 7.2 Hz. It is interesting to note that the film exhibited a significant DMMP detection capability at room temperature along with fast response (53 s) and a rapid recovery time (27 s).

C 022

Ultrasonic Sensor and LED Integration for Cyclist Safety

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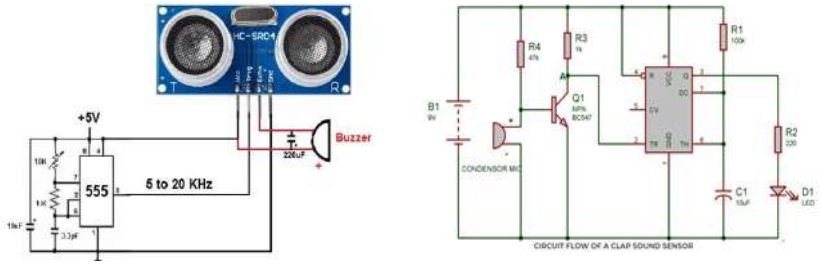
ABSTRACT

In this research, we introduce an innovative and comprehensive safety solution tailored for cyclists, focusing on enhancing their safety during nighttime rides. Our system combines cutting-edge technology, including ultrasonic sensors, clap sensors, and strategically integrated LEDs, to significantly improve visibility and awareness for cyclists on the road. The core component of our integrated safety solution is the ultrasonic sensor system, which plays a pivotal role in providing real-time information about the surrounding environment. By utilizing ultrasonic technology, our system effectively detects nearby objects, allowing cyclists to gauge distances and potential hazards even in low-light or dark conditions. This critical information empowers cyclists to make safer and more informed decisions while on the road. Complement the ultrasonic sensors, we have incorporated clap sensors that trigger an array of strategically placed LEDs on the cyclist's jacket. These LEDs create illuminated light signals that not only enhance the cyclist's visibility but also serve as an interactive signaling mechanism. The combination of ultrasonic technology and LED illumination ensures that the cyclist is not only visible to others on the road but can also actively communicate their intentions and actions, thereby improving overall safety.

Keywords: *Wearable devices, Cyclist safety, Ultrasonic sensors, LED illumination, Nighttime rides, Distance detection, Clap sensors.*



Block Diagram

C 023

Gold Dendrites Enriched with Gold Nanoclusters on Carbon Fiber Microelectrodes as Flexible Acetaminophen Microsensor

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ABSTRACT

Recent breakthroughs in the field of flexible fiber-based microelectrodes have paved the way for precise measurement of commonly utilized biomarkers. This study focuses on the creation of a nanoarchitectured gold-dispersed carbon-fiber microelectrode through a straightforward and efficient electro-deposition method, eliminating the need for surfactants, polymers, catalysts, or intricate procedures. The resultant gold-dispersed carbon-fiber microelectrode is employed as a signal transducer for the sensitive detection of paracetamol. Leveraging the distinctive structure and chemical properties of the surface-decorated microelectrode, it exhibits outstanding sensing capabilities, remarkable selectivity, an expansive detection range, and superior precision in electrochemically detecting paracetamol. This novel microsensor offers distinctive surface features, synergistic effects, and effective catalytic properties, rendering it suitable for practical applications in the analysis of paracetamol within human samples. In light of its impressive paracetamol sensing capabilities, this state-of-the-art microsensor carries the potential to revolutionize various aspects of the biomedical and pharmaceutical industries.

Keywords: *Microsensors; Gold nanodendrites; Carbon-fibre microelectrodes; Electrochemical deposition; Paracetamol detection.*

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C 024

Innovative Dual-Core D-Shaped Photonic Crystal Fiber Biosensor for Hemoglobin Monitoring and White Blood Cell Count Detection Using Surface Plasmon Resonance

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ABSTRACT

The advancement of biosensors is integral to precise detection and monitoring of critical physiological parameters essential for effective healthcare. Among these, monitoring hemoglobin levels and white blood cell (WBC) counts holds paramount importance. In this research proposal, an innovative bio sensing approach is presented, utilizing a dual-core D-shaped photonic crystal fiber (PCF) integrated with Surface Plasmon Resonance (SPR) for enhanced hemoglobin monitoring and WBC count detection. The PCF's unique design comprises a solid core surrounded by cladding with adjustable air holes, offering exceptional design flexibility while maintaining a flat surface and homogeneous nature, makingit highly suitable for bio-sensing applications. Integration of SPR within this PCF biosensor enhances accuracy, sensitivity, and overcomes limitations of conventional hemoglobinometers, such as the need forchemical substances, sample preservation methods, and prolonged analysis time. To characterize the biosensor, the finite-element method, implemented through COMSOL Multi-Physics- software, is utilized for analyzing light guiding properties and confinement loss characteristics for varying concentrations of hemoglobin and WBC counts. The observed peak wavelength shift effectively indicates concentrations of hemoglobin levels and WBC counts within the human body.

This innovative biosensor holds significant promise in healthcare diagnostics, promising non-disposable, accurate, and sensitive monitoring of crucial physiological parameters necessary for maintaining good health. It represents a significant step forward in biosensor technology, providing a pathway towards improved healthcare outcomes through real-time and precise monitoring of hemoglobin levels and WBC counts, facilitating timely interventions and personalized medical treatments.

C 025

Development of Doped and Undoped CeO_2 Based Quantum Dots for Fluorescence Sensing Applications

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ABSTRACT

Dopamine is a significant neurotransmitter which controls the central nervous system, body metabolism, hormonal and cardiovascular systems by passing messages in the nervous system. Abnormality in the concentration level of dopamine may result in several physiological and neurological dysfunctions leading to Schizophrenia, Parkinson Disease, Alzheimer's diseases, Huntington's disease, etc. Ferric ions have important roles in the transport of oxygen and enzymatic reactions. To some extent, the excess (hyperferremia) or deficiency (hypoferremia) of Fe^{3+} can cause serious health problems such as injury to kidney, hepatic cirrhosis, heart diseases, anemia, etc. Therefore, it is of urgent requirement for a novel sensor with selective, sensitive and quick determination abilities. Quantum dots with stunning optical, electronic and electrochemical characteristics have been widely used for the development of next generation fluorescent sensors for the selective, sensitive and interference free detection of important analytes. Herein, doped and undoped fluorescent CeO2 quantum dots were synthesized by sol-gel method for sensing of significant analytes such as dopamine and ferric ions. The probe's chemical and morphological characterization were conducted using XRD, FESEM, HR-TEM and FT-IR methods. Its electrochemical properties were investigated by various electrochemical techniques such as CV, DPV, EIS etc. Its electronic and optical properties were analyzed through UV-vis and fluorescence spectroscopy. The newly synthesized probe is expected to show impressive performance in terms of selectivity and sensitivity with respect to its sensing abilities.

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C 026

Facile Fabrication of Paper Based 2D WS_2 Nanosheets with Edge Site Defects for NO_2 Gas Detection at Room Temperature

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ABSTRACT

The exploration of materials towards gas sensing applications have been an era to focus in this 21st century due to the increased industrialization and automobilization [1]. The environmental protection agency (USA) has provided national ambient air quality limit around 100 ppb of NO_2 for a time period of 60 min. Long term exposure to high concentrations of NO_2 causes intense respiratory diseases and may even lead to cancer [2]. The main objective of this work is to develop an effective gas sensor material towards NO_2 gas. In recent times, 2D TMD (transition metal dichalcogenides) such as WS_2, MoS_2, CuS_2, $MoSe_2$ materials show fascinating properties in the field of gas sensors performing effective response towards gases such as NO_2, H_2S, NH_3. Among the above-mentioned materials, WS_2 shows effective response towards NO_2 even at room temperature. Heterostructures of TMD with metal oxides and carbon derivatives leads to interesting improvement in physical, chemical and electronic properties synergistically [3]. The fabrication of flexible substrates has gained much popularity in recent times. In this work, we have fabricated paper based WS_2 gas sensors for effective monitoring of NO_2 gas at room temperature. The results of the flexible gas sensitivity indicate the fast response and high stability of our devices in breathing detection and bending experiments. Furthermore, the devices can effectively distinguish bending stress changes and gas-sensitive response signals at the same time, realizing multifunctional sensing detection. Our work will be a reference for fabricating flexible sensors based on 2D materials.

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C 027

Enhanced Nitrogen Dioxide (NO_2) Sensing Properties of Chromium-Doped Bismuth Sulfide (Bi_2S_3) Nanomaterials

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ABSTRACT

The combustion of fossil fuels releases a variety of harmful substances into the atmosphere, which contributes to a wide range of respiratory illnesses in people. We need room-temperature gas sensors that can identify these dangerous gases precisely in order to detect the presence of the gas surrounding us. Nitrogen dioxide (NO_2) is a highly toxic and environmentally harmful gas, it is a major component in the creation of photochemical smog acid rain, and an air pollutant. Therefore, the development of efficient gas sensors for its detection is of paramount importance. Bi_2S_3, a semiconductor with a low band gap of 1.3–1.7 eV, has drawn a lot of interest because of its numerous applications in gas sensors, solar cells, electrical and optoelectronic devices, and hydrogen storage materials. With its vast surface area and strong surface activity, it has garnered significant attention in the field of NO_2 detection. In this work, a series of Cr-doped Bi_2S_3 samples with varying dopant concentrations were prepared through a simple hydrothermal method and its structural and morphological properties were studied using X-ray Diffraction, and Scanning Electron Microscopy.The Sensing studies showed that the Pure Bi_2S_3 good response towards NO_2 of 307% at 80ºC whereas the 5% Cr –doped Bi_2S_3 showed a good response of 1232% at 50°C with a good response time of 51s.

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C 028

In_2O_3/Cu_2O Heterostructure-Based Gas Sensor for NO_2 Detection at Room Temperature

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ABSTRACT

Metal oxides play a crucial role in detecting various gases by changing electrical parameters upon the adsorption or desorption of gas. The overall performance of metal oxide-based gas sensors improved by incorporating heterostructures. Moreover, the fabrication of p-n heterostructure materials is an efficient strategy for enhancing the gas sensing performance by facilitating catalytic activity, creating a charge carrier depletion and accumulation layer and increasing the rate of adsorption that produces a larger modulation in resistance. In this study, we fabricated flowerlike Cu_2O and In_2O_3/Cu_2O heterostructure thin films by facile hydrothermal method on an alumina substrate. The structural, optical and morphological properties were investigated using XRD, Raman analysis, FTIR, UV-Vis spectroscopy and SEM, it confirms that the p-type Cu_2O and n-type In_2O_3 were successfully combined and heterojunctions were formed at In_2O_3/Cu_2O interfaces. The flowerlike Cu_2O thin film exhibits a room temperature (RT) response for NO_2 gas up to 0.98 towards 5 ppm. Furthermore, the thin film of In_2O_3/Cu_2O heterostructure demonstrated a NO_2 gas response ~1.5 times higher than pristine Cu_2O. The In_2O_3/Cu_2O heterostructure displays excellent selectivity, quick response and recovery times (~1.26 s and 5.03 s). The gas sensing mechanism of heterostructure is thoroughly discussed and In_2O_3/Cu_2O could be considered as a novel and promising material for the practical application to detect NO_2 at RT selectively.

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C 029

Gamma-Induced La_2CuO_4 Perovskite for Rapid Simultaneous Detection Of N-Acetyl-P-Aminophenol and P-Aminophenol in The Presence of Ascorbic Acid and Uric Acid

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ABSTRACT

The development of efficient and selective sensors for the simultaneous detection of multiple analytes in complex biological and environmental samples has become imperative in analytical chemistry. This study focuses on the synthesis and characterization of a novel gamma-induced La_2CuO_4 perovskite- based sensor for the rapid and simultaneous electrochemical detection of *N*-acetyl-*p*-aminophenol (APAP) and *p*-aminophenol (PAP) in the presence of potential interferents, ascorbic acid and uric acid. The electrochemical response of APAP and PAP at the modified electrode was studied using cyclic voltammetry and square wave voltammetry techniques. Under optimization conditions, the SWV response of the modified electrodes showcased a wider linear response concentration range of 0.01 to 2000 µM for both APAP and PAP, respectively, with lower detection limits (LOD) of 0.004 µM for APAP and 0.007 µM for PAP. The fabricated electrode was successfully employed for real-time monitoring of APAP degradation in pharmaceutical formulations. Additionally, the sensor was used to quantify both APAP and PAP in various real samples, including industrial wastewater, biological samples, and tattoo ink.

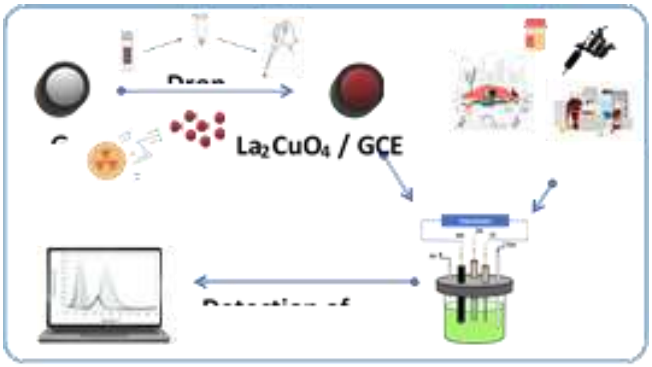

Figure. Schematic representation of the proposed work

C 030

WO_3 Coated Quartz Crystal Microbalance Sensor for Room-Temperature Sensing of NO_2

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ABSTRACT

Nitrogen dioxide (NO_2) is a major instigator of air pollution and is known for its detrimental impact on both human well-being and ecosystems [1]. Thus, the development of fast, sensitive, and reliable sensors for NO_2 is imperative. In this regard, Quartz Crystal Microbalance (QCM) holds great promise for gas detection at room temperature [2]. Among the various materials used in gas sensing applications, semiconductor metal oxides, particularly tungsten trioxide (WO_3) [3], have established themselves as prominent members of the semiconductor sensor community. The primary focus of this study centers on the growth of WO_3 thin film which involves the formulation of solutions with varying concentrations of WO_3, ranging from 30 mg/ml to 70 mg/ml. These solutions were subsequently deposited onto QCM surfaces through Chemical Solution Deposition (CSD). The study further delves into the sensor's response towards 10 ppm NO_2 gas. The QCM coated with a 70 mg/ml WO_3 solution exhibited the highest sensitivity, registering at 0.3 Hz/ppm. Additionally, the sensor displayed impressive response and recovery times, clocking in at 128 s and 206 s, respectively. Notably, all sensors showcased exceptional repeatability and a distinct selectivity toward NO_2.

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C 031

Textile Based Flexible Self-Powered Triboelectric Nanogenerator for Sweat Sensing Application

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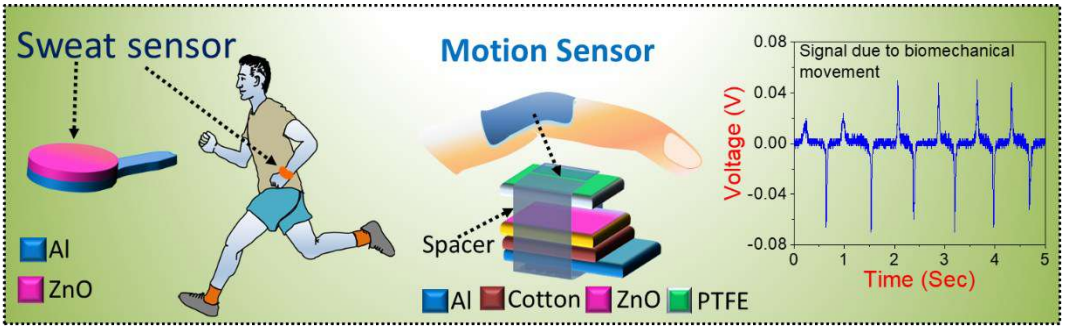
ABSTRACT

The devolopment of internet of things (IoT) based sensors also increases the demand of external power sources. Triboelectric nanogernerator (TENG) which works on the principle of contact-electrification and charge induction, is the one of the techniques to devoloped self-powered sensors through harvesting mechanical energy from our sorrounding environment or biomechanical movements, to reduce the excessive use of conventional power sources and to overcome the limitations of old battery techniques. In this work, we report a ZnO nanorod based single electrode triboelectric nanogenerator (STENG) grown on flexible cotton cloth for sweat sensing application. The sweat sensing capability of the as fabricated STENG has been observed through the variation of amount of saline water. The output performance of the STENG was changed due to variation of saline water quantity, which varifies the applicability of STENG for sweat sensing application. The increment in the output performance of STENG due to saline water has been expected due to the attachment of hydrated Cl ions present in saline water with ZnO, which improves the charge transfer mechanism. Our as fabricated STENG offers a limit of detection of 4.25 µL with sensitivity 0.015 V/µL. Next, for the real time applications of our as fabricated STENG, a prototype sensor has been attached in human body and operated upon biomechanical movement. Finally, the wireless data transmission through a microcontroler has been demonstrated.

Keywords: *Nanogenerator, ZnO, sensors, single electrode.*



C 032

WS_2 Nanosheet Incorporated PVDF-HFP Films for Efficient Solid-Liquid Interface Triboelectric Nanogenerator

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ABSTRACT

Energy Harvesting is one of the most important target of today generation. Looking on this context, enormous efforts have been forwarded towards harvesting energy from mechanical motion from various sources like human body movement, mechanical appliances and even natural events. Here we report, the energy harvesting process at Solid-Liquid interface based on principle of Triboelectric effect.WS_2 nanosheet embedded PVDF-HFP thin films have been developed through simple chemical technique and have been exploited in the application of solid-liquid interface TENG. Compared to bare PVDF-HFP, the incorporation of WS_2 has led to the elevation of the triboelectric property when contacted with normal water drops. Consequently, a progressive relationship between WS_2 content and the triboelectric output voltage has been observed. Upon varying the salinity of the liquid drop the output voltage can be tuned. It has been observed beyond an optimized salt concentration, the output gets degraded and thus the system exhibits strong candidature for the development of water TDS sensor.

C 033

Enhancing Lower Limb Rehabilitation Treatment through Chaotic Map-Based Compressive Classification of Wearable Sensor Data

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ABSTRACT

Rehabilitation treatment plays a pivotal role in enhancing the quality of life for individuals with lower limb impairments. In this context, the effective classification of lower limb data is essential for developing personalized and efficient rehabilitation strategies. Compressive classification, an emerging technique, has shown promise in efficiently processing and classifying such data. This paper presents a novel approach for compressive classification of lower limb data, using a random sequence generated by a unique chaotic map. The proposed methodology leverages the unpredictability and rich dynamic behavior of the chaotic map to generate random sequences, which are subsequently utilized to compress lower limb data. By doing so, it effectively reduces data dimensionality without significant loss of relevant information, while enhancing the classification performance. This approach is particularly advantageous for real-time applications, as it minimizes the computational burden associated with data processing. In this study, we provide a detailed description of the chaotic map employed for random sequence generation, the compression technique, and the classification framework. We present experimental results using lower limb data from rehabilitation patients to demonstrate the effectiveness and efficiency of the proposed approach. The outcomes indicate that our novel chaotic map-based compressive classification method significantly improves the speed and accuracy of lower limb data classification, thereby enhancing the potential for personalized rehabilitation treatments.

Keywords: *Wearable devices, Lower limb rehabilitation, Chaotic map, Data compression.*

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C034

Dynamic Capacitive touch security system for Autism Spectrum Disorder Using Wearable Smart Device

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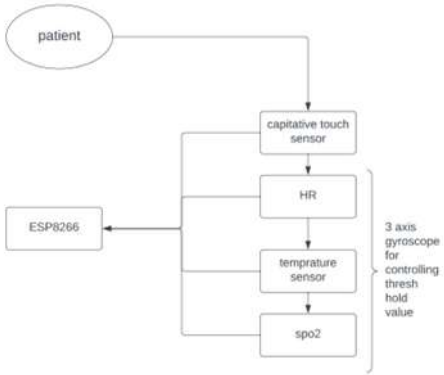
ABSTRACT

Autism Spectrum Disorder is a neurodevelopmental disorder, In general, handling ADs patients proves challenging due to a lack of awareness about their surroundings and difficulties with social interactions and a significant gap between the number of ADs patients and the availability of trained neurologists. This research presents a holistic approach for people suffering from Autism Spectrum Disorder by integrating Security alarm system with a wearable Capacitive touch sensor Device. Utilizing advanced machine learning techniques, our study explores the synergy between Capacitive touch sensor and wearable technology for security and ease . The wearable device, equipped with MAX30100 ,MLX90614 ,SIM900A or SIM800L, 3 axis gyroscope and Capacitive touch sensor. This system offers a touch sensor,temperature, heart rate, and sp02 detection system for situation when the patient is in difficult situation. Using the ESP8266 microcontroller with integrated other sensors, we can develop a cost-effective solution for guidance in Autism patients, aiding in remote monitoring and providing valuable data for healthcare practitioners. By combining the strengths of machine learning models and wearable devices, our approach provides a more comprehensive and effective solution for the security of Autism Spectrum Disorder patient .

BLOCK DIAGRAM



Keywords: *Wearable devices, Autism Spectrum Disorder, Capacitive touch sensor ,wearable device, ESP8266.*

C 035

Fabrication of ZnS Nanoparticle-Based Chemosensor to Detect Palladium (Pd) in Non- Aqueous Media & Cadmium (Cd) in Aqueous Media

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ABSTRACT

The presence of heavy metals in water and the food chain poses a serious threat to both ecology and human health. Industrial activities can cause heavy metals to become concentrated, degrading the air, water, and soil quality, and subsequently causing health issues in plants, animals, and people. This research aims to develop a ZnS nanoparticle-based chemical sensor for the detection of heavy metals in aqueous and non-aqueous media. ZnS nanoparticles possess exceptional optical properties, such as a wide bandgap and high photoluminescence efficiency. Various concentrations of cadmium (150μl, 250μl, 350μl, 450μl) in aqueous media and palladium (50μl, 100μl, 150μl, 200μl, 250μl) in non-aqueous media have been prepared and analyzed using a $4x10^{-6}$ M concentration solution of ZnS nanoparticles. The orange fluorescence of ZnS nanoparticles has shown a redshift along with a 265nm excitation peak, which is emitted at 527nm. The minimum crystalline size of the nanoparticles has been calculated to be 3.50nm using Scherrer's formula. The bulk ZnS NP has an average particle size of 147.9nm with an optical band gap of 4.1eV.

Keywords: *heavy metals, ZnS nanoparticles, chemical sensor, aqueous media, non-aqueous media, fluorescence quenching study.*

C 036

ZnO Quantum Dots-based Chemosensor to Detect Palladium (Pd) & Cadmium (Cd) Heavy Metals in Aqueous Media

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ABSTRACT

A research study has shown that heavy metals (Pd, Cd) can be detected in water using an instrumentational method. The study synthesized stable, water-soluble ZnO quantum dots using the sonication precipitation method, resulting in 2.50nm particles. A chemical sensor was then fabricated based on these quantum dots. The particle size was determined using the Scherrer formula from the P-XRD spectra. The ZnO nanoparticle was found to have a standard optical band gap of 3.37eV. The study also calculated the optical band gap of the QDs using Tauc's plot, which was found to be 5.8eV. To detect heavy metals, a fluorescence quenching study was conducted using a $5x10^{-6}$ M ZnO QDs solution. The sonication precipitation method had some defects, as evidenced by the emission spectra of ZnO QDs at 587nm. The pH was observed to be between 5-6, and the fluorescence had an orange-yellow color. The fluorescence quenching study was able to detect up to 1.66% concentration of heavy metals in the QDs solution. The study also observed the FRET effect, which occurs when electrons are shared between the donor and acceptor.

Keywords: *ZnO quantum dots, heavy metal detection, fluorescence quenching study, aqueous media.*

C 037

Non-Enzymatic Electrochemical Sensing of Conjugated Bilirubin in Serum

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ABSTRACT

Bilirubin conjugate is an important liver function biomarker of diseases like obstructive jaundice, Dubin-Johnson syndrome, Rotors syndrome etc. Electrochemical biosensing of bilirubin conjugate has been performed on a pencil graphite electrode (PGE) in 0.05 M tris buffer (pH 8.6). The disposable and low-cost pencil graphite electrode was employed for the first time to develop an electrochemical conjugated bilirubin (CB) sensor. The constituents of pencil lead, which include majorly graphite and kaolinite clay, provided an excellent electrocatalytic surface area for the effective and sensitive detection of conjugated bilirubin. The untreated pencil lead electrodes are selective in the detection of bilirubin conjugate. The PGEs exhibited a wide dual linear range of detection from 1 - 90 µM and 100 - 1000 µM with a sensitivity of 0.063 $\mu A \mu M^{-1} cm^{-2}$ and 0.03 $\mu A \mu M^{-1} cm^{-2}$ respectively. The PGEs also showed a good response in human serum samples when spiked with different concentrations of conjugated bilirubin. The sensor has the potential to be developed into a point-of-care device or a continuous monitoring device for bilirubin conjugate.

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C 038

Clinical Approach of Potentiometric Analysis for Sweat Electrolyte

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ABSTRACT

A non-invasive potentiometric sensor for real-time, *in-situ* monitoring of ions present in sweat has been developed. The device consists of a selective matrix for sweat sensors sensitive to changes induced by specific ions (Na^+, K^+, Ca^{2+}, Cl^-), connected to a system for reading and processing data. The device is portable and it includes a cross-platform user interface connected to IoT for data visualization. This device has the potential to greatly impact the fields of health, sports, and fitness by providing valuable information for disease prevention, performance optimization, and the development of healthy lifestyles. Robust potentiometric sensors can be obtained by using a conductive polymer support as an ion transducer and adding carbon nanostructures to the matrix membrane, providing a stable voltage output over time.

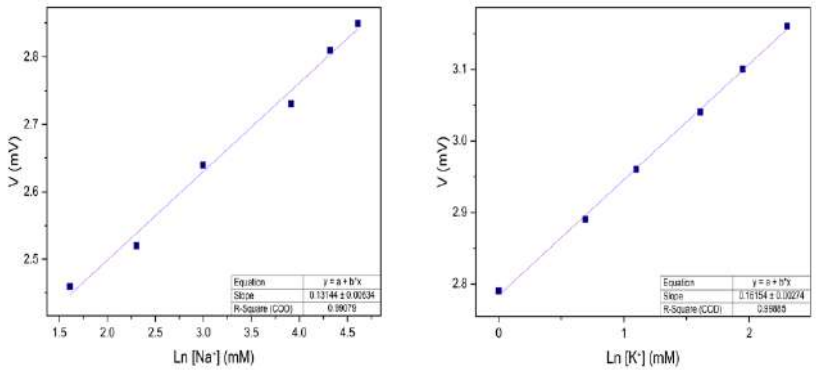

Fig.1. Calibration curves for Na^+ (left) and K^+ ions (right) measured in wearable potentiometric sensors.

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C 039

012 Facets Modulated LDH Composite for Neurotoxicity Risk Assessment through Direct Electrochemical Profiling of Dopamine

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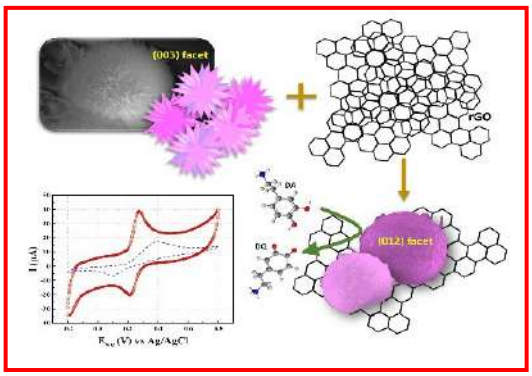
ABSTRACT

Rising concerns of pesticide-induced neurotoxicity and neurodegenerative diseases like Parkinson's, Alzheimer's, and Multiple Sclerosis, are exacerbated by overexposure to contaminated waterbodies. Therefore, evaluating the risk accurately requires reliable monitoring of related biomarkers like dopamine (DA) through electrochemical detection. Layered double hydroxides (LDHs) are an upcoming class of 2D layered materials that have gained much interest in the field of electrochemical applications due to their high catalytic activity, large specific surface area, tuneable composition and great biocompatibility. Layered double hydroxides (LDHs) have also shown great potential in sensors, however, to meet the challenges of rapid detection of large patient cohorts in real-time biological media, they should be further tailored to display superior analytical readouts. Herein, a ternary LDH was integrated with the sheets of thermally reduced graphene oxide (trGO), to expose more highly active edge planes of the LDH, as opposed to its generally observed inert basal planes. The improvement in detection performance through such a modulated structure property led to a 2-fold enhancement in the electrochemical activity exhibited by the face-on oriented LDH with trGO as compared to the pristine LDH material. Further, the fabricated sensor was employed for the direct detection of DA in real blood plasma samples. Moreover, it also exhibited exceptional selectivity towards the detection of DA with a limit of detection of 34.6 nM for a wide dynamic range of 0.001-5mM with exceptional stability retaining 88.56% of the initial current even after storage in ambient conditions for 30 days.



C 040

Ultrasensitive Detection of Chloramphenicol Antibiotic Using Functional Polymer Layers with an Aluminium Organic Framework

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ABSTRACT

The wide consumption of antibiotics, which are used to treat bacterial infections in humans and animals, expedites their accumulation in aqueous environments. Chloramphenicol (CAP) is one of the widely used broad-spectrum antibiotics against bacterial ailments like conjunctivitis, cholera, typhoid, etc., and also for veterinary treatments. The adverse side effects and increased risk of antibacterial resistance of CAP demand its proper monitoring in the aqueous environment. Metal-Organic Frameworks (MOFs) are extensively used as electrode material in various sensing applications due to their efficacious porous nature and tunable properties. However, pristine MOFs lack conductive attributes that hinder their wide usage in electrochemical applications. Electropolymerization of several aromatic monomers is a widely used strategy for preparing conducting electrode materials for various sensing applications in the past decades. Herein, we report a similar approach by using functionalized electropolymer to enhance the sensitivity of an Aluminium Organic Framework (DUT-4) for the selective detection of CAP. The combined strategy using the conducting polymer layer with the porous Al MOF provides surpassing electrochemical performance for sensing CAP with regard to the very low detection limit (LOD = 39 nM) and exceptionally high sensitivity (11943 μA mM^{-1} cm^{-2}). In addition, the fabricated sensor exhibited good selectivity, reproducibility and stability. The developed method was successfully evaluated in various real samples including lake water and river water for CAP detection with good recovery percentages even at lower concentrations.

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C 041

Targeting Selective Detection of Azithromycin Using Organic-Inorganic Hybrid Material as a Luminescent Probe

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ABSTRACT

Being a macrolide antibiotic, the antiviral and anti-inflammatory properties of azithromycin (AZM) were taken advantage of during the COVID-19 pandemic which led to the overuse of AZM resulting in excessive release and accumulation in the waterways and ecosystem causing unpleasant threats to humankind. This demands the necessity for a highly sensitive material being capable of recognizing AZM in wastewater. Mindful of the optical attributes of organic ligand structures, we have constructed a hybrid material by chelating Zn^{2+} with pyridyl benzimidazole (PBI). The prepared sensor material ZnPBI was characterized using various microscopic and spectroscopic techniques including XRD, FT-IR, HR-SEM, HR-TEM, etc. The proposed sensor material exhibits proficient detection performance selectively towards AZM with a very low detection limit of 72 nM. Two linear ranges between 0 – 70 µM and 70 -100 µM were observed corresponding to two different mechanistic pathways. To the best of our knowledge, the utilization of a metal-organic complex (MOC) for the fluorometric detection of AZM has not been explored so far. It is creditworthy to cite that the long-term structural stability of the sensor material was maintained for 100 days in water and it can be reused three times without any depreciation in the sensing activity. A combination of energy transfer routes, adsorption and electrostatic interactions for AZM detection are described extensively experimentally and theoretically which provides insights into the role of MOC as sensing probes.

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C 042

Fabrication of Magnetic Nanoclusters Modified Gold Electrode for the Impedimetric Detection of Serum Albumin

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ABSTRACT

Albumin is the most abundant protein in blood. Human serum albumin (HSA), with a molecular weight of 66.5 kD, is produced in liver. Serum albumin has essential physiological functions such as to maintain the osmotic pressure between blood and tissues and to transport those species such as hormones, fatty acid, etc. Therefore, albumin is a very important biomarker indicating the physiological condition of one's body. Additionally, iron oxide magnetic nanomaterials have been widely investigated because of their superparamagnetic property upon subjected to an external magnetic field. Consequently, we propose an Au electrode modified by iron oxide magnetic nanoclusters (MNCs) for the electrochemical detection of serumalbumin.

Thermal decomposition was applied to prepare uniformly distributed iron oxide nanoparticles. Afterwards, iron oxide magnetic nanoclusters (MNCs) were successfully prepared. The hydrophobic surfaces of the nanoclusters were turned into hydrophilic by appropriately chosen ligand. The hydrophilic nanoclusters were further conjugated with sulfo-SMCC (sulfo-*N*-succinimidyl 4-(*N*-maleimidomethyl) cyclohexane-1- carboxylate). Vi which, the electrode coated with SMCC conjugated MNCs (MNC@SMCC) were able to capture albumin. Impedance analysis on the electrodes at different stages was carried out. Thus, the calibration curve of impedance change against albumin concentration spiked in serum was established withexcellent linearity.

Detection of albumin concentration in the range of 1~10 g/dL is feasible by the as-prepared MNC@SMCC coated Au electrode. For stability test, the as-prepared sensor can maintain reproducibility for at least 30 days. To the 60 serum specimens received from NCKU hospital, the average recovery of 82% is achieved by the measurements from the as-prepared sensor.

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C 043

Single-Step Synthesis of N, B Co-Doped Graphene Oxide by Nanosecond Pulsed Laser Ablation in Liquid for Clad Modified Fiber Optic Gas Sensing Application.

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ABSTRACT

Fiber optic gas sensors have the advantages of room temperature sensing and their ability to detect gas at explosive and inaccessible locations. Nitrogen and boron co-doped graphene oxide (BNG) was synthesized efficiently and quickly by a single-step nanosecond pulse laser ablation(ns-PLAL) of graphene in ethanol. FT-IR and XPS confirm the nitrogen and boron doping on the surface of the graphene oxide. The optical properties of BNGs were studied using UV-Vis and Photoluminescent studies. The BNG possesses high photostability. FESEM confirms the spherical shape of BNG, and the average size of BNGs is found. XRD and Raman analysis carried out structural and crystallinity studies. The spherical-shaped BNG nanoparticle has been tested for sensitivity to room-temperature clad-modified fiber optic gas sensors with toxic gaseous like ammonia and ethanol. The gas sensing property of BNG was investigated using a fiber optic gas sensor and found to show good sensitivity and selectivity towards ethanol gas. The BNG nanoparticle demonstrates excellent characteristics for gas sensing due to its selective sensitivity and is a promising candidate for clad-modified fiber optic gas sensors.

Keywords: *PLAL, BNG, clad modified optical fiber, gas sensing, sensitivity*.

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C 044

Biomimetic Superoxide Sensor for Sensitive Detection of Superoxide Anion

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ABSTRACT

Reactive oxygen species (ROS) such as hydroxyl radical (O•H), hydrogen peroxide (H_2O_2), singlet oxygen ($^1O_2$) and superoxide anions ($O^{\bullet-}_2$) are direct measures of oxidative damage as their imbalance can cause signal impairment in cells, leading to several benign and malignant diseases like diabetes, atherosclerosis, cancer, autoimmune diseases, Alzheimer's, Parkinson's, etc… Among these ROS, $O_2^{\bullet-}$ is a short-lived oxygen intermediate, that is reported to be highly reactive and is found to take part in several physiological and pathological processes. $O^{\bullet-}_2$ is also well-known to function as a biomarker for certain types of tumors and cancers. Therefore, dynamic detection of $O^{\bullet-}_2$ is of utmost importance for pathological study, disease diagnosis, and health screening. Herein, we have designed and developed an electrochemical sensor using a novel copper oxide doped zinc-based metal organic framework (CuO-ZTF) that mimics the enzyme superoxide dismutase. The synthesized material was characterized using various spectroscopic and microscopic techniques such as X-Ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). Further, the CuO-ZTF was drop-coated on glassy carbon electrode (GCE) to construct the electrochemical sensor (CuO-ZTF/GCE). The electrocatalytic activity of the material was studied using cyclic voltammetry (CV) and $O^{\bullet-}_2$ was detected amperometrically at -0.2 V. The constructed sensor displayed a wide concentration range from 25 □M to 2.5 mM with a detection limit of 7.318 □M.

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C 045

Detection of Explosive Materials: TNP in Aqueous Media & TNT in Non-Aqueous Media by Using CDs-Based Chemical Sensor

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ABSTRACT

Explosions in different places are the destruction of the political department. Recently, there have been a number of ways to formulate explosive materials by using less and cheaper products. Day by day, the terrorist activities are increasing. The real challenge in forensic chemistry is to detect trace-level evidence, its proper collection, preservation, and scientific identification. In today's era, unauthorized use of explosive materials is continuously rising and hence a detailed description of the detection of explosive traces as forensic evidence has been elaborated. This research focuses on the detection of nitro group explosive materials with the help of a CD-based chemical sensor. The $4x10^{-5}$ M concentrated solution has been used to detect explosive materials having 3.33% concentration in aqueous media & non-aqueous media. The blue fluorescence absorbs at its highest intensity at 380nm wavelength. The absorption peak of CDs in water is at 350nm and the luminescence spectra between 400nm to 500nm show a maximum at 459nm with the strongest intense peak. The quantum yield of CDs is found between 10-17% in distilled water compared to pure CDs. By fluorescence quenching study, CDs based chemical sensor has been utilized to detect TNP in aqueous media as it makes hydrophilic chain and TNT in non-aqueous media.

Keywords: *quantum dots, explosives, fluorescence quenching study, sensor, aqueous media & non- aqueous media.*

C 046

Highly Sensitive NO_2 Gas-Sensor for Enhanced Selectivity by Nanoporous CuO@ZnO Heterostructures

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ABSTRACT

In the combustion of fossil fuels, various noxious gases are released. Therefore, it is revered to design gas sensors with excellent performance and low power consumption. In this work, we account the superior nitrogen dioxide (NO_2) sensing characteristics of pristine CuO and CuO/ZnO heterostructures at RT (30℃). The fabricated CuO/ZnO sensor manifested a maximum sensitivity of 337% for 5 ppm of NO_2 gas, relatively rapid response/recovery time of 15/25 s, and detection limit is to be 155 ppb at RT (30℃). The CuO/ZnO heterostructures reveals the outstanding response against NO_2 and imperceptible cross-response to other gases. Furthermore, the fabricated gas sensor has good repeatability, and excellent stability of 92%. The increased sensitivity was ascribed, owing to the synergistic effect of CuO and ZnO. Especially, the nanoporous heterostructure may promote NO_2 gas adsorption, and providing a large number of reaction center between chemisorbed oxygen species and NO_2 molecules.

Keywords: *Heterostructure, NO_2 gas sensor, Selectivity, gas response.*

C 047

DFT Investigation on Sensing the VOCs on Vacancy Induced, B, C, and N Doped Armchair Silicene Nanoribbon

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ABSTRACT

Volatile organic compounds (VOCs) play a vital role in the early detection of diseases. More than 200 VOCs are released in human breath and few of them are used as a biomarker. These kinds of VOCs are released due to the metabolic changes in the human body. VOC detection is a quick, noninvasive, and cost-effective method for early detection of many diseases. Nanomaterial-based sensors are efficient for sensing the VOCs with high selectivity and sensitivity. Among the class of materials, xenes are compatible materials for sensing the VOCs due to the high surface-to-volume ratio, high surface reactivity, and excellent electron mobility. Apart from graphene, silicene attracts many researchers due to its low-buckling nature from the xenes group. Silicene nanosheets pose a semi-metallic nature similar to graphene which makes this material lack tunable properties. But armchair silicene nanoribbons (ASiNR) have semi conducting behavior with tunable electronic properties also widely reported for sensing applications. This makes this material for sensing the VOCs in the exhaled breath. In the present work, we are using the DFT approach to study the ground state electronic properties and structural properties of pure ASiNR, vacancy-induced ASiNR, and doped (B, C, N) ASiNR. Then we studied the adsorption behavior of COPD breath biomarkers 3-hexanone and 3-methyl cyclopentanone towards all the systems. The structural stability of the system is confirmed through the formation energy. Then the adsorption energy, adsorption distance, charge transfer, and recovery time are also calculated. These results would give some insights into making a VOC sensor for the early diagnosis of diseases.

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C 048

Morphology Varied $SrTiO_3$ Supported on MXene ($Ti_3C_2T_X$) for Gas Sensing Study

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ABSTRACT

NO_2 (Nitrogen dioxide) is among the most hazardous gases and common air pollutants as declared by the World Health Organization (WHO) which is produced by combustion processes and exhaust fumes of cars. It can cause diseases such as respiratory irritation, emphysema, and bronchitis even at a low concentration [1]. Therefore, the development of ideal gas sensors with high stability, rapidity, repeatability, and sensitivity is desirable. ABO_3 type metal oxide perovskite have garnered attention due to their outstanding features. The semiconductor strontium titanate (STO) exhibits good thermal and chemical stability, high dielectric constant, superconductivity, large absorption coefficient with a band gap of 3.2 eV. These properties bestow SrTiO3 excellent potential in gas sensing application [2]. $Ti_3C_2T_x$(Mxene) has emerged as an outstanding support material improving the sensing property. They have a unique laminar structure, high surface area, conductivity, and excellent adsorption capability which helps in the ease of charge transfer during the sensing process. Focusing on these characteristics we have synthesized $SrTiO_3$ based on $Ti_3C_2T_x$ for the sensing of NO_2 gas. Moreover, the various morphologies of the $SrTiO_3$ have shown varied results on exposure to the same gas. Therefore, exploring the morphological behaviour of SrTiO3 on the MXene surface for gas sensing studies will give a broader knowledge about the material. It was observed that flower-based morphology gave a response of 63% with a fast response and recovery time. The synthesized material was confirmed by using sophisticated characterization techniques like Powder X-Ray diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FTIR), Raman Spectroscopy, UV- Visible Spectroscopy (UV-Vis), Scanning Electron microscopy (SEM), Transmission Electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS).

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C 049

Mn Doped ZnO Thin Films for Reagentless Biosensing Applications

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ABSTRACT

Although zinc oxide (ZnO) is a versatile material with applications in diverse fields, its potential in some processes is constrained by its poor redox capabilities. In this study, we use sol gel technique to fabricate Mn (a transition metal) doped ZnO thin films and further utilize them as platform for uric acid biosensors. The objective was to introduce manganese (Mn) into the ZnO matrix to enhance its redox properties, capitalizing on multivalent nature of manganese. The Mn-doped thin films of concentrations varying from 3%,5%,7% and 10% were prepared and further characterized using UV-VIS spectroscopy, FTIR, FESEM and Cyclic Voltammetry (CV) measurements. The Mn doped ZnO thin films with 7% Mn doping exhibited improved redox behaviour, as evident by the distinct redox peaks. These peaks were obtained in PBS solution in absence of redox mediators which are known to be hazardous and hence not suitable for fabrication of integrated biosensors. In order to immobilise the uricase enzyme, the 7% Mn doped composition was used, creating a highly sensitive and focused uric acid detection platform. Excellent performance was shown by the fabricated sensor in terms of sensitivity ($40\mu AmM^{-1}cm^{-2}$), selectivity (less than 5% deviation was found in presence of other known markers present in human sera), and shelf life (>10 weeks), enabling precise and sensitive uric acid detection. This study brings to light a different approach in developing point of care biosensors using transition metal doped ZnO thin films.

C 050

Copper-Modified Screen-Printed Electrode for Non-Enzymatic Creatinine Sensor

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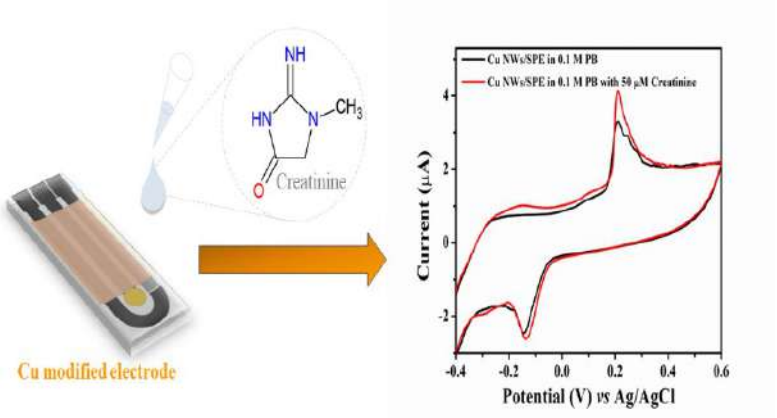
ABSTRACT

Chronic kidney disease (CKD) is a challenging health problem in the 21st century and creatinine detection plays a vital role in the early diagnosis of CKD. Copper nanoparticles form a complex with creatinine, which either adsorbs or desorbs on the surface. Disposable copper-modified screen-printed electrode was fabricated and tested in 0.1 M phosphate buffer. The sensor displayed excellent sensing towards creatinine with a detection range of 25-200 µM with a sensitivity of 4.5 µA μM^{-1} cm^{-2}. The developed sensor exhibited a stable response in the presence of common interfering molecules like ascorbic acid, glucose, uric acid, and urea. The fabricated copper-based non-enzymatic creatinine sensor is promising for point-of-care testing devices.



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C 051

Electrochemical Determination of Caffeine in Pharmaceutical Samples Using GO/SnTe Nanocomposite Modified Electrode

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ABSTRACT

The pursuit of simple, selective, and sensitive electrochemical sensors has received considerable attention in the pharmaceutical and food industries. Currently, several nanomaterials are used to modify the electrode surface due to their large surface area and more binding sites. Among the nanomaterials, tin telluride will be a potential one due to its greater conductivity and strong metallic characteristics over other elements in their family [1]. In addition, it also has a lower band gap, which can lower the analyte potential and detect even in trace quantity. Moreover, graphene oxide based nanocomposites act as a support material for the growth of metal nanoparticles and exhibited greater versatility because they are cost-effective, have a wide potential range, and possess relative electrochemical inertness and electrocatalytic activity in various redox reactions [2,3]. Caffeine (Caf) is a natural alkaloid stimulant to the central nervous and also used therapeutically in the treatment of migraine, in combination with nonsteroidal anti-inflammatory drugs and often analgesic pharmaceutical formulations because of its diuretic activity [4]. In this study, a facile GO/SnTe nanocomposite was developed and characterized by X-ray diffraction, Raman, FT-IR, energy dispersive analysis and scanning electron microscopy. Then, it was coated on a glassy carbon electrode (GCE), and thus produced the GC-GO/SnTe electrode. The electrochemical activity of the electrode was examined with caffeine obtained from pharmaceutical samples. The electrochemical features derived were a decrease in overpotential, an enhancement in electron transfer, excellent sensing ability and selectivity, a wide linear range, and a low detection limit.

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C 052

Development of Image Sensor for Pesticide Residue Detection on Grapes Surface

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ABSTRACT

Improper application of pesticides on grapes causes serious health issues and also pollutes the environment. Various analytical and laboratory methods like several types of chromatography techniques such as gas chromatography, and liquid chromatography available for the detection of pesticides in the samples of different fruits and vegetables. But such traditional methods require special laboratories and skilled persons. However, the present paper aims for a non-destructive, rapid and precise method of detecting pesticide residue distribution on grapes surfaces. The developed technique is based on image analysis of captured images of grapes using MATLAB. In the primary stage, it includes steps viz. image acquisition, display and exploration, geometric transformation and image registration. Further image filtering and enhancement are performed for contrast stretching and thresholding of acquired data. ROI is found using segmentation followed by object analysis and feature extraction techniques. Finally, texture analysis is carried out using gray level co-occurrence matrix (GLCM), a statistical method of characterization from pixel values. Thus the distribution of pesticides on the grapes surface is obtained. The results can further be compared with the image analysis of standard images of organic grapes to predict whether grapes are harmful or not.

Keywords: *Pesticide Residues on grapes, Image Processing, Non-destructive method, MATLAB, GLCM*

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C 053

Quantum Dot Based Nano-Biosensor as Wearable Devices

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ABSTRACT

Sensors are nowadays an universal tool in different areas of healthcare, environmental refinement and for the humanities, recent years have witnessed eloquent progress in the development of biosensor particularly with the integration of Quantum Dots. (QDs), into wearable devices. Both Quantum dots and nanoscale semiconductor particles which have gained eminence due to their peculiar optical and electronic properties and making them ideal for sensitive and selective bio-sensing. On the other hand nanotechnology has enabled the miniaturization of biosensor, facilitating their integration into wearable devices , which can continuously monitor variousb corporeal parameter. Further more the integration of nanotechnology has lead to the development of wearable devices like, biosensors that are comfortable unobstrusive and capable of long term monitoring for early diseases detection and persolnalized medicine, such devices have the potential to revolutionize healthcare by providing real time data. QDs with their unique electrostatic potential (ESP) properties of QDs have focused on enhanced signal to noise ratios , have revamped biosensor sensitivity and specificity , their application range from detecting biomarker for diseases to real-time monitoring of glucose levels in diabetics. The immense potential of biosensors based on quantum dots and nanotechnology is improving healthcare outcomes and enhancing our understanding of human biology. This flourishing field holds promise for the development of innovative wearable devices such as smart band, hearing aids ...etc that will have an abstruse impact on future healthcare, diagnostics and diseases management.

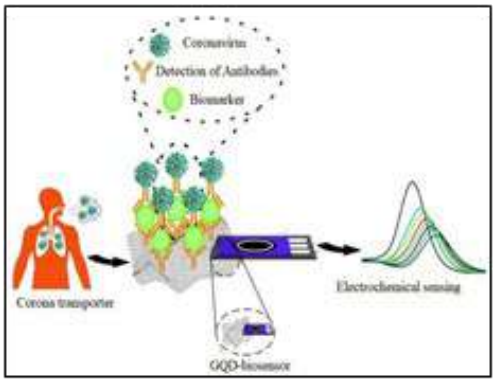

Fig 1.1 QD Chip for biosensing

Keywords: *Biosensor, Biomarker, Quantum dots, Nanotechnology, Sensitivity, Specificity.*

C 054

Hydrothermal synthesis of Nano CO_2SnO_4 Ternary Metal Oxide (TMO) Semiconductor for the Acute Ethanol gas sensing application

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ABSTRACT

In this present work CO_2SnO_4 Nanostructure has been synthesized by hydrothermal method with varying molar concentration of tin chloride ($SnCl_4$) as a source of Sn. The thick film of nano CO_2SnO_4 with tin chloride ($SnCl_4$) concentration was fabricated by using screen printing methodology. The structural properties of CO_2SnO_4 were confirmed by X-Ray diffraction and the formation of nano CO_2SnO_4 was confirmed by transmission electron microscopy (TEM). The surface morphology and surface characteristics of fabricated material analyzed using scanning electron microscopy (SEM) while the energy dispersive spectroscopy analysis (EDS) shows the chemical composition of the prepared thick film. The fabricated thick film of composition was tested for different hazardous gases like Nitrogen dioxide (NO_2), Ammonia (NH_3), Hydrogen Sulphide (H_2S), Ethanol (CH_3CH_2OH), and Methanol (CH_3OH). The thick film of CO_2SnO_4 thick film prepared at molar concentration (CO- 1M : Sn- 0.7M) shows the maximum sensitivity 89.63% to Ethanol gas at an operating temperature of 120 ^oC and concentration of 500 ppm. The rapid response and recovery were recorded for CO_2SnO_4 thick film gas sensor.

Keywords: *Hydrothermal Synthesis, Screen Printing Technique, Thick Film Preparation, Ethanol Gas Sensor, Reusability.*

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C 055

Exploring the Superior CH_4 Gas Sensing Performance of Metal Substituted Shell (M = Ni, Zn, Co) on CuO Metal Oxide Core Derived from CuM- Based Metal Organic Framework

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ABSTRACT

Methane (CH_4) with its explosive nature possesses potential threat in coal mines. Real-time methane monitoring is crucial because an explosion might occur if there is 4-5% methane in the air[1]. Towards this direction, substantial research has been done on chemiresistive type gas sensors based on transition metal oxides for the sensing of toxic gases because of their ease of altering the electrical conductivity upon interaction with analyte gaseous molecules[2]. Further, conventional metal oxide semiconductor-based gas sensors possess some limitations such as frequently include their small surface areas and high operating temperatures[3]. Hence, development of gas sensing materials with superior selectivity, sensitivity, reproducibility, fast response, and recovery time along with room temperature operation is necessary for practical usage. In view of this, metal organic frameworks (MOFs) have emerged as an alternative material with outstanding properties such as tunable pore structure, high crystallinity, incredibly large surface area, easy synthesis, and high gas accessibility. Hence, MOF derived core-shell heterojunction metal oxide materials can collectively reach upto the benchmark by enhancing surface area, sensitivity as well as lower response and recovery time[4]. This report revealed core-shell CuO/ZnO showed a comparatively higher response of S% = 12.9%, with a response and recovery time of 20 s, 25 s, respectively, towards 100 ppm of CH_4 than other cation substituted shell due to higher vacancy oxygen, larger pore diameter and high specific surface area. Further, to attain efficient room temperature activity with higher sensor response and lower response, recovery time, the core-shell structure was modified with 3-D graphene oxide (3DGO). The 3DGO-CuO/ZnO gas sensor showed comparatively higher response of 20.5% towards 100 ppm of CH_4 at room temperature, with the lowest response and recovery times of 8 s and 11 s, respectively.

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C 056

Modulating the Dual Emission Behavior of Azine Probes Using Micelles

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ABSTRACT

Organic fluorescent probes are progressively getting important due to their significant role in the detection and understanding of biomolecules due to their high selectivity, sensitivity and suitable for real-time investigation of living systems (1,2). Understanding their photophysical behavior are very challenging due to their excited state energies dependent on the microenvironment around the probes. The presence of excited state intramolecular charge transfer (ICT) and proton transfer (PT) pathways within the same organic molecule shows highly interesting photophysical properties and, consequently their utility and in applications also get enormously magnified several folds (3-5). Here, we have synthesized a symmetrical azine based dimer molecule (DEASAD) which contains both ICT and ESIPT pathways within the molecules. The photophysical behavior of DEASAD was studied both in solution as well as heterogeneous medium using micelles. Up to premicellar concentration, DEASAD shows dual emission due to the presence of both open and twisted enol forms as similar to be in protic solvents. After micellization, new anomalous longer wavelength emission is observed due to the formation of keto form in the excited state via ESIPT reaction. The complete studies through interaction of metal ion and control molecules (with and without ESIPT and ICT moieties) revealed the position and interaction of DEASAD with the charge of micellar stern layer. In contrast to the ionic micelles, the new anomalous longer wavelength keto form of DEASAD emission was absent in neutral micelles like Triton X-100. The present study may give a better insight into the future development of ESIPT based fluorescent probes for biological studies and also for improving surfactants coupled fluorescent sensors.

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C 057

Application of Machine Learning Algorithms for Water Quality Assessment

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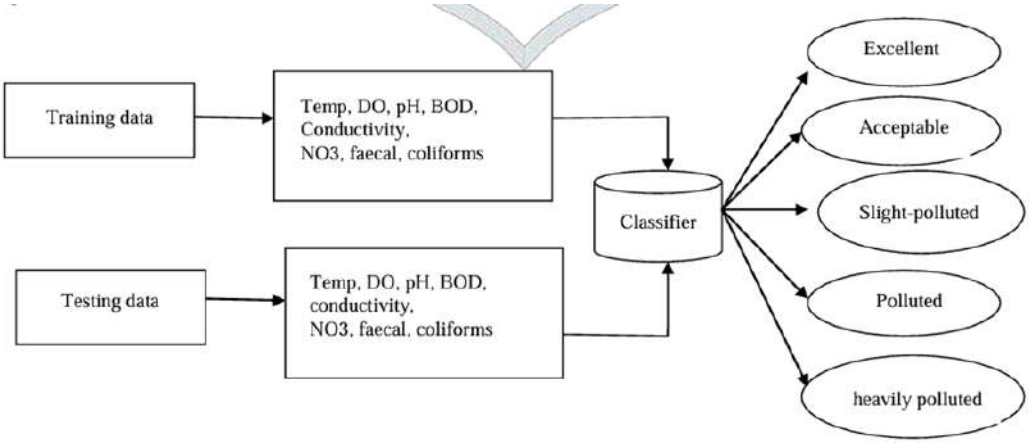
ABSTRACT

Water, a precious and essential resource, is unfortunately scarce in both developing and developed nations worldwide. It stands as the most crucial natural element on Earth, vital for human health. Various types of waste, including municipal solid, industrial, agricultural (such as pesticides and fertilizers), and medical waste, can lead to geo-environmental pollution, rendering water unusable for any living organism. Hence, the development of efficient methods to automate the assessment of water quality is paramount. The primary aim of this study is to utilize machine learning algorithms for assessing water quality. The Water Quality Index (WQI), a numerical expression employed to assess the quality of a specific water body, is employed in this research. The water quality parameters considered for evaluating the overall water quality and calculating the WQI include temperature, dissolved oxygen (DO) percentage saturation, pH, conductivity, Biochemical Oxygen Demand (BOD), nitrates (NO_3), fecal and total coliforms (TC). In this research, we utilized a supervised learning approach to create highly accurate predictive models from a labeled training dataset for determining water suitability, whether for consumption or other purposes. We consider a range of physiochemical and microbiological parameters as input features to characterize the water's condition and classify its suitability (either safe or unsafe). Methodologically, we approach the problem as a binary classification task, evaluating the performance of various machine learning models (such as Naive Bayes, Logistic Regression, k Nearest Neighbors, tree-based classifiers, and ensemble techniques) with and without class balancing techniques (such as the Synthetic Minority Oversampling Technique - SMOTE). We compare these models based on metrics like Accuracy, Recall, Precision, and Area Under the Curve (AUC).

Keywords: Water pollution, machine learning, decision tree, support vector machine.



C 058

Secure Wearable Biomedical Data Transmission: A Chaotic Map-Based Encryption Framework for Wearable Devices

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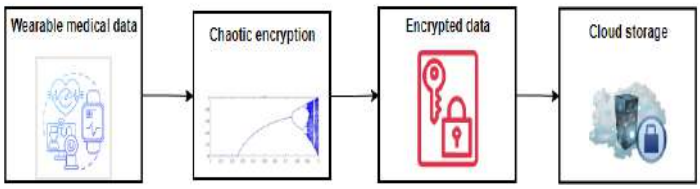
ABSTRACT

In the realm of biomedical instrumentation, wearable devices produce invaluable, yet highly sensitive, medical data. Given the prevalent storage of this information in cloud repositories, it becomes susceptible to security threats such as man-in-the-middle attacks. To mitigate this risk, our research introduces an innovative framework for encrypting medical wearable sensor data. This encryption process leverages a unique chaotic map to generate random sequences, ensuring robust security. Validation of these sequences is achieved through the meticulous examination of parameters, including the Lyapunov exponent and bifurcation analysis. This comprehensive approach aims to enhance the confidentiality and integrity of medical data in wearable devices, offering a promising avenue for safeguarding sensitive healthcare information in the digital era.

BLOCK DIAGRAM



Keywords: *Wearable sensors, encryption, chaotic map, digital healthcare, cloud security.*

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C 059

CO_2 Gas Detection by Nanostructured $ZrSe_2$ Sensor Synthesis by Hydrothermal Method and Its Characterization Study

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ABSTRACT

In the present research work, Zirconium diselenide ($ZrSe_2$) has been synthesised by hydrothermal method with varying the molar concentration of Zirconium oxychloride ($ZrOCl_2.8H_2O$) as a source of Zirconium (Zr) and Se powder as source of Selenium (Se) by using the surfactant as cetyl trimethyl ammonia bromide (CTAB) and reductant hydrazine hydrate, respectively. Thick films of nanostructured $ZrSe_2$ were developed on glass substrate using screen printing technique. The structural properties were studied by X-Ray Diffraction (XRD) characterization. The X-ray diffraction analysis revealed that hexagonal crystal structure and crystalline size was found to be 60.66 nm. The surface morphology of thick film was studied Field Emission Scanning Electron Microscopy (FESEM) and SEM images shows that grains of spherical and needle-like shaped and oriented in different direction with voids are present which create the porosity in the film surface. The quantitative elemental analysis did by Energy Dispersive X-Ray Analysis (EDAX). By UV-visible spectroscopy the average optical band gap of $ZrSe_2$ thick films was found to be 2.96 eV. The prepared $ZrSe_2$ thick films were tested for NO_2, H_2S, CO_2, NH_3 LPG, C_2H_6O (ethanol) and CH_3OH (methanol) gases at different gas concentration and different operating temperature. The film prepared with the molar concentration of 0.1:0.5 M shows the highest repose to CO_2 gas as compare to the other gases with 83.44 % sensitivity at an operating temperature of 160°C with 500 ppm gas concentration. The film shows quick response and recovery times of 8 and 38 seconds respectively.

Keywords: *Hydrothermal method, Zirconium diselenide, Thick films, Gas sensors, Nanostructures, Sensitivity.*

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C 060

Inelastic Electron Tunneling Spectroscopy of Protoporphyrin IX (PPIX) using Scanning Tunneling Microscope

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ABSTRACT

Inelastic electron tunneling spectroscopy (IETS) based on scanning tunneling microscope (STM) makes the measurement of single-molecular vibrational spectra possible. This is an excellent spectroscopic tool to detect biomolecules for ultra-sensitive medical diagnosis. A fraction of the electrons tunneling through the molecules excite molecular vibrations, resulting in inelastic tunneling component. Since electron-phonon coupling is stronger than electron-photon coupling, IETS offers high sensitivity as compared to optical detection schemes. That is, a single molecule monolayer is sufficient to generate the spectra. The obstacle for IETS to expand its applications to sensing is the thermal broadening known as the Jaklevic limit of temperature (5.4KBT) limiting its use at room temperature. Protoporphyrin IX(PPIX), a biosynthetic precursor to heme and chlorophyll can be incorporated into bioelectronics for modeling photosynthesis, diagnosis and therapy of cancer and photocatalysis applications. Elevated levels of PPIX in blood disturb the heme production pathway causing abnormal production of metal-free PPIX. Currently spectrophotometric method is employed to detect PPIX in blood,but it has its demerits. In the present work, IETS by STM was performed for PPIX deposited on highly oriented pyrolytic graphite (HOPG) for a range of temperatures. Deviation from the Jaklevic limit was noted for full-width half maxima corresponding to a peak around 400 cm^{-1}. Although evident peak broadening was observed at elevated temperatures, the peaks remain distinguishable extending possibilities for sensing applications. These observations are supported by vibrational modes calculated using density functional theory (DFT), Raman spectra, and infrared (IR) spectra

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C 061

Fabrication of CeO_2 and Cu_2O Films for Humidity and Bending Sensors by Using Solution Processes Based on Thermochemical Calculations

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ABSTRACT

Functional oxide films such as CeO_2 and Cu_2O are generally fabricated by dry processes or thermal decomposition of starting material solutions. These processes need high temperature, and the required temperature is above about 300ºC in the case of the CeO2 films. However, both of CeO2 and Cu2O can be formed from Ce^{3+} and Cu^{+} ions below 100ºC according to the thermochemical calculations as shown in Fig. 1. The films fabrication below 100ºC by the solution process opens the way to fabricate the films on low heat-resistant resin substrates such as polyethylene (PE) and polyethylene terephthalate (PET), and on porous substrates such as foams with maintaining their original structure. The CeO2 and Cu2O films were fabricated on the conductive PE foams and the flexible PET substrates by the G-LPD process[1] and the spin-spray process[2], which were developed by our group. The PE foams coated by CeO2 layers kept their original structure and perform humidity sensor properties[1]. The PET substrates coated by Cu2O films showed bending sensor properties with high resolution covering a wide curvature range[2]. Other than CeO_2 and Cu_2O, many kinds of oxides can be formed by the solution process. Our research enables to fabricate the functional oxide films on the porous and flexible resin substrates with maintaining their original structure.

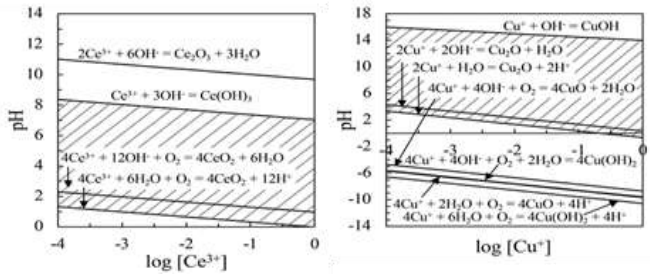

Fig. 1 Chemical equations from Ce^{3+}or Cu^{+} ions to their oxides orhydroxides with $\Delta_r G < 0$ at 60ºC andtheir precipitation equilibrium pH lines. CeO_2 and Cu_2O are fabricated in the dotted line area.

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C 062

Enhanced Ammonia Vapor Sensing with MXene-Decorated ZnO Thin Films at Room Temperature

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ABSTRACT

Metal oxide gas sensors are crucial for safeguarding human health and the environment against toxic and explosive gases. The integration of two-dimensional (2D) materials has emerged as a promising strategy to significantly enhance the performance of these sensors, allowing for higher sensor response, rapid response, and efficient recovery times. This study specifically aims to elevate the gas sensing capabilities of nanograin-structured ZnO thin films at room temperature. The approach involves incorporating MXene ($Ti_3C_2T_x$) through a drop-casting technique, thereby exploring the potential for tailored gas sensing measurements. Simultaneously, $Ti_3C_2T_x$ was etched using the Minimally Intensive Layer Delamination (MILD) technique and subsequently decorated onto the DC sputtered nanograin-structured ZnO thin film. This sequential process resulted in the generation of enhanced active sites, expanded surface area, and increased surface roughness. These enhancements collectively played a pivotal role in improving the gas-sensing capabilities of the composite material. The successful integration of $Ti_3C_2T_x$ nanoparticles and its impact on nanograin-structured ZnO thin films were thoroughly assessed through X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and field emission scanning electron microscopy (FE-SEM). The $Ti_3C_2T_x$ decorated ZnO thin film exhibited increased selectivity towards ammonia at room temperature compared with the bare ZnO. The selectivity studies of the $Ti_3C_2T_x$/ZnO sample involving ten different compounds, including ammonia, ethanol, isopropyl alcohol, formaldehyde, acetone, triethylamine, dimethylamine, xylene, and n-butanol vapors at a concentration of 25 ppm. The study revealed that ammonia demonstrates exceptional selectivity towards $Ti_3C_2T_x$/ZnO than bare ZnO and underscoring the synergistic effect of $Ti_3C_2T_x$ decoration and emphasizing significantly enhanced gas sensing capabilities. This finding suggests promising implications for the utilization of $Ti_3C_2T_x$/ZnO in advanced gas sensing applications.

Keywords: *ZnO chemiresistive gas sensor, $Ti_3C_2T_x$, MILD technique, synergistic effect, ammonia sensor.*

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C 063

Design, Simulation, and Fabrication of a Soft Capacitive Pressure Sensor

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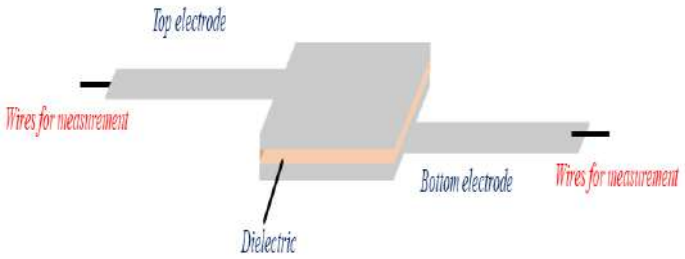
ABSTRACT

Flexible wearable devices are revolutionizing point-of-care health monitoring. Along with a wireless electronic network, these sensors can easily monitor the signals without causing any side effects on human health. Flexible and wearable capacitive pressure sensors are widely used to monitor heart rate, pulse, motion, and blood pressure, where the capacitance change in response to an applied pressure is monitored. In this work, we develop a highly sensitive capacitive pressure sensor using flexible electrodes and a microcylindrical array of PDMS as the dielectric material. Different microstructures are patterned and their effect on capacitance change for pressure monitoring is studied. Simulation studies are performed using COMSOL Multiphysics to evaluate the effect of different parameters in the microstructure of the dielectric like the thickness of the dielectric, spacing between the microcylinders, and geometry of the microcylinder. The optimized design of the dielectric is then microfabricated by photolithography and soft lithography and sandwiched between two flexible electrodes. The change in capacitive behavior in response to different pressures is analyzed using an LCR meter and the sensitivity, response time, and hysteresis of the sensor are evaluated.



Schematic of the capacitive pressure sensor

C 064

Flexible Printed Sub-Zero Temperature Sensor for Real-Time Monitoring of Cold Storage of Biological Specimens

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ABSTRACT

Our research focuses on the development of highly flexible sub-zero temperature sensors tailored for continuous and real- time monitoring in environments critical to biological storage applications. Particularly relevant for the preservation of biological materials, including blood stem cells, human epithelial cells, DNA, RNA, and mouse fibroblast cells, our sensors offer a robust solution for extended sub-zero storage (below -10°C). This innovation caters to diverse applications, ranging from cold storage in the food and beverage industry to pharmaceutical refrigeration and polar regions. The uniqueness of our sensor design lies in its flexibility, rendering it robust, conformable, wearable, and mechanically stable against deformation. Leveraging inkjet printing technology for the fabrication of temperature sensors brings advantages such as simplicity, scalability for volume manufacturing, cost-effectiveness, and compatibility with large-area substrates. The sensor's architecture involves using printed conductive graphene for temperature sensing on polydimethylsiloxane (PDMS) elastomer for the flexible substrate. A pivotal aspect of our fabrication process is the integration of photonic curing, significantly enhancing the graphene film's conductivity (up to ~142 S/m) (fig. 1(a)) after the printing process and ensuring a positive temperature coefficient of resistance within the sub-zero range from -30°C to 80°C (fig.1(b)). This positive correlation results in a notable sensitivity of approximately 0.12% per degree Celsius. Demonstrating exceptional flexibility, our sensors endure 200 continuous bending cycles with a bending radius of approximately 25 mm. Moreover, we successfully tested the wireless operation of these sensors, transmitting and monitoring real-time temperature data using a smartphone platform. This research, blending inkjet printing and photonic curing, establishes a cost-efficient approach to manufacturing sub-zero temperature sensors, holding great promise for applications demanding precise temperature control in the preservation of biological specimens.

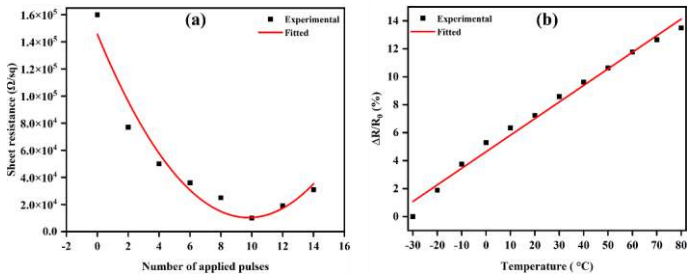

Figure 1. (a) Sheet resistance of printed graphene film at different nos. of applied photonic pulses. (b) Change in resistance (%) of the non-encapsulated sensor with temperature (from -30 to 80 °C)

C 065

SERS with Au and Ag@Au Nanoislands Film for Detection of Trace Chemical Molecules

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ABSTRACT

In this work, we present a cost-effective and novel method for making large-area surface-enhanced Raman scattering (SERS) substrates using thermal annealing of ultrathin gold (Au) and silver-gold (Ag-Au) films. The evolution of optical properties of thermally annealed Au and Ag-Au discontinuous films were investigated and correlated with morphological changes. Au with thickness of 5nm and Ag-Au films with 5nm thick each were deposited by electron beam evaporation and annealed at different temperatures at normal environment. Optical characterization of the samples was carried out using UV-VIS spectroscopy, surface morphology was analyzed with field emission scanning electron microscopy. Thermal annealing of these films formed high-density gold nanoislands (AuNI) and gold-coated silver nanoislands (Ag@AuNI) with average sizes ranging from 10nm to 45nm and 10nm to 50nm, respectively. The SERS response of the fabricated samples was carried out by using Rhodamine 6G (R6G) as Raman probe molecule. The experimental results showed that Ag@AuNI exhibits highest SERS signal as compared to AuNI due to the higher optical field confinement at SERS hot spots due to the presence of Ag. Our study found that the efficiency of Ag@AuNI in the detection of R6G achieved a detection limit (LOD) of 10^{-9}M. We believed that SERS platform with excellent sensitivity and high signal reproducibility demonstrates its potential to develop low-cost SERS substrates for their applications in biomedicine and medical diagnosis.

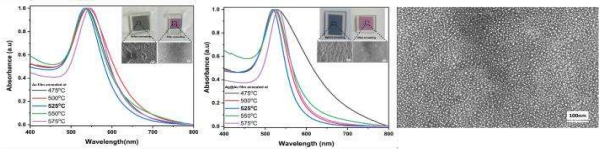

Fig. (A and B) Absorbance spectra of Au film with thickness of 5nm and Ag-Au film with thickness of 5nm each layer and annealed at different temperatures; (C) FESEM image of Ag@Au Ni which is thermally annealed at 525°C.

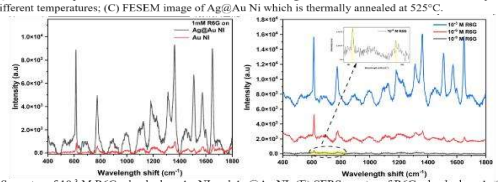

Fig. (D) SERS spectra of 10^{-3} M R6G adsorbed on Au NI and Ag@Au NI; (E) SERS spectra of R6G adsorbed on Ag@Au NI showing the minimum detected concentration as 10^{-9} M.

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C 066

Low-Dose X-ray Sensing Nature of Cs_4PbBr_6

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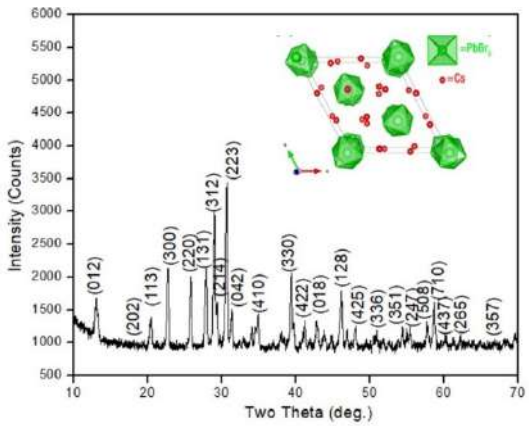
ABSTRACT

Single phase Cs_4PbBr_6 powder was synthesized using solid state reaction using CsBr and $PbBr^2$ as precursors. Phase purity and morphology of the sample was characterized respectively using powder X-ray diffraction and High-resolution scanning electron microscope. The obtained powder XRD pattern was indexed using JCPDS card 73-2478 using XRDA 3.1 software and the it was shown in figure. Also, spectroscopic investigation was performed using Raman and diffused reflectance spectroscopy. Since a scintillator is a radiosensitive luminescent material that can convert the incident energy of the radiation (high-energy photons) into ultraviolet or visible photons and constitutes a critical part of the radiation sensor[1, 2]. Thick film of Cs_4PbBr_6 (~100 µm) was coated on the top of commercial BPW-34 photodiodes and its performance was tested under the illumination of 70kv X-rays. The observed X-ray instigated photocurrent for the dose (mGy) exposed and the thickness of the film was accounted to estimated the sensitivity of the device developed.



Powder XRD pattern of solid-state reaction derived Cs_4PbBr_6 (Insert: Schematic illustration of the crystal structure)

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C 067

SERS-active Silver Nanowires with Network Alignment for Chemical Sensing

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ABSTRACT

The fabrication of efficient substrates composed of silver nanowires for surface enhanced Raman scattering (SERS) was accomplished through the utilisation of a drop-casting method followed by evaporation. The electron micrographs of these SERS substrates indicate that nanowires interweave with each other during evaporation and form monolayered and multi-layered network-like structures depending on the concentration of nanowires. It is of greater significance to utilise substrates with nanowire network alignment due to their possession of a higher overall surface area, an increased number of hotspots, and a higher laser utilisation efficiency, all of which enhance the SERS performance. X-ray diffraction pattern indicate that these nanowires possess fcc structure with preferential growth along (111) crystal plane and the absorption spectrum show a plasmon peak at 385 nm. SERS activity of these substrates was tested with probe molecules viz., p-nitrophenol (PNP) and methylene blue (MB) with excitation at 633 nm. The sensitivity of these substrates was investigated by varying the concentration of probe molecules. A maximum enhancement of 4.5×10^9 was observed for substrates prepared under optimum conditions. The observed enhancement in these substrates is attributed to the hotspots arising from nanogaps of ~10 nm formed due to interweaving at the network junctions. The minimum detection limits for PNP and MB molecules were down to 10^{-7} M with good linear responses.

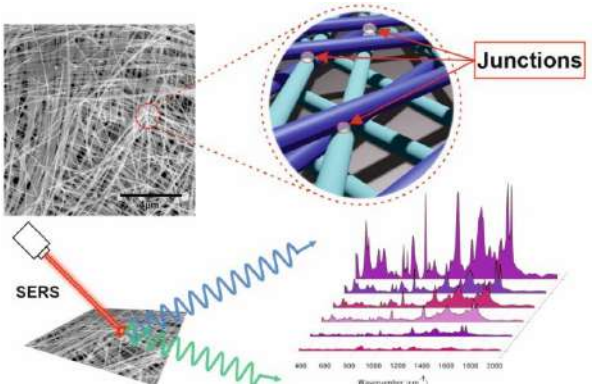

Fig 1. Illustration depicting a nanowire network featuring junctions (hotspots) formed within the network,accompanied by Surface-Enhanced Raman Scattering (SERS) spectra of PNP acquired at varying concentrations

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C 068

Recycling and Reusing Medical Waste: An Internet of Things (IoT) Cloud-Based Smart Hand Sanitizer Leveraging Triboelectric Touch Sensor

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ABSTRACT

As the globe watches a colossal medical waste pandemic on its doorstep, environmental plastic and waste pollution has steadily increased as a result of the COVID-19 epidemic. The extensive and mandatory usage of personal protective equipment such as masks, gloves, and PPE kits, tends to lack substantial and effective waste management systems, contributing to an increase in the earth`s pollution level composition. By repurposing COVID-19 scraps for green and sustainable development, this study effort introduces the notion of turning medical waste into a medium for energy harnessing while aiming to reduce the carbon footprint in this process. This work involved the fabrication of a 3D-printed contact-separation-based triboelectric nanogenerator using sterile, three-layered surgical masks and nitrile gloves for energy harvesting and sensing applications. Inside the three-dimensional construction was a piece of three-layered mask and nitrile gloves, representing the top negative and bottom positive triboelectric materials, with copper and aluminum serving as the corresponding electrodes (MG-CS TENG). The solenoid valve's opening and shutting to control the sanitizer flow was accomplished by pressing the MG-CS TENG pedal. By repurposing pandemic trash for energy harvesting and sensing applications while limiting the transmission of the coronavirus through appropriate hand sanitization, this study significantly contributes to disaster management efforts to control microplastic environmental pollution.

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C 069

Microring Resonator Sensor Utilizing Whispering Gallery Mode for Cancer and Diabetes Detection

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ABSTRACT

Contemporary optical sensing has been significantly advanced by the emergence of Whispering Gallery Mode (WGM)-based techniques, leveraging their rapid sensing capabilities and exceptionally high-quality factor. This study introduces a WGM-based optical sensor, designed to operate at a wavelength of 1.55µm, with a specific focus on detecting cancer cells in blood samples and diabetes markers in tear samples. It is reported that 20 million people affect cancer in every year and 450 million adults affect diabetes. The proposed sensor features a micro-ring with an approximate radius of 10µm intricately connected to a waveguide with a width of around 2µm. This miniaturized design not only ensures efficient performance but also facilitates seamless integration into compact and portable devices.. Theoretical analysis, conducted using the finite element method, delve into the sensitivity and quality factor of the proposed structure. The results demonstrate that the sensor exhibits a remarkable sensitivity and an impressive quality factor within the range of 2000. This high level of performance indicates the potential for the sensor's application in various sensing scenarios. Its robust capabilities make it a compelling candidate for detecting cancer cells in blood samples and diabetes markers in tear samples, showcasing its versatility and adaptability for diagnostic purposes. The study opens doors for further exploration and development of compact and efficient sensing devices for critical healthcare applications.

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C 070

Optimizing NO_2 Gas Sensor Performance: Investigating the Influence of Cobalt Doping on WO_3 Recovery Kinetics for Enhanced Gas Sensing Application

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ABSTRACT

In the realm of gas sensor research, the ongoing quest for outstanding performance remains a persistent focal point. Navigating the complexities of response and recovery processes poses a persistent challenge in attaining selectivity, elevated gas response and rapid response/recovery times within the atmospheric environment. Chemiresistive gas sensors based on metal oxide semiconductors are widely utilized, demonstrating efficient operation at moderate temperatures for the detection of diverse gases, including nitrogen dioxide (NO_2). A systematic investigation was conducted to explore the impact of cobalt (Co) doping in WO_3 and its influence on gas sensing properties. Intriguingly, the Co-doped WO_3 (CW3) sensor exhibited a remarkable and well-rounded gas sensing response of 14171% at 10 ppm NO_2, showcasing a seven-fold enhancement compared to the pure WO_3 sample at 200 °C. The findings demonstrated that the sensor exhibited an outstanding repeatability, selectivity and long-term stability of 95% over the period of 60 days. Moreover, CW3 sensor possessed a fast response and recovery time 15 / 22 s as compared to the CW sensor 22 / 154 s. The exceptional gas-sensing capabilities can be ascribed to the existence of defects within the oxygen vacancy structure. These defects effectively boost the surface reactivity of WO_3 nanoplates, thereby augmenting their sensitivity and enabling a broad-range sensing performance. The incorporation of cobalt in WO_3 nanostructures opens a novel avenue for enhancing the efficiency of gas sensors based on transition metal oxides. As a result, this research demonstrates considerable promise for utilizing environmental NO2 monitoring applications.

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C 071

Enhanced Ammonia Sensing of SnO_2 Thin Films through Mo Doping by Cost-Effective Nebulizer Spray Pyrolysis Method

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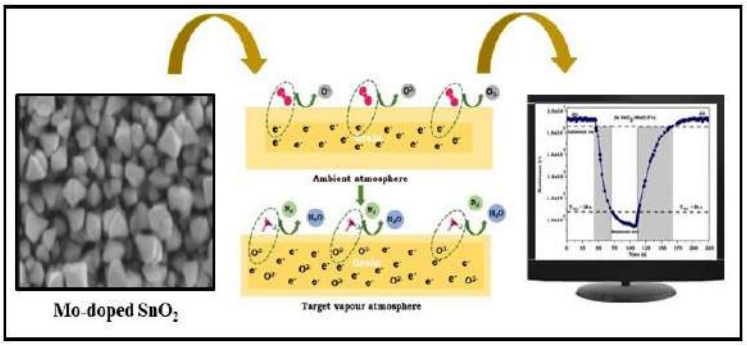
ABSTRACT

The presence of pollutants in air atmosphere causes health issues to human beings and other living organisms. There are several types of pollutants, such as gases, organic and inorganic particulates, and biological molecules. Due to the heavy industrialization and rapid economic growth in the world, these hazardous gases are evolved in our environment. Hence, the detection and control of toxic gases is of prime importance for human safety and environmental monitoring. Due to these interesting properties, studies are focused on the possibility to use this material in many field-like catalytic applications, conducting electrodes and gas sensors etc., In recent years, metal–oxide semiconductors such as SnO_2 [1], ZnO, TiO_2, NiO, WO_3 and CuO have been found as promising materials for cost effective gas sensing. Of these materials, Tin oxide (SnO_2) can be used to detect ammonia [2] vapour. However, in this Molybdenum (Mo) doped SnO_2 thin films of varying the doping percentage 0 to 1.5 wt% (in steps of 0.5 wt%) were successfully coated by Nebulizer spray pyrolysis at 350°C. The characterization studies such as, structural, optical, surface morphological, photoluminescence and elemental composition of the prepared SnO_2 thin films are taken along with their specifications for gas sensors applications.



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C 072

Investigation of Structural, Optical, Morphological, and Electrical Properties of La-doped SnO_2 Nanoparticles for Gas Sensing Application

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ABSTRACT

Metal oxide semiconductor materials are inevitable in gas sensing applications due to their wide range detection of volatile organic compounds and toxic gases. In our day-to-day life, gas sensors are useful in many active fields like healthcare, food processing, air quality monitoring, explosive detection, and agricultural industry. In this present work, we have synthesized the La-doped SnO_2 nanoparticles via the chemical co-precipitation method under the superlative conditions at different doping of La- concentrations (2%, 4%,6%, and 8%) and studied the structural, optical, morphological, and electrical characteristics. The prepared samples were characterized by XRD, FT-IR, UV-Vis, SEM, EDS, TEM, XPS, and I-V Measurement. The X-ray diffraction analysis confirms the formation of a tetragonal crystal system, rutile phase SnO_2, and the crystallite size was calculated using the Debye Scherrer formula. Crystallite sizes of pristine and La-doped SnO_2 are in the range of 40-56 nm. FT-IR analysis confirms the existence of Sn-O-Sn through the peak present at 601 cm^{-1}. UV-visible studies show the material's absorbance range between 275-263 nm, the shift due to the La-doping in the host material and their band gap from 3.28 to 3.58 eV. Scanning electron microscopy studies reveal the nanoparticle's morphology with agglomerated structures. Elemental dispersion X-ray spectroscopy confirms the presence of Sn, O, and La. Elemental mapping reveals the homogeneous distribution of elements over the surface. Activation energy is calculated from the temperature-dependent electrical conductivity and measured as a lower value which increases the adsorption sites on the surface of metal oxide semiconductors. The establishment of the polycrystalline nature of $SnO2$ was verified by the TEM analysis and the shape is in the nano cubical structure. X-ray photoelectron spectroscopy found the formation of Sn^{4+} in the synthesized samples. This investigation concludes that the La-doped SnO_2 nanostructures are the most suitable material for gas sensing applications.

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C 073

Pencil Graphite-based Electrode for the Detection of Salicylic Acid

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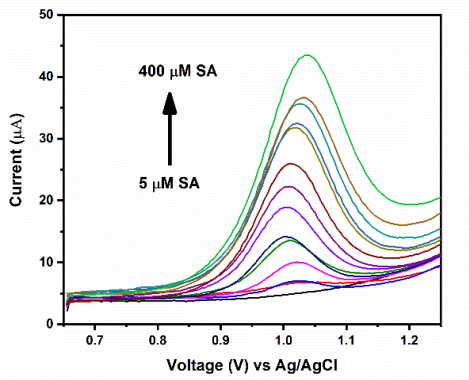
ABSTRACT

Biotic and Abiotic stress tremendously impact the major food crop yields worldwide. Early identification of these stresses in crops is essential to avoid yield loss. There are limited methods available for early detection of plant stresses. However, these methods are time-consuming, require complex instrument handling, and can be effectively performed only in laboratories. Plants produce different phytohormones against pathogens as a self-defence mechanism. Also, Monitoring the levels of such phytohormones in crops can help to understand plant physiology, such as seed growth, flower formation, seed production, and pathogen infection. Some of these phytohormones undergo electrochemical oxidation and reduction. Therefore, Electrochemical detection can be favourable and promising because it is a simple and fast method compared to other detection methods. Salicylic acid (SA) is one of the crucial phytohormones involved in various metabolic activities in different stages of a plant's life. SA is mainly involved in a plant defence mechanism as a signalling molecule. Also, the well-known anti-inflammatory drug aspirin is derived from salicylic acid. An overdose of aspirin will cause salicylate poisoning in the human body which can cause death. In this context, we attempted to detect salicylic acid by a pencil graphite-based electrode (PGE). Based on the obtained results, a fast and cost-effective way to detect the low concentration of salicylic acid is proposed.



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C 074

Fabrication of Nanostructured ZnSe/PANI composites for NO_2 Sensing Application

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ABSTRACT

Transition metal dichalcogenides (TMDs) have attracted tremendous research attention in the field of gas sensing. Nowadays ZnSe, has sparked great interest due to the high surface-to-volume ratio and high air stability as compared to other TMDs. Still, it suffers slow response and recovery at room temperature. The formation of hetero-nanostructure with metal oxides can modulate and overcome the inherent property by facilitate more interaction with gas molecules. Here, ZnSe/PANI nanocomposites were synthesized by hydrothermal method. The fabricated ZnSe/PANI sample exhibited an excellent response and recovery time as compared to that of the pristine ZnSe at room temperature. The fabricated sensor displays an excellent reproducibility, stability and superior selectivity to NO_2 compare to other interferents such as NH_3 and H_2S. This enhanced sensing performance is due to the heterostructure formation, enhanced interaction active sites and increased surface-to-volume ratio. Such improvement of ZnSe/PANI hetero-nanostructure sensors can be considered as a good sensor at room temperature.

Keywords: *Hetero-nanostructure, NO2 detection, gas molecules, room temperature*

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C 075

Room Temperature NO_2 Sensing via Co_3O_4/ZnO Heterojunctions

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ABSTRACT

Metal Oxide Semiconductors (MOSs) are widely used in gas sensing due to their unique advantages. However, their main drawback is the need for high operating temperatures and their low responsiveness at room temperature. In this study, we address this issue by combining p-type tricobalt tetroxide (Co_3O_4) with n-type Zinc Oxide (ZnO) in various molar ratios to create a p-n heterojunction through a simple one-pot hydrothermal method. We adjusted the Co^{2+}/Co^{3+} ratio to induce significant oxygen vacancies using a wet chemical synthesis route. Morphological and surface studies demonstrated improved oxygen vacancies, a high surface area, heterojunction formation, and the porous nature of the Co_3O_4/ZnO samples. Gas sensing experiments were conducted with different NO_2 concentrations (5-50 ppm). Notably, the 20% Co_3O_4/ZnO sample achieved a room temperature response towards 50 ppm of NO_2 without the need for expensive noble metals. We analyzed the band bending of the sensor after NO_2 exposure and evaluated the response/recovery kinetics. The paper discusses the potential mechanism behind the room temperature sensing and the enhanced performance of the proposed sensor. In conclusion, this research outlines an effective strategy for room temperature NO_2 sensing using metal oxide hybrids and the formation of p-n heterojunctions.

C 076

NiHCF/MXene-Based Electrochemical Sensor for the Trace Level Detection of Catechol in Real Water Sample

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ABSTRACT

Selective and sensitive detection of catechol is essential because the high concentrations of catechol in humans can cause cancer, DNA damage, swelling of internal organs, headaches, weariness, dizziness, skin irritation, and nausea. Electrochemical detection is one of the most prevalent technique for the detection of catechol in trace level due to its simple operation procedure, low cost, high sensitivity, requirement of less sample volume and rapid analysis. Hence, development of an efficient, stable and low cost electrocatalyst is required for electrochemical sensor/biosensor. Prussian blue (PB) and its analogues (PBAs) have gained great attention as viable electrocatalyst due to their advantageous properties such as tunable morphology, ease synthesis approach, 3D framework, abundant metal centres, and cost-effectiveness. However, practical application of these materials is limited due to their weak conductivity and low chemical stability in harsh condition. To overcome these limitations, in this work, we have synthesized a novel redox active nano heterostructure by in-situ growth of nickel hexacyanoferrate (NiHCF) on 2D MXene sheets NiHCF-MXene by a simple hydrothermal process. As prepared NiHCF- MXene was characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). Thereafter, a sensor was fabricated by drop casting of NiHCF-MXene on glassy carbon electrode (GCE) to obtain NiHCF-MXene-GCE. Further, the initial electrochemical characterization of NiHCF-MXene-GCE using cyclic voltammetry (CV) exhibited a well-defined redox peak with an anodic peak potential of +0.61V and a cathodic peak potential of +0.52V. Furthermore, amperometric response of the developed electrode shows broad linear ranges for the determination of catechol from 30 µM to 2.3 mM with the detection limit of 5 µM. Also, the modified electrode has demonstrated reasonable stability and reproducibility.

C 077

Electrochemical Patch for Continuous Chloride Monitoring and Sweat Rate Tracking

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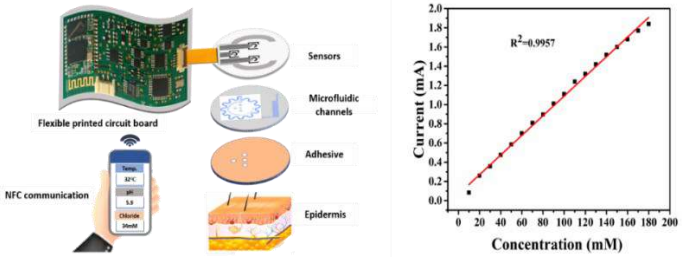
ABSTRACT

The advent of wearable sweat sensors has facilitated the continuous real-time monitoring of sweat compositions, enabling the tracking of electrolyte depletion and the quantification of electrolyte levels during physical activity or for individuals working in demanding conditions [1]. Meanwhile, the development of flexible electrochemical sensing devices, such as wristbands, headbands, patches, and tattoos, has progressed significantly [2]. In this work, a disposable, battery-free, flexible electrochemical patch has been developed for continuous chloride monitoring and sweat rate tracking. This patch is equipped with an NFC module, a temperature sensor, on-site signal processing circuitry featuring an analogue front end, and a sensor array. The chloride sensor comprises three screen-printed electrodes, which consist of a working electrode and an auxiliary electrode (both made of carbon paste), as well as an Ag/AgCl pseudo-reference electrode. The fabricated electrode was modified using silver and shows a linearity in the chloride concentration window, 0 – 180 mM. The modified screen-printed electrode (SPE) shows good sensitivity and no interference is shown. To boot, the sweat samples were prepared as per the standard used in Denmark, tested, and quantified the chloride ion levels. This affordable wearable platform can enhance the understanding of physiological aspects for athletes, healthcare professionals, and individuals operating in mobile settings.



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C 078

Indirect Conversion X-Ray Sensing Capabilities of $CsCu_2I_3$ Coated BPW-34 Photodiodes

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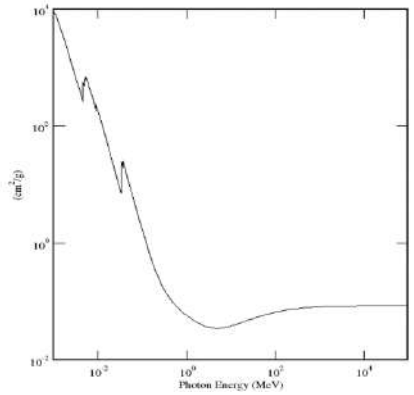
ABSTRACT

X-ray sensors play a central role across diverse fields, including medical imaging, security, research, and industrial applications[1]. The sensing of X-rays can be achieved through direct or in-direct conversion processes. Over the past decade, there has been a surge in research, focused on copper-based scintillators due to their impressive luminescent properties and cost-effectiveness[2]. In the present work, indirect conversion X-ray sensors was developed $CsCu_2I_3$ coated BPW-34 photodiodes with four different thickness of coatings. Diode current was measured under the illumination of X-rays using an intra-oral X-ray machine as source for X-rays, in order to explore the effect of thickness on the sensor developed. Prior to device fabrication, as-prepared $CsCu_2I_3$ was characterized using XRD, TEM, Raman, and FTIR analysis. The thickness of coatings was examined using SEM analysis. Since, attenuation is dependent on thickness of the coatings. The observed effect of thickness was explained with a possible mechanism to explain the insights on the design and performance of our X-ray sensor.



Energy dependent X-ray attenuating nature of $CsCu_2I_3$

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C 079

Integrated Electrode System for Printed Electrochemical Multiple Analytes Sensors for the Real-Time Monitoring of Toxic Heavy Metal Ions, Biomolecules, and Carcinogens

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ABSTRACT

The on-site monitoring of various analyte species in the diversity of fields by EC sensor requires considerable improvements in sensitivity, selectivity, and accuracy along with its inherently fast, compact, portable, and cost-effective properties. Herein, we are trying to meet the aforementioned needs by developing various nano-functional materials based on graphene quantum dots (GQD) and metal nanoclusters (MNC). These includes the preparation of different types of GQD and MNC-based materials, their characterization, developing modified electrodes using the prepared materials, studying their EC sensing properties, and examining the reasons/mechanisms behind the effective sensing behaviors. Thus, we successfully developed GQD and MNC-based materials and further explored the electrochemical sensing technique for detecting the toxic heavy metal ions in water bodies and biologically relevant molecules. Further, the studies were extended toward developing an integrated electrochemical screen-printed sensor electrode for real-time monitoring. Then, we are designing and developing novel ink materials for working, counter, and reference electrodes in the integrated electrochemical sensor for the selective and simultaneous sensing of the analytes. The studies will extend further to develop a multiple analytes sensor, simplifying the technology. The use of various templates such as paper, plastic-coated paper, and plastic materials for the sensor films must also be explored to get cost-effective and flexible sensors for versatile real-time applicability.

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C 080

Enhanced Detection of Hydrogen Peroxide Using Composite Electrospun Nanofibers

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ABSTRACT

Recent studies shows that over consumption of hydrogen peroxide (H_2O_2) has serious effect on the environment and humans. Electrospun nanofibers have large surface area and porosity, which enhances the sensitivity and rapidity for the detection of various chemicals. In this work, H_2O_2 is detected using electrospun polyvinyl alcohol (PVA) nanofibers embedded with gold nanoclusters (AuNCs). Though most reported sensors rely on immersion technique [1], here we adopt the method of incorporating AuNCs within the nanofibers. The prepared nanofibers showed wide emission in the red region (λ_{max}=645nm). The SPR band of gold was invisible, which can be attributed to the strong capping behaviour of BSA. The fluorescence quenching was observed with increase in concentration of H_2O_2, with an LOD of 230pM, which is higher than the reported literatures. This quenching happens because H_2O_2 interacts with BSA by proton-exchange, thus reduces its capping nature, which causes morphological change of gold from cluster form to nanoparticle form. This was further established using confocal microscopic images and thermogram plots. Thus, PVA-AuNCs nanofibers can be used as an excellent platform to replace the conventional sensing substrates.

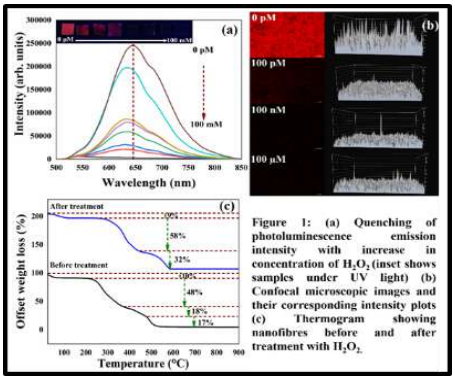

Figure 1: (a) Quenching of photoluminescence emission intensity with increase in concentration of H_2O_2 (inset shows samples under UV light) (b) Confocal microscopic images and their corresponding intensity plots (c) Thermogram showing nanofibres before and after treatment with H_2O_2.

Keywords: *Gold nanoclusters, electrospinning, photoluminescence, sensors.*

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C 081

Non-Enzymatic Wearable Patch for Continuous Glucose Monitoring

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ABSTRACT

Monitoring glucose levels in the body is crucial for the prevention and treatment of diabetes. Most of the sensors in the market rely on finger-prick blood samples and are enzymatic, limiting their use for non-invasive, continuous monitoring. In this work, we have developed a smart wearable continuous glucose sensing platform utilizing non-enzymatic sensing signal technology. The mainchallenge associated with non-enzymatic glucose sensing is to maintain an alkaline pH, which is achieved using a pH control electrode. The electronic circuit is developed on a flexible platform and houses a potentiostat to provide the necessary potential for the electrochemical reaction. The electrochemical sensors, along with a sweat handling patch will be integrated with the flexible electronics to develop the smart wearable system for the continuous non-enzymatic monitoring ofglucose in a non-invasive manner. The wearable also consists of an NFC chip, and printed super capacitor array, where the NFC chip harvests energy from a mobile phone and the power is stored in the super capacitor, to power the wearable patch as and when needed. The glucose measurementis taken at regular intervals and the results are when a mobile phone is nearby, the result is sharedto the mobile application.

C 082

Highly Efficient Fe_2O_4/ZnO@Ag Magnetic Nanocomposite Used Peroxidase Mimicking for Colorimetric Detection of H_2O_2 and Glucose

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ABSTRACT

The design and development of multifunctional ferrite nanomaterials with numerous components and features are in high demand for a range of more efficient biosensing platforms capable of performing several jobs in multiple nanosystem. We present a multifunctional biosensing device for sensitive colorimetric detection of H_2O_2 and glucose based on magnetic ferrite nanocomposites. Fe_3O_4/ZnO@Ag had enzyme mimicking inherent peroxidase-like catalytic activity. When compared to natural enzymes, magnetic composites could be employed across a wider pH and temperature range and were more stable over time. Importantly like activity through the catalytic oxidation of peroxidase substrate 3,3,5,5-tetramethylbenzidin (TMB) in the presence of H_2O_2 producing a blue-colored solution. On the basis of this colored-reaction, we have developed a simple, cheap, highly sensitive and selective colorimetric method for estimation of glucose using Fe_3O_4/ZnO@Ag.

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C 083

Thermoelectric Properties of Ag_2S/Ag_2Se Composite Growth on Carbon Fabric for Wearable Thermoelectric Application

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ABSTRACT

The wearable devices have been increasingly attractive in wearable electronics due to their advantages of environmental friendliness and foldability. Till date, the state-of-the-art thermoelectric depends on inorganic semiconductors that shows high electron mobility but lack in mechanical stability. Therefore, in this study we have done composite growth of Ag_2S/Ag_2Se on the carbon fabric and also we have studied its wearable thermoelectric properties. The crystallographic analysis was performed for all samples through XRD and confirmed the Orthorhombic Ag_2Se and mono-clinic Ag_2S. Further, the morphological analysis was performed to confirm the growth of Ag_2S/Ag_2Se on the carbon fabric, therefore from the FE-SEM the growth of the Ag_2S/Ag_2Se composite was confirmed and also the elemental mapping of all the samples showed even distribution of all the elements such as Ag, Se, S, C. Room temperature hall measurement has been taken for (25%, 50%, 75%) Ag_2S/Ag_2Se composite samples to investigate the electrical properties such as carrier concentration and mobility. The enhancement in the power factor was seen due to the enhancement in the electrical conductivity. The analysis shown that Ag_2S/ Ag_2Se composite offers promising wearable thermoelectric properties.

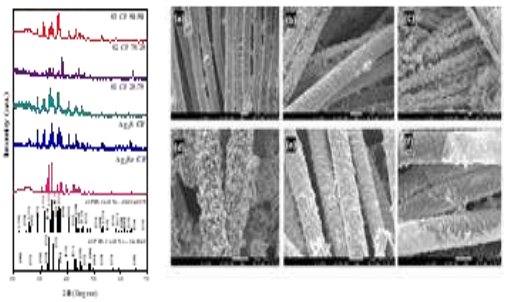

Fig .1 Shows XRD and FE-SEM of Ag_2S/Ag_2Se composite on carbon fabric

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C 084

Tailoring Zinc Stannate Morphology for Fabricating Highly Sensitive NO_2 Gas Sensor

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ABSTRACT

In recent times, there has been a noticeable rise in the number of toxic gases and their concentration [1], precipitating adverse impacts on both human well-being and the ecosystem which spurred the scientific community to develop gas sensors capable of detecting harmful gases. In this study, we explore the synthesis and gas-sensing capabilities of zinc stannate, an inverse spinel, in three distinct morphologies: spherical nanoparticles, nanoflowers, and octahedral-like structures. The fabricated devices, forming an ohmic contact with a gold electrode, exhibited a notable decrease in resistance upon exposure to nitrogen dioxide (NO_2) at room temperature, indicative of a p-type sensing material and a body-controlled type device. Among these morphologies, zinc stannate nanoparticles, particularly in a spherical configuration, demonstrated the highest sensor response of 66% to 5 ppm of NO_2 with a response and recovery times of 23 s and 83 s, attributed to their enhanced surface area. Notably, the nanoparticle-based sensor exhibited exceptional selectivity for NO_2 over gases like NH_3, SO_2, and CO. Furthermore, the sensor displayed a low detection limit of 450 ppb at room temperature, underscoring its high sensitivity. The reversible and stable response to NO_2 gas at room temperature underscores the potential efficacy of zinc stannate nanoparticles as sensitive and selective gas sensing material.

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C 085

Exploring a Cyanoquinoxaline 1,4-Dioxide Based System as a Fluorophore and Demonstration of its Wide-Ranging Applications

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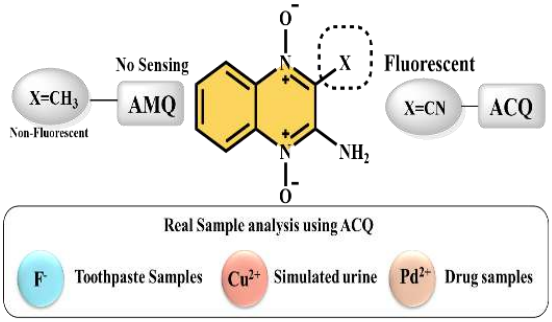
ABSTRACT

Use of small organic fluorophores in real sample analysis provide a versatile and effective means of studying a wide range of substances. In this study, the selection of a cyanoquinoxaline-1,4-dioxide-based molecule (ACQ), was primarily driven by its water solubility, easy synthesis and vibrant colour that lends itself well to visible light sensing. Initially, detailed photophysical analysis of 2-amino-3-cyanoquinoxaline 1,4-dioxide (ACQ) was carried out, followed by their exploration in the detection of various ions. It showed selective detection of cations Cu^{2+} and Pd^{2+} in aqueous environment, while the sensing of F^- was conducted in DMSO. Stern–Volmer plot analysis highlighted static quenching as the primary mechanism for detection of $Cu^{2+/+}$ and F^-. On the other hand, lifetime measurements indicated the coexistence of static and dynamic quenching during selective Pd^{2+} sensing. The stoichiometry for ACQ and ions binding was determined as 2 : 1 for Cu^{2+} and $Pd^{2+,}$ while a 1 : 1 ratio is observed for F^-. Limit of Detection (LOD) was obtained as 0.75 µM, 7.6 µM and 0.53 µM for Pd^{2+}, Cu^{2+} and F^- respectively. Our study was further extended for real sample analysis of Cu^{2+}, Pd^{2+} and F^- in simulated urine, drugs and commercially available toothpaste samples, respectively.



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C 086

Electrochemical Behaviour of Propyl Gallate at a Mercaptoacetic Acid Self Assembled Gold Electrode

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ABSTRACT

Electrochemical techniques are one of the widely used platforms for the determination of various compounds due to its short response time, simplicity in operation and possibility of miniaturization. Antioxidants are a group of food additives which play an important role in food industry. Among the various antioxidants, determination of the antioxidant Propyl gallate (PG) is important because excessive use of this can result in potential health problems [1]Gold is the substrate of choice because of its inert properties and its formation of well-defined crystal structures, which strongly influence the generation of self-assembled monolayers. [2] The greatest advantage of SAM is that the preparation of SAM in the laboratory is very easy and simple method. The current study, presents a SAM modified gold electrode for the selective and sensitive determination of propyl gallate. [3]

SAM based voltammetric sensor has been fabricated via cyclic voltammetry and electrochemical studies were conducted using SWV measurements. Mechanistic aspects were derived using LSV.A SAM based voltammetric sensor for the determination of antioxidant propyl gallate (PG) has been developed. The credibility and mechanistic aspects behind the processes have been investigated.

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C 087

Tailored Co_3O_4 Nanoparticle-Coated Optical Fibers for Enhanced Sialic Acid Sensing: An Application towards Cancer Detection

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ABSTRACT

Here, we have demonstrated an optical fibre sialic acid sensor-a biomarker for cancer detection. Flattened PMMA fiber coated with Co_3O_4 nanoparticles (NPs) of varied sizes i.e. of ~12nm, ~22nm and ~40nm are used as sensing probes. The Co_3O_4 nanoparticles were synthesized using a simple chemical route method and centrifuged to separate the product [1]. In order to collect the required Co_3O_4 nanoparticles of various sizes, the isolated products were first dried at ambient temperature and then calcined at various temperatures of 300°C, 700°C, and 1000°C for 4 hours. A detailed structural analysis demonstrates that the NPs are cubic phase-stabilized. The morphological investigation (HR-TEM) demonstrated that the nanoparticles exhibit a spherical shape and their size increases as the annealing temperature increases. Raman and Fourier-transform infrared spectroscopy **(**FTIR) Spectroscopy are also used to characterise the properties of the synthesised nanoparticles. The sensing probes (F-300, F-700 and F-1000) are connected to the optical setup for the sensing application. For all the fiber configuration the sensor showed a dynamic linear range of sialic acid concentration from 5 – 30 mg/dL. The limit of detection for the fibers F-300, F-700 and F-1000 are found to be 3.77mg/dL, 8.25mg/dL and 11.87mg/dL with sensitivities 1.59 µA/mg/dL, 0.60 µA/mg/dL and 0.34 µA/mg/dL respectively. Finally, we used COMSOLE multiphysics simulation to comprehend the sensing mechanism of this designed sensor. The advantage of this sensor-device is the sensing response time reflected to be within a few-seconds. Patients with adrenal cancer had lipid-bound sialic acid concentrations of 119.5 mg/dL, while those with endometrial cancer have serum sialic acid concentrations of 78.1 mg/dL [2]. The observed LoD values are much less than the stated concentration of sialic acid in cancer patients and hence can be used as sensor for the detection of the cancer.

Keywords: *Optical fiber, sialic acid sensor-device, Co_3O_4 nanoparticles.*

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C 088

ZnO/B-g-C_3N_4 Nanoplatelet/Nanosheet Heterostructures for the Electrochemical Detection of Metol in Real Sample Analysis

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ABSTRACT

One of the most important organic molecules is metol [4-(methylamino)phenol sulfate], which finds extensive usage in various applications as a monochromatic material. People, plants, and animals are all affected by it, and it raises serious environmental concerns (1). Developing a straightforward, quick, affordable, sensitive, and hands-on technique for metol determination in water bodies is of the utmost importance in the current scenario (2). A low-cost fabrication strategy is presented in this work for the synthesis of a zinc oxide nanoplatelet (ZnO) embedded into boron-doped carbon nitride nanosheetmaterials (ZnO/2D-BCN) utilizing a high-performance electrochemical sensor. The quantitative and qualitative information about the nanostructure of ZnO/2D-BCN were systematically analyzed further by using standard spectroscopic techniques such as XPS, XRD, FT-IR, EDAX, and Raman spectroscopy. 2D-nonstructural was observed to have a nanoplatelet/nanosheet through FE-SEM and TEM. Electrochemical sensors' performance was analyzed by using cyclic and differential pulsed voltammetry techniques. The fabricated ZnO/2D-BCN has peculiar intrinsic structural features, both connectivity and characteristic synergistic effect of B-dopants 2D-structure, which perturb mass transport with highly efficient electrochemical pathways. In addition, the electrochemical sensors of metol and its electrocatalytic mechanism were scrutinized further, which confirmed a fast electron transfer event. The as-prepared ZnO/2D-BCN exposed superior sensing conclusion through LOD (8.6 nM) in a wide-ranging linear 0.039−1617 (μM) as well as a remarkable sensitivity of 0.804 μA μM^{-1} cm^{-2}. Additionally, other sensing parameters such as remarkable repeatability, electrodes' reproducibility, materials' stability, and a remarkable selectivity toward metol have been performed. Furthermore, the practical feasibility of as- made ZnO/2D-BCN/GCE has been inspected with biological and environment samples such as blood serum, human urine, river, pond, industry, and tap samples as a real sample, revealing excellent rational recovery outcomes.

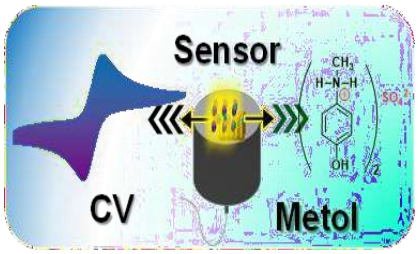

Figure: Diagrammatic sketch of the electrochemical sensors Metol

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C 089

Smart Gloves for Gesture Based Communication with Versatile AI Technology

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ABSTRACT

In India, a significant challenge looms large as approximately 63 million individuals in the mute community struggle to effectively communicate with those outside their immediate social circles due to the limited prevalence of sign language knowledge. The primary concern stems from the scarcity of accessible products that can empower completely mute individuals to engage, communicate, and lead fulfilling lives. Additionally, a secondary issue arises in the absence of efficient communication tools between caregivers and the device users, making it challenging to share crucial information like location or daily activity updates when necessary. Moreover, the dearth of affordable solutions exacerbates the situation, rendering the few available products prohibitively expensive for many in this community. Addressing these multifaceted challenges requires innovative and cost-effective solutions that can bridge the communication gap and enhance the quality of life for the deaf and mute population in India. The smart gloves are equipped with speakers in the right hand glove to signal different sentences and in the left hand glove to signal to access artificial intelligence through glove while also monitoring the wearer's pulse for distress, automatically sending location-based emergency messages to caretakers and nearby individuals if the pulse exceeds or falls below the threshold. Furthermore, it enable users to send messages to caretakers, and activate lights in dark environments for enhanced visibility.

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C 090

Chemiresistive SnS_2/SnO_2 Heterostructures for Enhanced Room Temperature NO_2 Gas Sensor

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ABSTRACT

The current work investigates the sensing behavior of the SnS_2/SnO_2 nanocomposite for NO_2 detection at room temperature. The SnS_2 and SnS_2/SnO_2 nanocomposites was successfully synthesized via the solvothermal method. The morphological analysis confirms the formation of SnO_2 nanoparticle-like structure deposited on the SnS2 flower-like structure. The compositional analysis confirms the interaction between the SnS_2 and SnO_2. The selectivity results reveals that the fabricated sensor showed peculiar selectivity towards NO2 gas molecules. The impact of the SnS2 flower-like structure coupled with the SnO_2 particles (SnS_2/20 wt.% SnO_2) enhanced the rapid response time of 135 s towards 2 ppm of NO_2 gas molecules. The proposed gas sensing mechanism explains the synergy of electronic and geometric effects along with the formation of heterojunctions. The fabricated sensor showed 348.37% of enhanced sensing response over pristine SnS_2 with 96% of stability. These results certify that this could be an effective technique to increase the utility of the SnS_2 as a room-temperature gas sensor.

Keywords: *SnS_2/SnO_2; hierarchical architecture; nanoparticle; NO_2 gas*

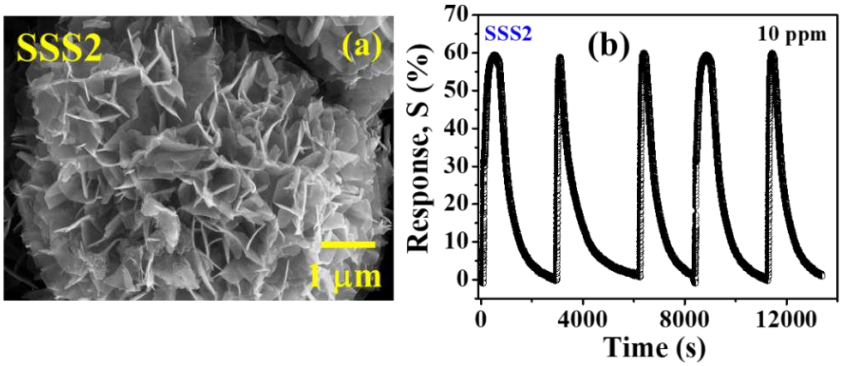

Figure: (a) HRSEM image of SnS_2/20 wt.% of SnO_2 (b) Repeatability of SnS_2/20 wt.% of SnO_2 sample towards 10 ppm of NO_2.

C 091

Recent Advances in Carbon Nanomaterials-Based Electrochemical Sensors and Biosensors

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ABSTRACT

In this presentation, we will focus on the electrochemical behavior and electroanalytical applications of laser-scribed graphene electrodes, as well as screen-printed electrodes modified through microwave-assisted functionalization of carbon nanofibers and various types of carbon blacks. Noteworthy advancements, such as the non-enzymatic oxidation of glucose, nanomolar detection of dopamine, and a negative shift in the oxidation peak of electroactive molecules, characterize these electrodes, setting them apart from conventional methodologies.

The structural and morphological characterization of sensors based on various carbon nanomaterials, employing techniques such as Raman spectroscopy, transmission electron microscopy (TEM), and scanning electron microscopy (SEM), will be elucidated. The increasing prominence of these carbon nanomaterials can be attributed to their superior performance, including a decrease in applied potential or peak-to-peak separation, improved peak intensity, and reduced resistance in electron transfer. Key features contributing to their success include nanostructure, low electron transfer resistance, a high number of defect sites, stability, tunable properties, and cost-effectiveness.

This presentation will also provide a brief overview of our latest work on the design, preparation, and electrochemical sensing applications of these carbon nanomaterials. Furthermore, challenges and future perspectives in this field will be outlined and discussed.

C 092

$C_3H_7NH_3PbI_3$@PVDF Porous Piezo-active film: A Wearable Potential Bio-Sensor

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ABSTRACT

Recently, sustainable energy sources have become top most concern worldwide to meet the huge requirement of power. At similar time frame, micro-sensors especially wearable biosensors, environment monitoring, space monitoring sensors, etc. are potentially used in our day-to-day life.[1] Therefore, harvesting low power in large scale unit is also important as the demand of low-powered based sensors is huge in every corner of daily life. Piezoelectric energy harvesting can serve the requirement of low yet regular power harvesting by scavenging mechanical energy from surroundings.[2] The inclusion of the sol-gel derived Propylammonium lead iodide[3], (C3H7NH3PbI3) in polyvinylidene difluoride (PVDF) induces significant enhancement of the ferroelectric phase content i.e β phase (~66.7 %) of the film. This composite was employed in the fabrication of piezoelectric energy harvester (PEH) that generates ~ 80 V open circuit voltage (VOC) and 17.8 μA/cm2 short circuit current (JSC) under hammering with free hand and the obtained outcome is substantially large compared to that of a PEH made of neat PVDF. The flexibility of PEH provides an added advantage for the film to be used as wearable bio-sensor. Moreover, the photo-active piezo response of the photodetector made of the aforesaid composite is remarkable enough to serve as a photo-detector.

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C 093

Investigation on III-Nitride Semiconductors Based Methane Gas Sensing at Room Temperature

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ABSTRACT

Methane (CH4) is one of the greenhouse gases and second highest contributor to global warming. It is a colorless, odorless and flammable gas, an explosive in the concentration range of 4.9 - 15.4 vol%. Therefore, it is important to monitor and control the exposure of CH4 in the atmosphere. Besides developing real time and reliable CH4 gas sensor is inevitable [1, 2]. III- Nitride semiconductors are thermally stable and chemically inert when compared to metal oxides [3]. In this work, Aluminum Nitride (AlN), Gallium nitride (GaN) and Aluminum Gallium Nitride (AlGaN) alloy were prepared for CH4 gas sensing at room temperature. The AlN, GaN and AlGaN were successfully prepared by chemical vapor deposition (CVD) method. The XRD pattern reveals that synthesized AlN, GaN and AlGaN has a Hexagonal structure, the average crystallite size was found to be around 4-6 nm. In case of AlGaN alloy there was a shift in the XRD peak to the higher angle, which can be attributed to Aluminum (Al) substitution in GaN crystal lattice. The SEM- EDAX spectrum also confirms the incorporation of Al. The band gap of pure AlN, GaN and AlGaN was calculated from UV-Visible spectra and it was found to be 6.2, 3.41 eV and 3.80 eV, respectively. These synthesized materials were coated on interdigitated electrodes (IDE) to study the sensing parameters at room temperature. The sensing response for AlGaN alloy was found to be more than 80% when compare to AlN and GaN which exhibit less than 40% response for 15000 ppm CH4 gas.

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C 094

Silver Nanoparticles Impregnated rGO-Wedged CNT Nanocomposite for Electrochemical Detection of Etilefrine Drug

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ABSTRACT

Etilefrine (ET), 2-ethylamino-1-(3'-hydroxyphenyl)ethanol hydrochloride, is an α- and β-adrenergic sympathomimetic drug often used as a cardiac stimulant, and it improves heart rate and vein wall tension. Therefore, ET is increasingly used as a stimulant by some athletes practicing endurance sports, and the World Anti-Doping Agency included ET in the list of prohibited stimulant drugs. In this study, an electrochemical biosensor for the detection of ET at trace levels from physiological fluids has been designed using nanoAg (nAg) impregnated reduced graphene oxide (rGO)-wedged multi-walled carbon nanotube (CNT) composite. A simple one-pot synthesis approach has been employed to synthesize the composite from CNT, GO and silver nitrate with the use of a green reducing agent, L-ascorbic acid. Extent of nanoAg in the composite was optimized in the range of 2.5 to 15.0 wt%, and 5.0 wt% Ag was found optimum for electrochemical sensing of ET. The as-synthesized composite, nAg-rGO-CNT, was drop-casted on glassy carbon electrode with Nafion binder to fabricate the electrodes. Cyclic voltammograms (CVs) of 10 µM ET in aq. 0.1 M PBS (pH 7.0) recorded at different scan rates (10 – 110 mV/s) have shown an irreversible oxidation peak at ~0.7 V vs. Ag/AgCl (Fig. 1A). Differential pulse voltammograms were recorded at different trace concentrations of ET, 0.117 to 7.5 µM, and a very prominent intense peak was observed at the concentration of as low as 0.117 µM ET (Fig. 1B). From the plot of differential peak current vs ET concentration, the low-detection-limit of ET was determined to be 0.010 µM ET. The stability, selectivity and trace level analysis in physiological fluids of the fabricated electrode for efficient electrochemical sensing of ET would be established.

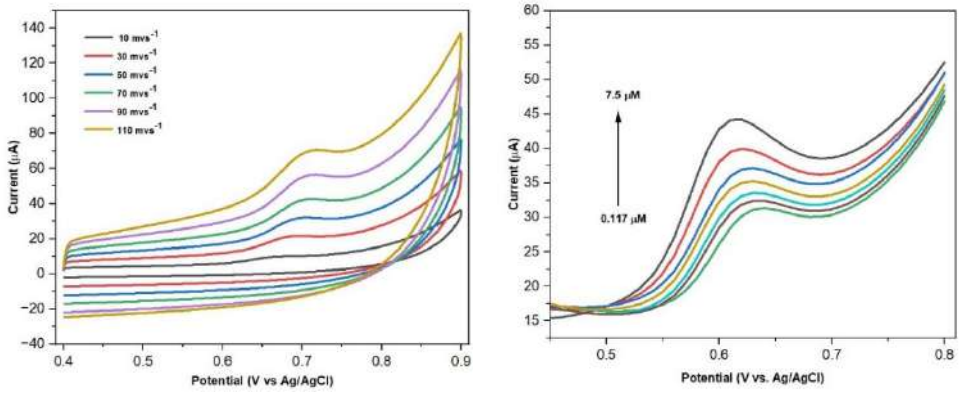

Figure 1. (A) CVs of 10 µM ET (scan rate = 10 to 110 mV/s) and (B) DPVs of 0.117 to 7.5 µM ET at nAg-rGO-CNT/GCE in aq. 0.1 M PBS (pH 7.0).

C 095

Impact of Bismuth Doping on Hexagonal Nickel Oxide Nanoporous Plates for Room Temperature Gas Sensing Applications

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ABSTRACT

Nickel Oxide (NiO) has shown great attention in the field of gas sensors because of its chemical stability, strong oxidizing property and excellent catalytic activity. Herein, we report the influence of bismuth (Bi) doping on the hexagonal NiO nanoporous plates to examine their gas sensing properties at room temperature (RT). The pristine and Bi-doped NiO were successfully synthesised through hydrothermal method. The prepared sensing materials were subjected to diverse characterization techniques to assess their structural, morphological, chemical states, and surface area properties. The gas sensing performance of a sensor utilizing both pristine and Bi-doped NiO were systematically investigated. The hexagonal nanoporous structure of NiO contributes to an augmented gas adsorption capacity by offering a greater number of active sites for interaction with the target gas.

Keywords: *doping; nanoporous; response; gas sensor*.

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C 096

Trace Level Electrochemical Analysis of Arsenic(III) in Real-Time Samples Using an Unmodified GCE

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ABSTRACT

Arsenic contamination has grown drastically on a global scale in the past decade and its contamination in groundwater, above the World Health Organization's recommended maximum allowable limit of 10 parts per billion, is thought to afflict approximately 108 countries. Due to the significant health risk of As(III) poisoning from drinking contaminated water, robust and reliable sensors are of importance since drinking contaminated water poses a serious health risk for As(III) poisoning. This study focused on increasing the sensitivity of the glassy carbon electrode (GCE) by optimizing the other factors and establishing a favourable environment for the electrochemical detection of As(III), after examining all the limiting factors that emerged from the process of enhancing the sensitivity of GCE by modifying its surface. Optimization of deposition potential, time, pH resulted in achieving lower limit of detection(LOD), explained by Fig.1. LOD is found to be around 0.84 ppb, lower than the permissible limits set by W.H.O i.e. 10 ppb. Subsequently, this study was employed to identify As(III) in water in real time, a result that ICP-MS verified.

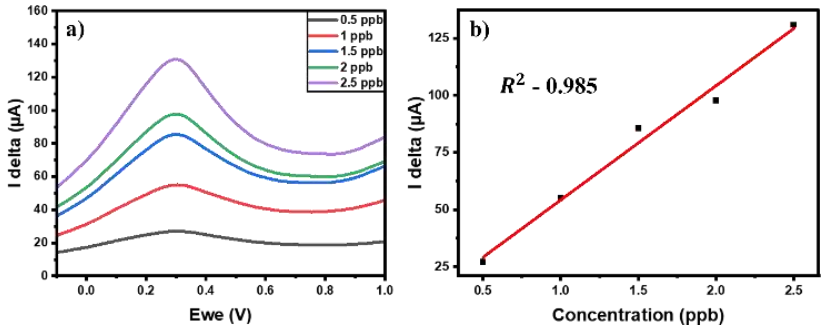

Fig.1. a) Square Wave Voltammograms b) Calibration plot of As(III) at different concentrations

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C 097

Sensitive and Selective Impedimetric Detection of E. coli using Bacteriophage-Immobilized Gold Electrode

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ABSTRACT

A simple yet effective electrochemical sensor has been designed for the detection of E. coli ST155 strain using AuNP/bacteriophage modified gold electrode. The simple surface modification has allowed seamless translation of the developed sensor into a disposable point-of-care device using screen-printed gold electrodes. Two differently charged AuNPs were synthesized using different capping agents, such as cysteamine and sodium citrate, and named Cys-AuNP and Cit-AuNP, respectively. An increased peak current was observed after the immobilization of AuNPs on the gold electrode irrespective of their surface charges owing to the highly conductive nature of AuNPs. However, changes were observed in the binding of bacteriophage over both surfaces through EIS studies. A better binding of bacteriophage was observed for the Cit-AuNP-modified gold electrode. These observations suggest that the bacteriophage may be positively charged and hence tends to have an affinity towards the negatively charged Cit-AuNP surface. Further studies confirmed that the Cit-AuNP-modified gold surface has a higher increase in the RCT after adding bacteria. This developed biosensor sensitively detects the E. coli ST155 strain with a detection limit of 104 cfu mL-1 in 2 µL of the sample. The specificity of the developed sensor was tested using three other bacteria, such as Pseudomonas aeruginosa, Proteus vulgaris, and Enterococcus faecalis. In addition, the same approach on gold screen-printed electrodes shows a detection limit of 102 cfu mL-1 in 5 µL of the sample. The versatility of the technology allows it to adapt to detect various organisms by selecting bacteriophages suitable for capturing the targeted bacteria.

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C 098

Enhancing Piezoelectric Properties of PVDF Polymer-Based Membrane Through Integration of ZnO Nanorods for Flexible Sensing Devices

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ABSTRACT

The utilization of PVDF in flexible sensors underscores its pivotal role in enabling lightweight and conformable devices for diverse applications, ranging from healthcare to structural health monitoring. This study focuses on the synthesis and fabrication of a piezoelectric PVDF polymer-based membrane, incorporating ZnO nanorods to enhance its piezoelectric properties. ZnO nanorods, with an approximate diameter of 100nm, were synthesized using a surfactant-assisted hydrothermal method. Four different weight fractions of ZnO (0%, 1%, 5%, 10%) were integrated into the PVDF matrix to investigate their influence on the piezoelectric behavior. The crystallinity of the PVDF/ZnO composite polymer membrane was analyzed through XRD and FTIR characterizations. Piezoelectric and dielectric studies revealed an enhanced polarization behavior in the PVDF/ZnO membrane with the addition of ZnO nanorods. The results suggest that the PVDF/ZnO polymer membrane holds significant potential for applications in flexible sensing devices.

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C 099

Electrochemical Incorporation of PVA-ZnO Nanocomposite on Screen Printed Carbon Electrode as Dopamine Sensor

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ABSTRACT

In the current study, a zinc oxide (ZnO) and polyvinyl alcohol (PVA) screen-printed carbon electrode (SPCE) nanocomposite (SPCE/PVA/ZnO/DA biosensor) was utilised to create an improved electrochemical dopamine (DA) sensor. Several factors influenced the choice of PVA for the biosensor. These factors include its solubility in water, its capability to enhance electrical conductivity, its potential to provide the biosensor surface with increased electronic density due to the presence of free -OH groups. These groups function as a protective layer, repelling anionic interferents present in the biological medium. Additionally, the ability to control the PVA content in the electrodeposition bath enables the regulation of ZnO growth and crystallization. The SPCE/PVA/ZnO sensor that was developed was examined using FE-SEM and EDX. With a low detection limit of 25.0 µM, the wide linear range from 25.0 µM to 1000µM was used for the voltammetric determination of dopamine. SPCE/PVA/ZnO has shown satisfactory performance in evaluating dopamine within real-world samples. The use of PVA/ZnO presents itself as a suitable material for crafting electrochemical sensing devices tailored for dopamine detection.

C 100

2D Inorganic $CsPbBr_3$ Perovskite for Effective Optical Gas Sensing of NH_3

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ABSTRACT

Recent years have seen an immense rise in the interest of 2D perovskite nanomaterials due to their exotic optical properties. Therefore, it has attracted a significant attention in the field of optical gas sensing. Here, we synthesized two-dimensional $CsPbBr_3$ perovskite nanomaterial and examined its optical characteristics. In particular, it exhibits highly intense green emission (494 nm) excited at a wavelength of 402 nm. The optical band gap of synthesised 2D $CsPbBr_3$ perovskite nanomaterial is determined to be 2.64 eV calculated from the Tauc plot. A direct spin coating preparation of a $CsPbBr_3$ thin film was used to create an efficient ammonia sensor. Our optical sensor device based on 2D- $CsPbBr_3$ has demonstrated high selectivity towards ammonia gas with an indication of a direct correlation between the amount of ammonia and emission intensity at ambient temperature. Our First principles simulations support these experimental findings and provide further insights into the adsorption of ammonia molecules on the surface of 2D-$CsPbBr_3$.

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Study of Growth Method Influence on the Performance of the Vibration Sensor

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ABSTRACT

ZnO nanorods are grown vertically on FTO substrates (H) using hydrothermal method and the ZnO nanorod powder is deposited on FTO substrate (P) using doctor blade method. The PEDOT: PSS is further spin-coated on the ZnO layers for both H and P device to form p-n junction. The XRD pattern of both the devices shows wurtzite hexagonal phase of ZnO. The H sample reveals its unidirectional 1-d nanostructure through the intense diffraction peak of (002) plane. The FESEM images confirms the growth of nanorod morphology. Optical properties were investigated for bandgap analysis. The photoconductivity study confirms the formation of p-n junction. This also showed the better transporting properties of the charge carriers of H than P device. The vibrational experimental analysis reveals the better performance of H device than P.

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Fabrication of Disposable Screen-Printed Electrochemical Sensor Based on Chitosan Based Conductive Ink for Arsenic Heavy Metal Ion Detection

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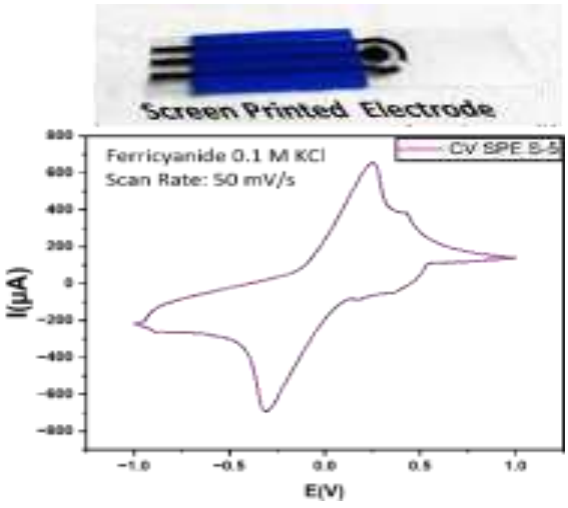
ABSTRACT

Heavy metal contamination was a serious concern in several parts of the world because of its significant health risks when ingested into human body either directly or indirectly through food chain. The present work involves developing an electrochemical sensor for arsenic heavy metal detection. This work outlines a sustainable and optimized approach for fabricating screen-printed electrodes using Polyethylene Terephthalate (PET) recyclable plastic as the non-conductive substrate and a formulated chitosan-based conductive ink. The low-cost and biodegradable chitosan, derived from shrimp shell waste, was used as binder which was dissolved in diluted acetic acid to create dispersions with varying weight/volume ratios. The graphite and laser ablated multilayer graphene was used as conductive material. The ink's electrochemical performance is evaluated through cyclic voltammetry after each preparation, allowing for a comprehensive understanding of its behaviour. The screen-printing process utilizes a stencil mask, involving design in software, creation with a vinyl cutter plotter machine, application on the PET substrate, and subsequent drying in a vacuum oven. This eco-friendly and efficient fabrication process demonstrates promise for applications in detection of heavy metals. This work contributes to sustainable electrode manufacturing methodologies with potential implications in the field of wastewater treatment technology.



C 103

ZnO-rGO Nanocomposite Coated Twisted Fiber Optic Sensor for Uric Acid Detection

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ABSTRACT

An increased level of uric acid (UA)in human blood serum can cause critical health issues like gout disease; hence its detection becomes very crucial. In the present work, an interferometry-based low-cost fiber optic biosensor for the detection of UA is proposed. The middle portion of the developed fiber sensor is flattened and twisted (single, double and multiple times) using our home-made arrangements and then coated with ZnO-rGO nanocomposite layer. The nanocomposite is characterised by using X-ray diffraction (XRD), Scanning electron microscopy (SEM), UV absorption spectroscopy (UV) and Photoluminescence spectroscopy (PL) techniques. It is found that the sensor is more sensitive when it is both flattened and twisted for one or two times, but when it is twisted for more than two times, the transmission at the output drops to almost zero. The proposed biosensor shows a limit of detection of 1.6 mg/dl which is less than the normal range of UA in blood (2 mg/dl to 8.5 mg/dl), and sensitivity of 11.76 nW/(mg/dl). The sensor also exhibits a linear behaviour in the concentration range from 2 mg/dl to 10 mg/dl with a regression coefficient of 98%.

Fig 1: SEM image of flattened and twisted fiber

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C 104

Flexible Reversible Thermochromic Membrane based on Europium doped Strontium Aluminate Materials for Temperature Sensing Applications

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ABSTRACT

In this work, flexible, reversible thermochromic membranes were created using a europium doped strontium aluminate ($SrAl_2O_4.Eu^{+2}$, Dy^{+3}) material. These membranes showed excellent thermochromic performance along with a remarkable heat storage capacity. In this composite membrane, the polymer matrix material was a polyvinyl alcohol (PVA)/water-soluble polyvinylpyrolidine (PVP) composite, whereas the functional fillers were strontium aluminate europium doped ($SrAl_2O_4.Eu^{+2}$, Dy^{+3}) materials. By using a thermogravimetric analyzer (TGA), differential scanning calorimeter (DSC), field-emission scanning electron microscope (FE-SEM) the thermal stability was experimentally examined. Moreover, the effects of $SrAl_2O_4.Eu^{+2}$, Dy^{+3} contents on the thermochromic performance, thermal property, and durability was also examined. The results showed that matrix membranes had a balanced distribution of $SrAl_2O_4.Eu^{+2}$, Dy^{+3}. However, the fabricated flexible thermochromic membranes could change color in response to variations in the outside temperature, they demonstrated perfect thermochromic capability. As the concentration of $SrAl_2O_4.Eu^{+2}$, Dy^{+3}, increased, the thermal stability and mechanical performance of the membranes declined. Water resistance increased dramatically, according to study on static water contact angles (WCAs). An intuitive temperature colorimeter was developed with the aid of a flexible thermochromic membrane that possesses the capacity to control temperature and retain heat. It is possible that this temperature sensor will be worn on the body. Thus, there is a lot of promise for the future use of the produced thermochromic membrane in thermal regulation, energy storage, early breast cancer diagnosis, and wearable temperature sensors

Keywords: Flexible reversible thermochromic membrane, Temperature-sensitive, Thermal and energy storage, Early breast cancer

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Highly Responsive Detection of NO_2 at Low Operating Temperature via Al-Modified MoO_3 Nanorods

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ABSTRACT

Molybdenum trioxide (MoO_3) is a recently emerging n-type, 2D-layered material with stable orthorhombic phase. The unique atomic arrangement of MoO_6 octa-hedral units combined by edge and corner sharing leads to layers via covalent interaction and Van der Walls interaction. In addition, the direct band gap ≈ 3.3 eV and unique chemical, electrical and optical properties gathers focus towards utilization of MoO_3 in various applications. Particularly, MoO3 gains immense attention in gas sensing owing to its stability, and high sensitivity. However, the high operating temperature limits the exploitation of MoO_3 based gas sensors. Therefore, in this work we have implemented a facile strategy of incorporating Al in MoO_3 and attained higher response of 1500% for 10 ppm NO_2 at low operating temperature of 170 °C. The Al incorporation has led to 10 folds enhancement in response as well as reduction in the operating temperature which is mainly attributed to the defects and oxygen vacancy generated in the MoO_3 nanorods. Thus, the obtained results suggest feasibility of the fabricated sensors for low temperature NO_2 detection.

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C 106

Advancements in Microcantilever Technology: Fabrication and Characterization for Biosensing Applications

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ABSTRACT

The paper describes the development of a biosensor using a micro-cantilever array chip designed with MEMS (Micro-Electro-Mechanical Systems) technology. The device consists of four layers: polysilicon coated with gold, which serves as a piezoresistor. This design enables the detection of quantifiable deformation in response to applied tensile and compression forces. The range of resistance detection spans from 0 to 85 K ohms. Experimental analysis revealed that the maximum change in resistance occurred when the concentration of biotin adsorption exceeded 90 µg/mL. However, the device was still able to detect resistance changes at lower concentrations as well. Based on these findings, it was concluded that the device is suitable for use as a Biosensor. This biosensor offers potential applications in various fields such as medical diagnostics, environmental monitoring, and biochemical analysis, where sensitive detection of biomolecules is crucial.

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C 107

Enhancement of Acetaldehyde Detection on Doping Pristine WO_3 Thin Films with Gallium by Spray Pyrolysis

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ABSTRACT

Pure WO_3 and gallium doped thin film for gas sensing were deposited by a direct, one step process. The deposited films were characterized for optical, structural, morphological and gas sensing studies. The orthorhombic phase of WO_3 and gallium doped WO_3 films were highly crystalline. The Ga doped samples have high surface roughness and grain size than the pristine WO_3, contribution to the increase of the adsorption of gas molecules. Doping gallium results in an increase in donor carrier density, which signifies a red shift due to the decrease in the band gap. FE-SEM analysis reveals that filamentous structured porous thin films exhibit larger pores, facilitating increased adsorption of gas molecules. A novel sensing response of 98.09 % was obtained at room temperature for Acetaldehyde gas by 0.075 % gallium doped WO_3 thin film.

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C 108

Single and Mixed phase Co_2SnO_4 Thin Films Gas Sensing Performance Toward Volatile Organic Compounds at Room Temperature

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ABSTRACT

Revolutionized modern industries evolved to develop tremendous potential chemi - resistive gas sensors to safeguard human health, food spoilage, and air quality. Binary metal oxide semiconductors play a pivotal role in chemi-resistive gas sensors as a sensing layer, but they are failed to compete in real-time flexibilities such as cross-selectivity, lower operating temperature, and limit of detection. To overcome all these hindrances, ternary metal oxide spinel as a sensing layer has gained enticing attention due to its high thermal stability, dual cationic nature, superior physiochemical behavior, etc. In this work, we have deposited cubic spinel Co_2SnO_4 and SnO_2/Co_2SnO_4 thin films via the facile chemical spray pyrolysis method. Deposited films were scrutinized by Powder X-ray diffraction, UV-Vis Spectroscopy, Atomic force microscopy, Water contact angle measurement, Morphological study, and Gas sensing performances. Higher defect rate, a narrowed bandgap, higher surface roughness, hydrophilic nature, and smaller nano-grain morphology facilitate more target gas molecule diffusion on the Co_2SnO_4 film surface. Among various volatile organic compounds, dimethylamine has higher electron cloud density in nitrogen atoms, lower bond strength (308 kj mol^{-1}), and rapid degradation ability of Co^{2+} in tetrahedral site on cubic spinel Co_2SnO_4 thin film results to achieve high sensor response ($S = I_{gas}/I_{air} = 640$ @ 1 ppm) at room temperature.

C 109

Modelling and Optimization of MEMS based Piezoresistive Biosensor

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ABSTRACT

The proposed work utilizes the sensing mechanism that can detect biological quantity by using deformation and subsequent compatible output for read-on-chip devices. More specifically, a change in the surface stress due to the immobilisation of the target analyte molecules, which causes the cantilever to deflect; & will enable measurement of strain in the form of a change in resistance between two conducting points at the base of the cantilever with respect of stress-concentrated region (SCR) concept of punching into piezoresistive cantilever.

This paper is focused on the design aspects of microresonators with different shapes and microcantilevers; A piezoresistor connects both resonator and cantilever; subsequently takes the binding load and transduces as an electrical signal. Optimization of dimensions, selection of materials and input parameters are thoroughly modelled to realize the ultra-fast sensitivity and read-on chip compatibility of piezoresistive biosensors. The biological quantity concentration is measured by converting it into voltage through the implementation of piezoresistor-based cantilevers arranged in a Wheatstone bridge configuration. COMSOL Multiphysics Software tool v 5.2 is used to carry out this modelling and simulation studies. For the current investigation, piezoresistive microcantilever of dimensions; length: 100-150µm, diameter: 10-50µm, thickness: 1-5µm, for the materials of SiC, SiO2 has been modelled against the applied load ranging from 50N to 200N. Based on simulation results, it is found that SiC added piezoresistive cantilever has the highest sensitivity of range 8-12 mV/mg. Furthermore, the piezoresistive microcantilever with stress-concentrated regions (SCR) of circle is found to exhibit higher sensitivity of 6mV/mg in comparison with SCR's of triangle, square. The optimised dimensions of the cantilever and selective materials exhibiting high sensitivity are explored for real-time biosensor development applications involving DNA. Proteins, various viruses etc. These microcantilevers will provide label-free sensing of biomolecules which is a direct & faster way of biological detection than non-label-free sensors.

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Piezoelectric PVDF Polymer for Sensor Applications

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ABSTRACT

Wearable sensors are a kind of sensors which can be attached to human body directly and via clothes to monitor the human physiological movements and to recover some intensive disease [1, 2]. Among different types of wearable sensors, self-powered sensors attracted because they can function without external power sources and piezoelectric sensors are a type of self-powered sensor [3].Piezoelectricity is a phenomenon in which the electricity is produced by applying mechanical force (Pressure or stress) and vice versa. Out of many piezoelectric polymers, Polyvinylidene fluoride (PVDF) and its copolymers are the most important semicrystalline piezoelectric polymer due to their mechanical stability and bio compatibility which plays key role for wearable sensor applications.Piezoelectric PVDF has four crystalline phases α, β, γ, δ which depends on crystallisation condition. Among these phases, polar β phase exhibit piezoelectricity due to its non centrosymmetric crystal structure [2]. Piezoelectric PVDF wearable sensor having advantages like light weight, air permeability, good functionality and durability. Some applications of PVDF piezoelectric wearable sensors are nasal sensor for identification of respiratory rate, belt shaped sensors to monitor cardiorespiratory signals [4].

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C 111

Advances in 2D Nanomaterials for High-Performance Photodetectors

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ABSTRACT

Light and its interaction with things around us is a fundamental part, not only small particles but also for complex systems as well. Most of the complex creatures around us are equipped with a pair of photodetector arrays connected to nervous system helping them to navigate the world and process information acquired around them which is limited to very narrow range of the available spectrum. Photodetectors are becoming increasingly significant in our daily life because of the rapid development in electronic and information technologies. Basically a photodetector absorbs photons of particular frequency causing a change in its electrical conductivity. An array of such photodetectors can be created with accompanying electronics to create an image sensor which is better suited for human processing. Photodetectors can be designed in variety of ways. One of the ways is by using 2D nanomaterials which leads to a very small, efficient and broadband photodetector. In 2004, the advent of graphene sparked a wave of research on 2D materials. Graphene and graphene-like 2D layered materials such as black phosphorus, transition-metal dichalcogenides, oxides, chalcogenides, and so forth have attracted tremendous attention due to their unique crystal structures, physical and optical properties. But graphene has zero band gap and low absorbance lead to low switching ratio and short carrier life time which limits its application in optoelectronic devices. Objective of the work is to investigate the promising 2D materials for photodetection and to find a way to improve their usability in commercial applications. The process of mastering the art of fabricating nanoscale flexible photodetectors and hopefully to come up with small, faster, efficient commercially usable products to complement the demand surge in medical, military, communications and biotechnology. It would also be interesting to study Mxenes for photo detecting, which can show responsivity 1200 times higher than graphene, good conductivity, hydrophilicity, and large specific surface area.

Keywords: *Mxene, Photodetector,*

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Remote Asthma Patient Health Monitoring System by Using IOT Technology

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ABSTRACT:

In this project, we developed an improved asthma patient tracking system that continuously tracks patient health data via the Internet of Things. An ESP32 microcontroller served as the system's main component. To gather patient data, we also integrated sensors into the system, including the MQ-135 air quality sensor, the DHT11 sensor, the MAX30100 pulse sensor, the heart rate sensor, and the LM- 35 temperature sensor. The collected information is easily transferred to the web app dashboard via Wi- Fi. Patients can check their data via the dashboard and send the data report straight to their doctor's profile. The doctor can review the patient's report and use it as the basis for prescriptions and health advice. If abnormal readings are found, the doctor will automatically alert the patient and advise whether or not to visit the hospital. With health monitoring kits, physicians may monitor their patients' conditions from a distance and provide prompt care to lower the likelihood of complications and prevent hospital stays. The elderly, those with chronic diseases, and those prone to illness will find this helpful.

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Smart Campus Integration with Arm and Iot Technologies

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ABSTRACT:

The Smart Campus system proposed in this project combines Internet of Things (IoT) technologies with ARM 7 architecture to provide extensive control and monitoring. The system uses edge devices based on ARM architecture to integrate Internet of Things (IoT) sensors for temperature monitoring, allowing for accurate management of lights, fans, and air conditioning systems. To further improve campus safety, sophisticated security measures including access control systems and video cameras are put in place. A web application is also integrated, offering a centralized platform for these systems' real-time monitoring and control. With the help of an intuitive online interface, users will be able to remotely administer and monitor campus resources in an intelligent and energy- efficient learning environment created by this comprehensive strategy.

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Cloud-Based QR Code Security Smart Vehicle Parking Management System

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ABSTRACT:

The Cloud-Based QR Code Security Smart Vehicle Parking Management System is an innovative solution that aims to provide security to parked vehicles. It transforms the urban parking management system and improves the security of vehicles. It is an innovative solution that could address many of the challenges faced by drivers and parking operators in urban areas. The system consists of a hardware setup powered by an ESP32 microcontroller and a web-based interface that allows users to search and find available parking slots, as well as make reservations. For added security, a unique QR code is generated for every reservation. The system also provides administrators with comprehensive analytics and utilization trends to optimize parking area management. Overall, the Smart Vehicle Parking System is a seamless, efficient, and secure solution that addresses many of the challenges faced by drivers and parking operators in urban areas.

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D 001

Energy Storage and Electrocaloric Effect Properties in Sm^{3+} and Fe^{3+}Substituted Pseudo-Binary BCZT Ceramics

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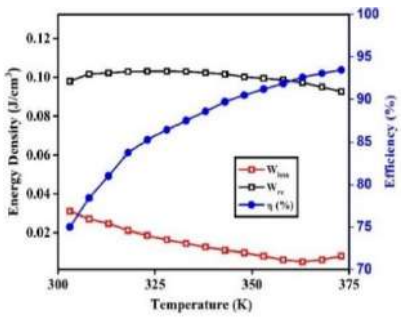
ABSTRACT

The polycrystalline ceramics having composition $0.45BaTi_{0.80}Zr_{0.20}O_3$-$0.55Ba_{0.69}Ca_{0.30}Sm_{0.01}Ti_{0.99}Fe_{0.01}O_3$ prepared using conventional solid-state reaction route has been analysed for their energy storage and electrocaloric properties. The phase formation of the prepared sample was confirmed by X-ray diffraction (XRD). The temperature dependent dielectric permittivity 'ε' shows diffused phase transition. Observance of ferroelectricity at temperatures above T_c suggests presence of nano-Polar Regions in the studied sample. Efficiency (η) determined from the P-E loops increases with increase in temperature while W_{loss} shows a reverse trend. The measured value of W_{rec} is 0.10 J/cm^{3}and 'η' was found to be 94%. Electro-caloric effect 'ECE' was investigated using indirect method and the adiabatic change in temperature 'ΔT' was found to be 0.34K at 25kV/cm having electro-caloric coefficient = 0.0136 K cm kV^{-1}. These results suggest that this composition can be used in energy storage and electro-caloric applications.

Keywords: *Dielectric; ferroelectric; electro-caloric effect; energy storage*



Energy densities and efficiency of simultaneously substituted BCZT ceramics

D 002

Magnetic and Magnetocaloric Properties of $Tb_2Co_{0.84}In_{3.24}$ Alloy

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ABSTRACT

Amid the environmental and energy crisis, efficient green fuel liquefaction demands efficient magnetocaloric materials. A magnetocaloric material with a large isothermal entropy change ($-\Delta S_M$), minimal hysteresis loss, and a wide working temperature range (ΔT_{FWHM}) makes a suitable magnetic refrigerant. In an attempt to study a new magnetic refrigerant, R_2TX_3 is one of the best choices because it belongs to the interesting intermetallic series of compounds known for their various magnetic ground states, crystal structures, and magnetocaloric properties. In the effort to study the magnetic and magnetocaloric properties of the new compound Tb_2CoIn_3 from the R_2TX_3 series, $Tb_2Co_{0.84}In_{3.24}$ alloy is formed. The sample is prepared using the arc melting technique followed by annealing at 1073K for a week. The alloy consists of the major phase (76.6%) $TbCo_{0.64}In_{1.99}$ with an $HfCuSi_2$ structure (space group – *P4/nmm*) and the minor phase (23.4%) $TbCo_{0.24}In_{1.46}$ with the $MgCu_2$ structure (space group – *Fd-3m*). The major phase $TbCo_{0.64}In_{1.99}$ and the minor phase $TbCo_{0.24}In_{1.46}$ are off-stoichiometric compositions of RTX_2 and RT_2 compounds, with lattice parameters comparable to their parent compounds. Considering the good magnetocaloric properties of RTX_2 and RT_2 compounds andthe enhanced magnetocaloric properties of alloys, magnetic, magnetocaloric, and magnetoresistive properties of the $Tb_2Co_{0.84}In_{3.24}$ alloy are studied. The metallic alloy exhibits ferrimagnetic transitions around T_1 = 250K, followed by antiferromagnetic transitions at T_2 = 54K, and T_3= 9.2K, respectively. The high-temperature magnetic transitions at T_1= 250K might be due to the minor phase $TbCo_{0.24}In_{1.46}$, as Rco_2 compounds have near-room-temperature magnetictransitions, whereas other transitions could be from the major phase $TbCo_{0.64}In_{1.99}$. Investigation ofmagnetocaloric properties denotes an alloy with $-\Delta S_M$ of 1.29 J/kg K, with a relative cooling power of 215 J/kg, and with a wide ΔT_{FWHM} of 167 K for ΔB=90 kOe .

D 003

Half-Metallicity in 2D NiMnAs Half Heusler Nanosheet for Spintronics Applications

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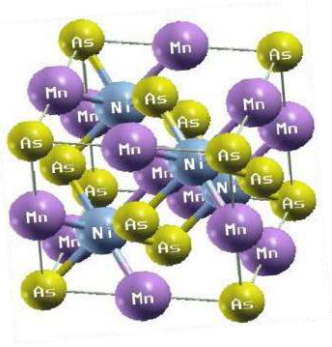
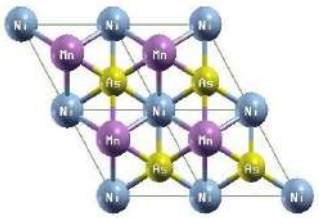
ABSTRACT

A novel 2D NiMnAs half Heusler nanosheet with half-metallicity for spintronic device applications is proposed through first principles calculation. Investigation of Bulk and 2D NiMnAs nanosheet has been performed through Quantum Espresso code based on Density Functional Theory-plane wave basis set approach. Band structure and density of states results were used to study the confinement effects. Comparing bulk NiMnAs with 2D NiMnAs change of structure is observed from fcc to trigonal is observed due to confinement effects. Half metallic nature of the bulk structure is undisturbed while moving to 2D nanosheet however, half metallic gap is found to increase from 0.5 to 1.2 eV due to the restricted motion of the electrons in one direction. Thus, NiMnAs nanosheets are demonstrated to be a promising material for spintronics applications with 100% spin polarisation near Fermi level with integer magnetic moment of 4 μ_B and large half metallic gap. Two-dimensional nature of atomically thin, flat surfaces and potential to form van der Waals hetero junctions paves the way for nanoscale device fabrication.

Keyword- *2D, half-Heusler, halfmetallicity, nanosheet, pseudopotential*





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D 004

Structural, Optical and Magnetic properties of 'Sm' doped Lithium Ferrites Prepared by Hydrothermal Method

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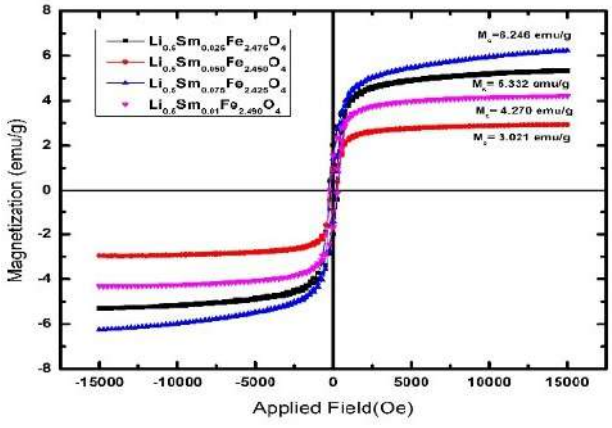
ABSTRACT

Samarium doped Lithium ferrites with chemical formula $Li_{0.5}Sm_xFe_{2.5-x}O_4$(x = 0.025, 0.050, 0.075 and 0.10) were prepared using hydrothermal method followed by calcination at 750^0C/4hr. The structural, optical and magnetic properties of the prepared ferrites were studied using XRD, FTIR, UV- Visible and VSM characterizations. The formation of cubic beta phased lithium ferrites was observed for all samples. The lattice parameter of the ferrites increased from 8.970 ^{0}A to 8.999 ^{0}A with increase in the 'Sm' addition. The FTIR spectroscopy confirms the A-site and B-site lattice vibrations perfectly. The optical band gaps of the ferrites range from 1.94 eV to 2.03 eV. The saturation magnetization (Ms) values vary randomly with Sm doping from 3.02 emu/g to 6.25 emu/g. The Ms values of the prepared ferrites indicated the low ferromagnetic nature of the ferrites. The coercivities of the ferrites varies randomly similar to saturation magnetization from 156.30 Oe to 294.09 Oe. The retentivity of the ferrites varies from 0.9428 Oe to 2.008 Oe randomly with Sm doping. These ferrites having low saturation magnetization and small coercive field can be used as transformer cores, transducers and inductor applications.



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D 005

Investigation on Physical Properties of Cobalt Oxide Nanoparticles and Their Super CapacitorApplications

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ABSTRACT

We report the structural, optical, electrical, thermal, magnetic and electrochemical properties of the cobaltoxide nanoparticles, prepared by co-precipitation method. The prepared cobalt oxide nanoparticles have been characterized by scanning electron microscopy, X-ray diffraction, X-ray electron spectroscopy and Fourier transform infrared spectroscopy. The prepared cobalt oxide nanoparticles exhibit spherical shape,crystalline normal cubic spinel Co_3O_4 phase and two band gaps 1.5 and 2.5 eV. The electrical properties have been determined using Hall effect and discussed. The thermal decomposition of the cobalt oxide nanoparticles sample have been analyzed using thermogravimetric analyzer. The room temperature paramagnetic behaviour of the cobalt oxide nanoparticles has been observed and this may arise from the spins of Co^{2+} ions and distortion of spin ordering, induced by thermal energy and reduction in particlesize. The capacitive performance of Co_3O_4 electrode has been analysed using cyclic voltammetry and electrochemical impedance spectroscopy. The maximum specific capacitance was found to be 29 Fg^{-1} at the scan rate of 5 mVs^{-1}. The results of our work may aid the development of the magnetic semiconducting cobalt oxide nanoparticles for electronic, magnetic, and super capacitor applications.

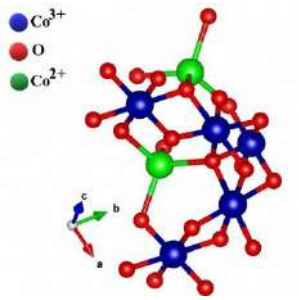

Figure 1: Crystal structure of Co_3O_4 nanoparticles obtained from XRD data

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D 006

Effect of Electrode Stress on the Structural and Ferroelectric Properties of the PZT Thin Films

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ABSTRACT

Lead zirconate titanate is a promising material for MEMS devices, such as piezoelectric micromachined ultrasonic transducers (pMUT). In this work, $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) thin film are deposited on silicon substrates with different buffer layers ($Pt/Ti/SiO_2/Si$ and $Pt/TiO_2/SiO_2/Si$ structure) at two different substrate temperatures using RF magnetron sputtering. Subsequently, the deposited PZT thin films are annealed at different temperatures using a rapid thermal annealing (RTA) process to form the perovskite phase. The multiple heat treatments develop thermal stress in the layers due to the mismatch in thermal expansion coefficients. The induced thermal stresses may affect the structural and ferroelectric/piezoelectric properties of the deposited films, which may be undesirable for device performance. In this work, we explore the stresses developed by the electrode deposition and buffer layers and how it affects the structural, ferroelectric and piezoelectric properties. The developed stresses are quantitatively assesses using x-ray diffraction and Raman spectroscopy. The effect of stresses on the ferroelectric properties are studied by analyzing remanent polarization and coercive field of P-E loops.

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D 007

Phenomenological Effect on the Structural and Electrical Characteristics of $CaCu_3Ti_{4-x}Nb_xO_{12}$ ($0.00 \leq X \leq 0.20$) Electroceramics

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ABSTRACT

$CaCu_3Ti_{4-x}$ Nb_xO_{12} (CCTNO), colossal permittivity (CP) material with Nb concentrations x=0.00, 0.05, 0.10, 0.15, 0.20 are synthesized by conventional solid-state reaction method, sintered at 1030 for 4 h. X-ray diffraction (XRD) confirms the cubic phase with *Im*3 space group. Field emission electron microscopy (FE-SEM) reveals that grains are highly dense with minimum porosity. Energy dispersive X-ray (EDX) spectroscopy confirms the presence of elements in the synthesized electroceramics. Oxidation states of the existing elements in the sample are confirmed by X-ray photoelectron spectroscopy (XPS). The effect of doping concentrations on the dielectric and electrical properties is analyzed and the maximum dielectric constant is obtained at the x = 0.15 doped concentration of Nb. Conductivity analysis is done and activation energy is estimated by the slope of the plot between the inverse of temperature and dc-conductivity. Negative temperature coefficient resistance (NTCR) behavior is confirmed by impedance spectroscopy. Nyquist analysis concludes the behavior of grains and grain boundaries in the synthesized ceramics. The non-Debye nature of the synthesized electroceramics is confirmed by the Modulus analysis

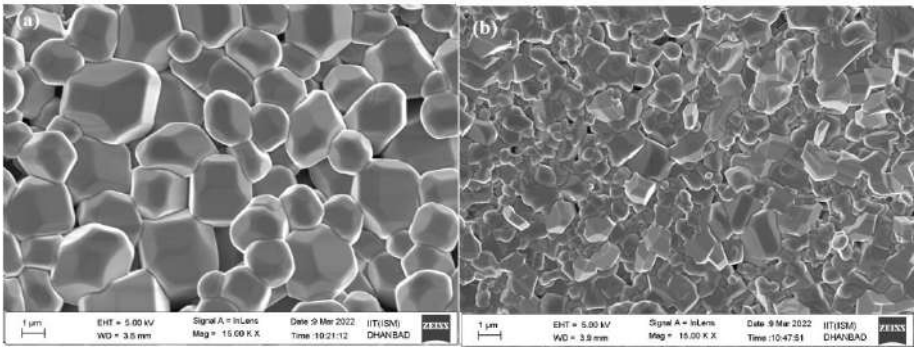

Fig. 1: FE-SEM images of (a) undoped and (b) x = 0.15 concentration of Nb-doped CCTO

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D 008

Dissecting the Effect of Synthesis Pressure and Chemical Ordering on the Ferroelectric Property of $Ca_{(2-x)}Mn_xTi_2O_6$ Complex Perovskite System

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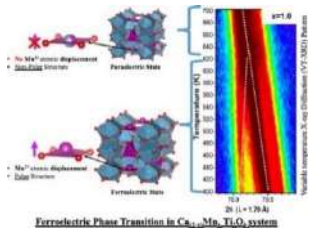
ABSTRACT

Quadruple perovskites (QPv) hailing as one of the most complex forms of perovskites; have promised the possibilities of hosting interesting physical phenomena including a structure-sensitive property like ferroelectricity in the past [1]. However, QPv's are less prominently studied for its specific chemical ordering and atomic co-ordination which were accessible only at extremely high synthesis pressures (> 7 GPa) in the past [2] before *Lee et al.* (2018) [3] synthesized a unique A-site ordered QPv ferroelectric $Ca_{(2-x)}Mn_xTi_2O_6$ (CMTO) system under Spark plasma Sintering (SPS) using a synthesis pressure of 100 MPa. Hence, creating a wide range of pressure phase space (7 GPa up to 100 MPa) yet to explore towardsunderstanding the trend of complex chemical ordering of QPv's with synthesis pressure. With this study, a detailed exploration of synthesis parameters (pressure, temperature, synthesis tools) is carried out, where various synthesis tools (like HPHT, HP-SPS, SPS) were used to synthesize the CMTO phases. Phase matching and chemical compositional analysis are performed followed by structural analysis by Rietveld refinement providing insight into the evolution of lattice parameters and cation displacements as a function of composition and processing conditions. Temperature trends of the ferroelectric to paraelectric structural phase transition for CMTO were probed by in-situ variable temperature powder X- ray diffraction (VT-XRD) data analysis. Finally, the interplay between synthesis conditions, cation compositions, and chemical ordering was discussed.



Ferroelectric Phase Transition in $Ca_{2-x}Mn_xTi_2O_6$ system

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D 009

Investigation of the heating efficiency of Mn-Zn Fe_2O_4 magnetic nanoparticles

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ABSTRACT

Ferrites are one of the most promising materials in the biomedical field due to their biocompatibility, rendering them useful in applications including hyperthermia for the inhibition of cancer cells, among which $MnFe_2O_4$ was found to be better than Fe_3O_4 [1,2]. Here we report MnZn nano ferrites as a potential material for magnetic nanoparticle hyperthermia. The MnZn nano ferrites with average grain sizes in the range of 7-16 nm showed saturation magnetization larger than 40 emu/g. The low coercivity of ferrite samples $H_c<90\ Oe$ suggest the superparamagnetic nature [3]. The hyperthermia response of the samples was carried out using the hyperthermia setup and the infrared thermography at an applied ac field of 8 kA/m and a frequency of 500 kHz. $Mn_{0.7}Zn_{0.3}Fe_2O_4$ ferrite exhibited higher heating efficiency when compared to all other ferrites such as Fe_3O_4 and $MnFe_2O_4$. The effective specific absorption rate (ESAR) value obtained in the range of $27-38\times10^{-9}W/gOe^2Hz$. The hyperthermic efficiency was also calculated using the theoretical model.

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D 010

Comparative Study on Hard/Soft Ferrite Composite Prepared by One-Pot Sol-Gel Auto-Combustion Method and Physical Mixing

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ABSTRACT

(100-x) $SrFe_{12}O_{19}$/x $CoFe_2O_4$, where x = 0, 10, 20, 30, and 100 wt.% composites of hard-soft ferrite phases were prepared by one-pot sol-gel auto-combustion method and physical mixing. The effect of synthesis methods on the microstructure of the composites as well as their electrical and magnetic properties have been evaluated. Crystal structure and microstructure of the composites have been investigated using X-ray diffraction and Scanning electron microscope. Hard/soft composites prepared by both methods, shows the presence of $SrFe_{12}O_{19}$ and $CoFe_2O_4$ phases, with the absence of the impurity phase. Maxwell-Wagner's two-layer model is used to describe the dielectric properties of the material, such as dielectric constant (ε'), dielectric loss, and AC conductivity. Complex impedance analysis (Nyquist plot) and equivalent circuit modeling revealed that both grains and grain boundaries significantly contribute to the overall conduction mechanism.[1–3] Magnetic hysteresis loops were measured with vibrating sample magnetometer (VSM) at room temperature (300 K) and low temperature (10 K). Magnetic parameters such as saturation magnetization (M_s), squareness ratio (SQR), remanence (M_r), and coercivity (H_c) were determined. The M-H loops were smooth, and the dM/dH vs. H curves show a single peak, indicating the presence of exchange coupling between hard/soft phases.

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D 011

Synthesis and Investigation of Structural, Magnetic, and Dielectric Properties of $Co_xNi_{1-x}Fe_2O_4$ Ferrite

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ABSTRACT

$Co_xNi_{1-x}Fe_2O_4$ ferrites (x= 0, 0.2, 0.4, 0.6, 0.8, 1) were prepared by a sol-gel auto-combustion method. The structural properties of the as-synthesized nanoparticles were characterized using X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), and Fourier transform infrared spectroscopy (FTIR). The X-ray diffraction patterns confirmed single phase formation of spinel structure and the average crystallite size were observed to vary between 38 nm to 44 nm. Fourier-transform infrared spectroscopy (FTIR) analysis of the nanoparticles revealed an absorption band between 450 cm^{-1} and 588 cm^{-1}. Electrochemical impedance spectroscopy (EIS) studies show that the charge transport phenomenon in ferrite materials is mainly controlled via grain boundaries, which have higher resistance than the interior of grains[1–3]. Dielectric properties of the cobalt-doped nickel ferrite nanoparticles were studied in the frequency range of 20 Hz to 1 MHz. Magnetic analysis were performed using a vibrating sample magnetometer, which shows substituting the Co^{2+} ions in nickel ferrites further increases their specific saturation magnetization (M_s), remanent magnetization (M_s) and coercivity (H_c). The law of approach to saturation magnetization is applied for the estimation of magnetization of the materials.

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D 012

Controlling the Magnetization Reversal Dynamics using Ultrafast Spin-Orbit-Torque

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ABSTRACT

Over the last couple of years, the field of spintronics has dramatically evolved to compete with the semiconductor-based memory technologies [1,2]. It has the advantages of non-volatility, faster speed, and energy efficiency. One of the branches of spintronics is the use of spin-orbit torque (SOT)-induced magnetization switching. Current pulses, majorly in the range of *~ns*, are used to switch the magnetization via domain wall driven dynamics. However some recent experiments explored a completely different magnetization switching dynamics using *~ps* current pulses [3,4]. We have used micromagnetic simulation [1,4,5] to study the mechanism of ultrafast SOT-induced magnetization reversal in the presence of a symmetry breaking in-plane magnetic field. The time-resolved magnetization dynamics is shown in Fig. 1a where the magnetization crosses zero in ~30 ps and complete switching occurs in ~70 ps without any activation delay. The gaussian current pulse with a 10 ps full-width-half-maxima is shown in black. Spatial magnetization profile (in Fig. 1b) shows a coherent rotation of magnetization in between 20-30 ps where the magnetization of the entire magnetic dot abruptly switches without creating domains. The red (blue) colour signifies positive (negative) magnetic saturation. Additional simulations revealed the importance of current density and pulse width in the observed switching mechanism. The newfound knowledge contributes to our fundamental understanding of the ultrafast SOT-driven magnetization reversal phenomenon.

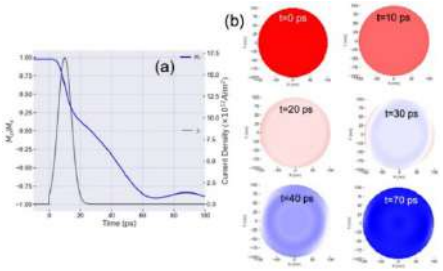

Fig. 1: (a) Time-resolved magnetization dynamics of SOT-driven device and (b) the corresponding magnetization reversal mechanism

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D 013

Comprehensive Study of Magnetocaloric Properties with Critical Exponent Analysis in Nanocrystalline $Pr_{0.6}Y_{0.1}Ba_{0.3}MnO_3$ Manganite

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ABSTRACT

Perovskite manganite have various applications in future technologies such as spintronics, magnetic sensors, storage media, colossal magneto-resistance, thermo-electric, and magnetic refrigerants. Double exchange interaction and super-exchange interaction play a vital role in the aforementioned properties. The magnetic and magnetocaloric properties of nanocrystalline $Pr_{0.6}Y_{0.1}Ba_{0.3}MnO_3$ (PYBMO) manganite synthesized via sol-gel wet chemical route have been investigated. X-ray diffraction pattern analysis has confirmed that our sample exhibits an orthorhombic crystal structure with a Pnma space group. The Williamson-Hall method was used to compute the crystallite size and lattice strain, which came out to be ~ 25 nm and 0.00127 respectively. The transmission electron microscope (TEM) was performed to elaborate structural and morphological studies. The temperature-dependent magnetic measurements have been carried out within 2 K - 300 K at 0.05 T applied magnetic field, exhibiting a ferromagnetic to paramagnetic phase transition with a transition temperature (T_C) ~ 128 K. The paramagnetic Curie-Weiss temperature was found to be 164 K. The experimentally and theoretically calculated effective magnetic moment is ~ 5.9 μ_B/f.u. and ~ 5.38 μ_B/f.u. respectively. The M-H isotherms in a protocol of 0 T → 5 T → -5 T → 5 T indicate ferromagnetism at 2 K, although the linear hysteresis loop corresponds to the paramagnetic behavior at 300 K. The second-order magnetic phase transition was affirmed by the positive slopes of Arrott plots. The classical Maxwell theory was used to compute the magnetic entropy change, and hence further calculating the magnetic cooling capacity. The collapsing behavior of Franco's curves presents the universality in magnetic entropy change, which corroborates the second-order phase transition in PYBMO, theoretically. Several methods, including the Modified Arrott plot, scaling theory, and the Kouvel Fisher approach, have been employed to determine the critical exponent values.

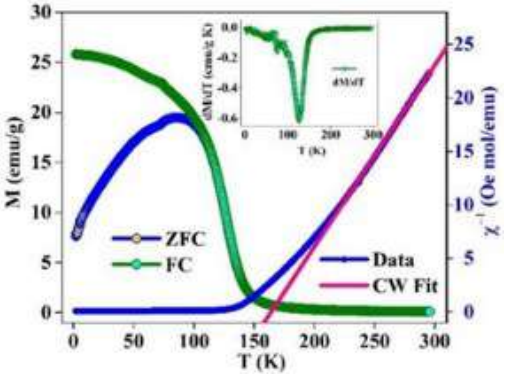

Fig. Temperature dependence of ZFC and FC magnetizations for nanocrystalline Pr0.6Y0.1Ba0.3MnO3 sample at applied field of 0.05 T. The right-side axis depicts the inverse susceptibility (χ-1) versus temperature (T) plot. The inset displays the dM/dT versus T plot.

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D 014

Structural, Dielectric, Ferroelectric and Magnetodielectric Properties of Fe Doped (BaSr)TiO_3 ceramics.

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ABSTRACT

Due to their intriguing physiochemical characteristics and wide range of possible uses in devices including actuators, sensors, transducers, magnetic data storage, and non-volatile memories, multiferroic materials are receiving a lot of attention these days [1-2]. Multiferroic properties arise when magnetic metal ions are substituted in the lattice of ABO_3-type ferroelectric ceramics. It has been found that ions with valences smaller than 4 substituting at the Ti site exhibit acceptor character with charge deficiency compensated by doubly ionized oxygen vacancies [2-4]. The present work deals with analyzing the impact on structural, dielectric, and ferroelectric properties of, Fe-doped lead-free $(Ba_{0.95}Sr_{0.05})TiO_3$. Multiferroic coupling was studied in terms of magnetocapacitance (change in dielectric properties with applied magnetic field) with the substitution of Fe at the Ti-site in BST. X-ray diffraction (XRD) study shows the tetragonal structure of BSTFe samples. SEM shows that grains are homogeneously non-uniform with the least porosity. The dielectric properties and curie temperature decrease with an increase in Fe doping. All BSTFe sample exhibits a ferroelectric nature at room temperature. The maximum value of magnetocapcitance is 6 % for the Fe=0.05 sample at 100 Hz.

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D 015

Theoretical Exploration of Half-Metallic Ferromagnetism and Optical Properties in Novel Half Heusler RbXSb (X = V, Nb and Ta) alloys

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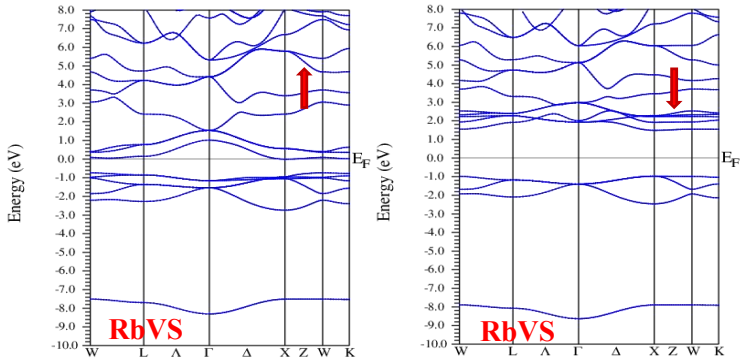
ABSTRACT

In this study, we conducted a comprehensive theoretical analysis using density functional theory (DFT) to explore the structural, mechanical, electronic, magnetic and optical properties of RbXSb (X = V, Nb, Ta) alloys. The electronic structures of RbXSb (X = V, Nb, Ta) were modeled using the generalized gradient approximation (GGA) and the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential implemented in WIEN2k code. Based on the total-energy calculations, all of these alloys are stable in the α phase. According to spin-polarized calculations, all the alloys favor a ferromagnetic state. The spin-polarized band structure shows the alloys as perfect half-metallics with indirect band gaps of 1.89 eV, 1.64 eV and 1.59 eV in RbXSb (X = V, Nb, Ta) respectively exhibiting 100% spin-polarization at the Fermi level obeying Slater-Pauling rule with total magnetic moment of 3.00 μ_B. The magnetic moment mainly originates from the strong spin-polarization of n*d* electrons of X (V, Nb, Ta) atoms and partial involvement of n*p* electrons of Sb atom. Dielectric spectra also indicate the semiconductor behavior of the alloys with various intense peaks. Optical absorption and conductivity were found to be maximum in the UV region of the spectrum. Half Heusler RbXSb (X = V, Nb, Ta) alloys, could be potential material in spintronic and optoelectronic devices



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D 016

Improved Iron Oxide Mesocrystals for Magnetic Hyperthermia

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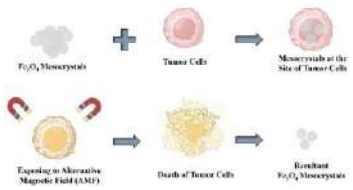
ABSTRACT

Magnetic nanoparticles are widely used for biomedical applications, especially for cancer treatment via magnetic hyperthermia, wherein the magnetic nanoparticles are exposed to an alternative magnetic field to produce heat to diagnose cancer [1]. Superparamagnetic nanoparticles were attempted to achieve by, size control that can have numerous advantages, such as preventing particle agglomeration and providing optimal heating power. Nevertheless, constraints to achieve the desired size with higher magnetization under the applied magnetic fields are challenges [2]. Self-assembly of nanoparticles with crystallographic features is a promising new design strategy to enhance material properties [3]. Spatially separated and crystallographically oriented nanoparticles form mesocrystals, and we applied this design strategy for hyperthermia application. We have synthesized Fe_3O_4 mesocrystals using the modified polyol method withethylene glycol as a solvent and $FeCl_{3.6}H_2O$ as the iron precursor. The XRD data confirmed the formationof Fe_3O_4, which is well-matched with the JCPDS card number 00-019-0629. The SEM images showed the hierarchical structure with oriented attachment of particles, which confirms the mesocrystal formation via a nonclassical route. The vibrating sample magnetometer (VSM) study showed the room temperature behavior of the Fe_3O_4 mesocrystal, confirming the particles soft ferromagnetic nature. We have successfully synthesized mesocrystals with slightly misaligned magnetic nanoparticles with low coercivity and notablesaturation magnetization. Further optimization with concentration and additives is required to obtain the particle with tunable size to reach a superparamagnetic nature. Thus, we expect that the mesocrystals design with superparamagnetic nature can enhance the hyperthermia treatment potentially to treat cancer.



Schematic representation of magnetic hyperthermia using mesocrystals

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D 017

Structural, Optical and Magnetic properties of multilayer $BiFeO_3$ /$BaTiO_3$ thin film by chemical solution deposition technique

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ABSTRACT

Multilayer Bismuth Ferrite ($BiFeO_3$ or BFO)/Barium titanate ($BaTiO_3$ or BTO) thin films were deposited on corning glass substrates by using a sol-gel spin coating technique. The samples were prepared by deposition alternate layers of BFO and BTO onto the substrates. The structural studies of the samples were carried out by using x-ray diffraction techniques. As-deposited films were found to be amorphous that crystalizes to pure phase after post deposition annealing at 500°C in air. Optical and magnetic studies of multilayer sample and 6 layers, as well as individual BFO and BTO thin films were carried out. The X-Ray Diffraction pattern confirms pure phase polycrystalline structure of the sample with preferred orientation along (100) plane. The crystallite size calculated from the x-ray diffraction data were found to be increase with increase in number of layers. The band gap decreases with increase in the number of layers. The optical band gap of the BTO thin film can be tuned with the inclusion of BFO thin film layer in different configuration. Magnetic properties of Multiferroic bilayer of $BiFeO_3$ (BFO)/ $BaTiO_3$ (BTO) were studied. It was found that saturation magnetization (Ms)of heterostructure thin films of BFO/BTO were found to be increased when BTO layer is fabricated over BFO layer. The results were analyzed in the light of reported results by other workers.

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D 018

Exploring the Structural, Microstructural and Magnetic Properties of Double Perovskite Structured Yb_2FeCrO_6 Compound

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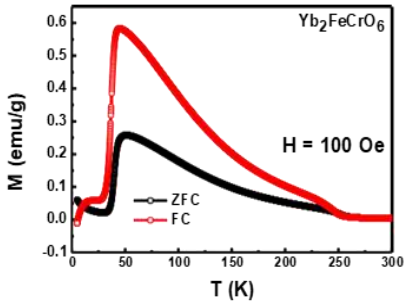
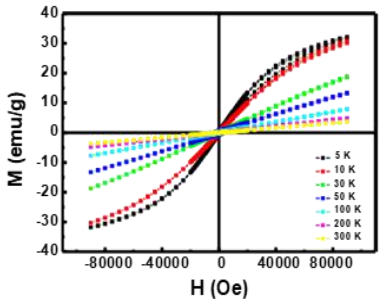
ABSTRACT

In this study, the novel double perovskite structured Yb_2FeCrO_6 (YBFCO) compound was synthesized using the conventional sol-gel method to investigate its structural, microstructural, and magnetic properties. The X-ray diffraction (XRD) patterns revealed a distorted orthorhombic crystal structure with the *Pbnm* space group. The field emission scanning electron microscopy (FESEM) images displayed a homogenous microstructure with grains of varying sizes. The energy-dispersive X-ray (EDX) spectrum confirmed the presence of all elements in the sample. The diffuse reflectance spectrum indicated the semiconductor natureof YBFCO, with a direct optical band gap of 1.92 eV. Furthermore, the temperature-dependent magnetic properties of the sample were analyzed over a range from 5 to 300 K. The results revealed two distinct magnetic transitions. The first transition occurred at approximately 248 K, denoted as T_{N1} (Néel transition temperature), and was associated with antiferromagnetic behavior arising from the canted antiferromagneticordering of the Fe^{3+}/Cr^{3+} sub-lattices. A second transition, T_{SR}, was observed at around 45 K, resulting fromthe competition between interactions involving Yb^{3+} ions and the anisotropic field of Fe/Cr. Notably, the M-H loops exhibited a hysteresis behavior without reaching saturation magnetization. This behavior can beattributed to the coexistence of ferromagnetic and antiferromagnetic components within the YBFCO compound.





D 019

Effect of Annealing Al Thin Film in Oxygen Environment: Microstructure, Transport and Magnetic Properties

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ABSTRACT

Metal-Oxide compounds have garnered significant attention from researchers over the past few decades due to their exotic electric and magnetic properties. These properties can be finely tuned by introducing defects into the crystal structure [1]. This work reports the effect of annealing Al thin film in oxygen environment on its microstructure, transport and magnetic properties. First, thin films of aluminum (Al) were deposited on a silicon (Si) substrate at room temperature using DC magnetron sputtering. The thickness of these films was 40 nm determined from X-ray reflectivity (XRR). Subsequently, the as-deposited films were annealed at temperatures above 600°C in an oxygen environment for different time periods [2]. The annealed films were then subjected to a series of characterizations, including microstructure, chemical composition, transport, and magnetic properties. X- ray diffraction (XRD) studies were conducted to confirm the crystallinity of the films and identify the different phases of aluminum oxide formed after annealing [3]. Temperature-dependent resistivity studies were performed within a range of 80 K to 300 K, revealing a negative temperature coefficient of resistivity, indicates the semiconducting nature of the films [4]. Also, the positive value of magnetoresistance is observed. Additionally, Hall resistivity measurements were carried out to determine the majority carrier concentration and its mobility. Magnetic studies revealed the paramagnetic nature of the Al thin films with feeble signal of ferromagnetism at room temperature. On the contrary, appearanceof clear ferromagnetic hysteresis loop confirms the presence of strong ferromagnetic interactions between the spins at room temperature after annealing in oxygen environment. Present work is significant in the sense that it provides a promising way to synthesize the Al_2O_3 film from Al with a possibility of tuning it's magnetic and transport properties for application as magnetic semiconductor in spintronics devices.

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D 020

Investigation on the Structural, Dielectric, Energy Storage, and Electrocaloric Properties of Environment-Friendly BCZT ceramics

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ABSTRACT

This study delves into a $Ba_{0.98}Ca_{0.02}Zr_{0.07}Ti_{0.93}O_3$ (BCZT) ceramic synthesized through the solid-state reaction method for its energy storage, and electrocaloric properties. The study presents empirical evidence illustrating the changes in the aforementioned properties in response to change in temperature and an electric field. Analysis through X-ray diffraction and Rietveld refinement confirms the co-existence of tetragonal and orthorhombic phases in the BCZT ceramic. Notably, at maximum transition temperature ($T_m \approx$ 373 K) and 1 kHz, the ceramic displayed a high dielectric constant of ≈14,655 and low dielectric loss of 0.04. In addition, BCZT ceramic exhibited a recoverable energy density (W_{rec}) of 544.6 mJcm^{-3} at T_m, with an energy efficiency of 97.50 %. The study further explored the electrocaloric effect in BCZT using an indirect approach based on the Maxwell relation at 20 kV cm^{-1}. It revealed a significant adiabatic temperature change of 1.136 K and isothermal entropy change of 1.24 Jkg^{-1}K^{-1} at T_m. These findings suggest that BCZT ceramics hold great potential as eco-friendly solid-state refrigeration materials for future technology development.

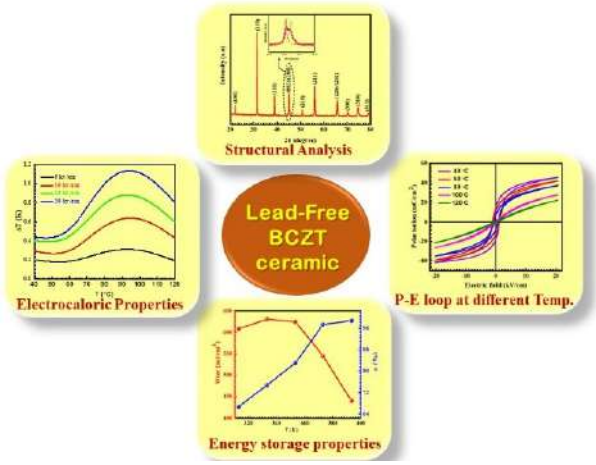

Fig.1: Structural analysis, P-E loop at different temperature, energy storage and electrocaloric properties.

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D 021

Rare-Earth Substitution in Nickel Cobalt Ferrite Compound: Effects on Structural and Magnetic Properties

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ABSTRACT

In this study, ferrites with the compositional formula $Ni_{0.5}Co_{0.5}Fe_{0.95}R_{0.05}O_4$ (where R= Pr, Sm & Ho) were prepared through the solid-state method and characterized their properties. These samples were sintered at 1250^0C for 4hrs. X-ray diffraction patterns were used to confirm the presence of single phase cubic structured compound [1]. In addition, structural parameters such as lattice parameter and crystallite size were calculated from rieveld analysis using fullprof software and the lattice parameter values are found to increase with the doping of rare earths. In UV-visible spectra, a decrease in bandgap energy was observed with rare earth element doping. Upon analyzing the micrographs using scanning electron microscopy (SEM), it was estimated that the average grain size of all samples and the presence of elements are confirmed with EDAX data. Raman spectra of the compounds exhibit five Raman modes and the positions are well matching with the literature. The shifting in Raman peaks clearly indicates the effect of rare earth doping on the undoped compound. Room temperature hysteresis loops indicate the increase in magnetic properties and it is due to the high magnetic moment of rare earth elements [2].

Key Words: *Ferrites, X-Ray Diffraction, Raman Spectra*

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D 022

Terahertz Generation Through Organic and Piezoelectric Nonlinear Optical Crystals

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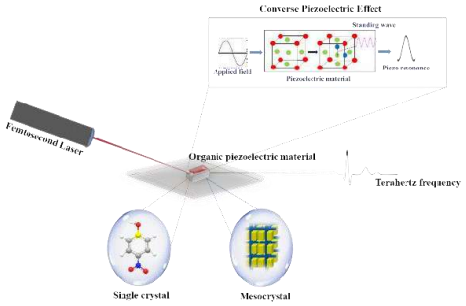
ABSTRACT

The Terahertz (THz) quantum efficiency of organic nonlinear optical (NLO) single crystals can be enhanced selectively by utilizing inverse piezoelectric effect and mesocrystal form of single crystals. THzradiation falls in the electromagnetic spectrum between microwaves and infrared region, with frequencies ranging from 0.1 to 10THz. This ultra-high bandwidth can connect IoT devices and used for short range communication effectively. This can enable data rates that are significantly faster than what is achievable with current wireless technologies. Organic π-conjugated crystals are appealing materials for terahertz (THz) application, yet their quantum efficiency remains a challenge, with a relatively low value of less than3%. When an external AC is applied to NLO materials with inverse piezoelectric behaviors, they exhibit apiezo-resonance at low frequency. This develops a coupling between electromagnetic field and lattice-wavein the material which governs the wave propagation of the incident THz beam by modulating its phase transfer function and significantly reduces power required to generate THz. An organic and piezoelectric nonlinear optical single crystal were grown by slow evaporation method. The crystal structure and optical quality were confirmed by single crystals X-ray diffraction and UV-Vis transmittance study. The hyperpolarizability value was theoretically obtained using density functional theory calculations. The preparation of crystals in the form of mesocrystals, second harmonic generation and THz measurement areunder progress to confirm the suitability of materials for THz generation.



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D 023

Structural and dielectric study of lead-free Nd doped $BaTiO_3$ (BT) ceramic

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ABSTRACT

Nd doped $BaTiO_3$($Nd_xBa_{1-x}TiO_3$) where x= 0.03, 0.05, 0.07 has been synthesised successfully through solid state reaction method. XRD has been performed to determine the structure of synthesised sample which confirmed crystalline structure of prepared sample. Dielectric constant as well as tangent loss has showed dispersive behaviour at low frequency region whereas nearly constant behaviour at high frequency region. The high value of dielectric constant at lower frequencies was possibly due the space charge polarization. AC conductivity is found to have increasing trend as the frequency and temperature increases. The Nyquist plot of impedance showed semi-circular arcs having centre lying below the real axis and the radius of the semi-circular arc gets decreased with temperature indicating the semiconducting behaviour of the sample.

Keywords: *Ceramic, ac conductivity*

D 024

Investigating Electronic, Magnetic and Structural Properties of Nano and Bulk Materials

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ABSTRACT

Micro-M-magnetics is a field of study that deals with the behavior of magnetic materials at the microscopic level. In this study, simulations are being performed using the Object-Oriented Micro-Magnetic Framework (OOMMF) to investigate the magnetic and electric properties of these materials. The aim of this research is to better understand the fundamental properties of magnetic materials and how they can be used in various applications such as data storage, sensors, and spintronics. The simulations involve modeling the behavior of magnetic domains and evaluating their response to external stimuli such as electric fields. The results of these simulations will provide insights into the complex interactions between magnetic and electric fields and aid in the design of new materials with tailored magnetic and electric properties.

D 025

Defect Induced Ferromagnetism and Visible Emissions in Ag Doped ZnO Thin Film

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ABSTRACT

We investigate the effect of Ag doping in structural, optical, morphological, and magnetic properties of ZnO thin films. Pure and Ag doped ZnO thin films were prepared by RF magnetron sputtering and investigated their structural, optical, magnetic, and morphological properties. The X-ray diffraction analysis (XRD) revealed hexagonal wurtzite structure of fabricated films. The surface of the undoped ZnO thin film is made up of tiny nanostructures while the surface morphology of Ag doped ZnO thin films revealed that the average size of the nanostructures increases with Ag concentration. Photoluminescence (PL) analysis showed the presence of donor defects (Oxygen vacancy and zinc interstitial) in singly ionized state. It was found that pure ZnO thin films exhibited diamagnetic nature where 1 and 3 at. % Ag doped ZnO thin films exhibited ferromagnetic behavior at room temperature. Correlation between PL and VSM results indicated that the donor defect contributes to the ferromagnetic behavior of Ag doped ZnO thin films. The bound magnetic polaron (BMP) model was proposed to explain the defect assisted ferromagnetism in Ag doped ZnO thin films.

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D 026

Aerosol Deposition of Functional Thick Films on Metal and Polymer Substrates

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ABSTRACT

To miniaturize functional devices, electroceramic components must be reduced in size down to the micrometer range. The aerosol deposition (AD) process (Figure 1a) offers a cost-effective way to deposit dense, micrometer-thick films at room temperature, enabling the integration of ceramic components on substrates such as metals and polymers. In this context, relaxor-ferroelectric (1-x)Pb $(Mg_{1/3}Nb_{2/3})O_3$–$xPbTiO_3$ (PMN–100xPT) materials exhibit excellent electromechanical properties as well as energy storage and conversion capabilities suitable for electrical generators, capacitors and electrocaloric refrigerators. In this work, PMN–PT thick films were deposited on low-cost stainless steel [1] and flexible polymer substrates (Figure 1b) [2]. The films exhibit a relaxor-like hysteresis loop of polarization versus electric field, which makes them promising for energy storage applications. PMN–10PT films on polymer substrates exhibit a recoverable energy density of ~10 Jcm^{-3} at ~1000 $kVcm^{-1}$. The energy storage properties of these films remain stable after 105 bending cycles at 1.0 % bending strain (Figure 1b) [2]. In addition, PMN–10PT films [3] and PMN–10PT/La-Fe-Si based alloy composites (Figure 1c) on polymer substrates show promising caloric properties, which are presented in this contribution. An analysis of the energy storage and piezoelectric properties of AD-processed PMN–35PT [4, 5] and lead-free $BaTiO_3$-based thick films is also discussed.

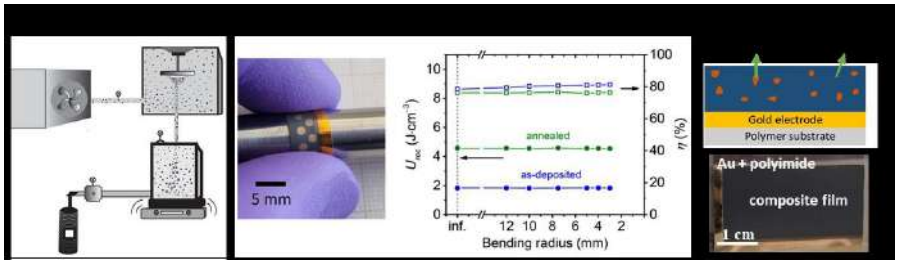

Figure 1: (a) Aerosol deposition process, (b) PMN–10PT thick film on a polymer substrate and their recoverable energy density (Urec) and efficiency (η) versus bending radius measured at ~500 kV·cm−1 [2] (c) PMN–10PT/La- Fe-Si-based intermetallic alloy composite thick film on polymer substrate.

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D 027

Domain Wall Pair to Skyrmion Conversion in a Typical Junction Geometry Useful for Racetrack Memory Devices

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ABSTRACT

In order to meet the ever-increasing demand of data processing speed and storage capacity, it is important to develop energy efficient magnetic memory devices [1]. A new class of memory storage device that was proposed in 2008 known as the "Racetrack memory (RM)" uses chiral spin textures such as domain walls (DWs), skyrmions etc., are known to be robust and energy efficient [2,3]. In this work using micromagnetic simulations (OOMMF) [4], we present the results of DW pair to skyrmion conversion in a specially designed magnetic nanotrack consisting of a wider nanotrack sandwiched between narrow nanotracks (Fig 1). We consider two systems in which DW pairs are stabilized on either left or right side of the wider nanotrack and we study their dynamics for the current applied along -/+ x direction. DWs experiences spin transfer torques and eventually sets into motion. We choose the material parameters corresponding to Co/Pt [5,6]. Interestingly, our results show that the DW pair stabilized on the left side of the wider nanotrack is depinned from the lower edge of the narrow nanotrack whereas the DW pair on the right side of the wider nanotrack is depinned from the upper edge of the narrow nanotrack. We observe that in both the systems the DW pair gets converted into three skyrmions, each having topological charge, Q = -1 (cf. Fig. 1 (a-h)). Further on reversing the current direction, the initial conversion time and the trajectory of the skyrmion also get affected due to the geometrical constraints. The controlled creation and dynamics of skyrmions plays crucial role in achieving high data processing speeds along with low power consumption.

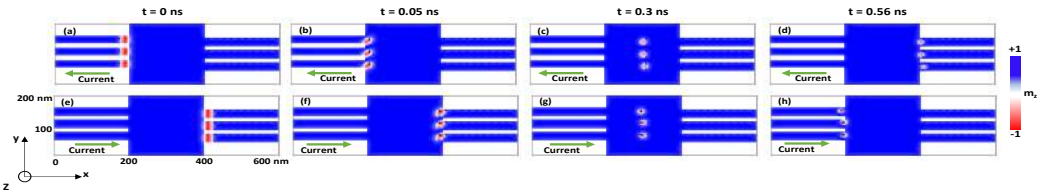

Figure 1(a) – (d): Formation and dynamics of skyrmion when the current is applied along -x axis and the pair of DWs are stabilized in left narrow nanochannels. (e) – (h) Shows their formation and dynamics when the current is applied in the +x axis and the pair of DWs are stabilized in right narrow nanochannels.

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D 028

Design of Multiferroic Oxide Superlattice as a Photovoltaic Material by Using First-Principles Calculations

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ABSTRACT

Multiferroic materials with perovskite structures are also promising for photovoltaic devices. In particular, hybrid improper ferroelectric mechanism in oxide superlattices $(LaFeO_3)m/(CaFeO_3)n$, (where, m and n = 1,2 and 3) induces microscopic polarization and also can tune the electronic structure as metal to insulator transition. These results are promising because it opens the possibility of tuning the optical properties with the electric field. By using Density functional theory calculations and WEIN2K simulations, we have studied the electronic, magnetic and optical properties of $(LaFeO_3)m/(CaFeO_3)n$ superlattices. In (1/1) superlattice, in addition to the primary order parameters, rotation (Q_{R+}) and tilt (Q_T) distortions along $a^0a^0c^+$ and $a^-a^-c^0$, we have discovered a polar charge disproportionation mode (QACD) which is analogous to the A-type antiferromagnetic ordering. We have found that when the QACD mode couples with the tri-linear coupling QTri, the system goes to a low symmetry (Pc) structure with lower energy than QTri ($Pmc2_1$). By using mBJ potential, the analysis of electronic properties shows the indirect semiconducting band gaps of 0.6 eV to 1 eV for (1/1) superlattice which are suitable (Eg< 3.0 eV) for absorption of visible light. Further, we have discussed the band structure and optical transitions to analyse the optical absorption spectrum for a whole range of $(LaFeO_3)m/(CaFeO_3)n$ superlattices. This enhances their absorption in the visible light region, allowing them to be used in optical device applications.

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D 029

A Comparative Study on the Magnetic Properties of Single and 1-D Array of $La_{0.7}Sr_{0.3}MnO_3$ Nanospheres using Micromagnetic Simulations

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ABSTRACT

Controlling the dipole interactions among magnetic nanospheres are of fundamental concern for the future development of spintronic applications, and high-density storage devices [1]. In this work, we explore the magnetization reversal of solely La0.7Sr0.3MnO3 (LSMO) magnetic nanosphere with a diameter of 10 nm and compared its result with one-dimensional (1-D) array LSMO structure consisting of same size nanospheres. In addition, the impact of varying the distance among each nanosphere (ranging from 0 to 5 nm) in 1-D array LSMO structure on the magnetism has been investigated. Magnetic hysteresis loop and spin-configuration results were generated for single and 1-D LSMO structures using micromagnetic simulations Mumax3 [2]. The simulation results on the hysteresis loop revealed the coercivity (Hc) value is ~ 0.06 T, and it remains unchanged when magnetic field is applied along x- and z- direction in single LSMO nanosphere (see Fig 1(a)). Interestingly, the hysteresis loop of 1-D LSMO structure displayed around three times of enhancement in Hc compared to a single LSMO nanosphere when the field applied along z-direction (i.e., along the chain-direction). Such enhancement of Hc could be due to stronger dipolar interaction among nanospheres in 1-D array structure. However, the value of Hc reduces to zero along the perpendicular to the chain direction (i.e., x-direction) indicating the anisotropic nature of magnetism in 1-D array LSMO structure (see Fig. 1(b)). Spin-configuration results showed the coherent and gradual rotation of spins for solely nanosphere and for 1-D array of nanospheres perpendicular to chain-direction, respectively. More importantly, the value of Hc reduces with increasing the distance between spheres in 1-D array structures, and its value is found to be same as single nanosphere when distance among nanospheres is large. This characteristic is attributed to the weakening of dipolar interaction and each nanosphere in 1-D array behaves like a single sphere at large distance. The present study unveils that the low-dimensional nanostructures can be deliberately designed for manipulation of magnetic properties effectively.

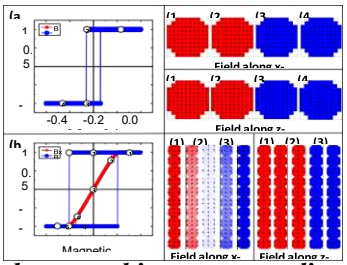

Fig 1: Simulated hysteresis loops and its corresponding spin configurations of LSMO (a) single sphere and (a)chain- like structure (10 nano-spheres) with applied field direction x- and z (Bx, Bz) respectively.

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D 030

Predictive Design of High Polarization Low Switching Barrier Hybrid Improper Ferroelectric Double Perovskite Oxides

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ABSTRACT

Multiferroic oxides with co-existing ferromagnetic and ferroelectric long range order are materials of high technological importance. The primary challenge is identifying materials with a functional coupling between electrical polarization and magnetization at room temperature. Despite a massive surge of research activity in this field, the number of potential materials is still limited. This is due to the scarcity of compounds that can act as possible parent candidates in the search for new multiferroics. In this direction, ordered double perovskite materials with general chemical formula AA'BB'O_6 (where A is an alkaline-earth or rare-earth ion, BB' are transition metal ions) hold high promise. Here, we take up the case of ferromagnetic insulating double perovskites RKFeOsO6 where Ln represents Y, Sm, Gd, Dy and Tm respectively. Our first-principles study predicts the replacement of R3+ ion by layered stacking of AA' ions belonging to lanthanide and alkali metal series makes the material polar. The calculated polarization is found to be substantial, with promises for strong polarization−magnetization coupling. We have identified and discussed the role of a key distortion associated with anti-ferroelectric displacement of planer oxygen ions in stabilizing layered AA' phase. Also, the insights gained from atomistic simulations conducted on this $RKFeOsO_6$ provided a comprehensive understanding of the switching process with applications in temperature-driven magnetic devices. The polarization switching (P) of $RKFeOsO_6$ occurs at a very high temperature of ~1150 K through a phase transition, from a polar (P21) phase with $\vec{P}+$ to $\vec{P}-$ via a non-polar P4/n phase [1]. The mechanism suggests that even though the HIF is established by the primary order parameters such as QR+ and QT, the switching is a two-step process in which P~ switches from [010] to [$0^{-}10$] via switching path driven by out-of-phase rotation (QR−, a0a0c− when QT = 0 or, a−a−b− when QT = 0). We utilize this information for 159 DPOs to estimate the switching barrier (Es) using the Nudge Elastic Band (NEB) method with reference structures as the fully distorted P21 and the phase with QR− distortion P4/n phase. In this 159 NEB calculated DPOs dataset, 67 are perfectly insulating and ferroelectric polarization is calculated using Berry phase formalism. In this work, we introduce a predictive learning strategy based on importance sampling to overcome this limited data for predicting polarization and switching barrier. Overall, in this framework, our predictive models identify candidates with high polarization and low switching barriers from a pool of double perovskite oxides, suitable for future investigation for their potential applications in spintronic devices [2].

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D 031

Development of Eco-Friendly Magnetoelectric Composites for Energy Harvesting Applications

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ABSTRACT

Eco-friendly Magnetoelectric (ME) composites with the combination of ferroelectric $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and ferrimagnetic $Y_3Fe_5O_{12}$ (YIG) were prepared to enhance the electric, magnetic and ME properties. Desired Crystalline structures of the NBT, YIG and composites (1-x)NBT- (x)YIG, (x=0.2, 0.4, 0.6 & 0.8) was confirmed from X-ray diffraction (XRD) patterns and Raman spectroscopy. Magnetic hysteresis loops confirm the ordered magnetic behaviour of the prepared samples. Morphological studies show the uniform distribution of both ferroelectric and ferrimagnetic grains in the composites. Hysteresis loops reveals that soft magnetic nature of YIG with showing remanent magnetization (M_r), saturation magnetization (M_s) and coercivity (H_c) values as 9 emu/g, 35 emu/g, and 15.07 Oe respectively. Further, we are focusing on dielectric and magnetoelectric characteristics of the (1-x) NBT- (X) YIG, (x = 0.2, 0.4, 0.6 & 0.8) composites.

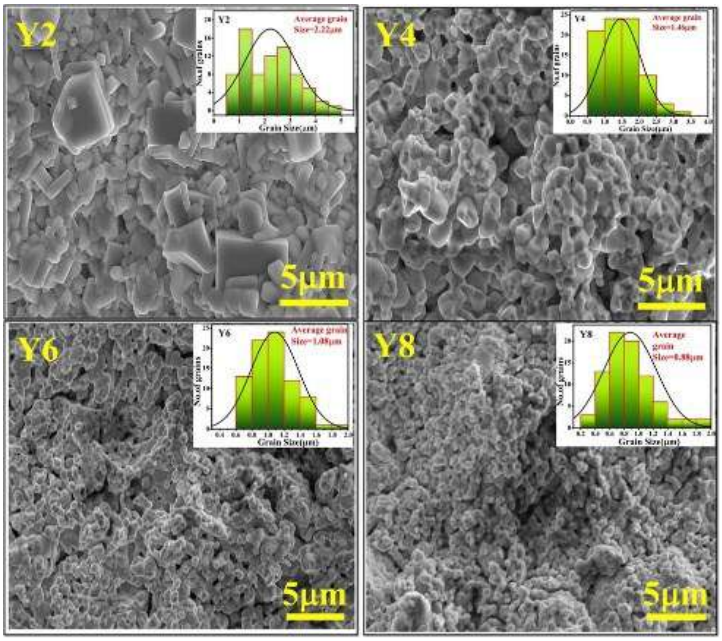

Fig 1. HR-SEM images (inset grain size distribution curves) of the (1-x) NBT- (x) YIG, (x = 0.2, 0.4, 0.6 & 0.8)

D 032

Exploring Magnetism in Ru-doped Canted Antiferromagnet Copper Pyrochlore Vanadate

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ABSTRACT

Low-dimensional spin systems are of great interest in quantum magnetism owing to their appealing magnetic phenomena. There has been significant attention given to these systems experimentally and theoretically [1-4]. Most recent studies have focused on chemical doping of high-spin orbit elements in frustrated magnetic materials to enrich their magnetic properties. Herein, we synthesized pure pyrochlore copper vanadate (α-$Cu_2V_2O_7$) and Ru-doped α-$Cu_2V_2O_7$ using conventional solid-state route. Synthesized samples were found to be crystallizing in orthorhombic structure with the Fdd2 space group, despite the fact that pyrochlore copper vanadate crystallizes in various crystal phases. The magnetization measurements of α-$Cu_2V_2O_7$ system revealed interesting magnetic features like reduced magnetization than calculated theoretically from spin moment of Cu^{2+}, canted antiferromagnetic nature owing to the existence of DM-interaction, etc,. Furthermore, the temperature- and field-dependent magnetization (i.e., M(T) and M(H)) behaviors of Ru-doped α-$Cu_2V_2O_7$ samples showed interesting features such as enhanced frustration parameter, constant magnetic transition temperature (TC), and signature of antiferromagnetic coupling at low field region in M(H) with regard to the pure α-$Cu_2V_2O_7$. Thus, the present work explores in detail about synthesis, structural, and magnetic properties of high spin-orbit coupling element (Ru)-doped pyrochlore copper vanadate.

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D 033

Resistive Switching in Perovskite Heterostructures: A Review

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ABSTRACT

Multilevel resistive switching in memristive devices is vital for applications in non-volatile memory devices. Resistive switching based resistive random-access memories (RRAMs) is one of the auspicious candidates for high speed, low power consumption, artificial synapse, and high density. There are two types of working mechanisms in RRAM: valence change mechanisms (VCM) triggered by the drift-diffusion of oxygen anions and electrochemical metallization mechanism (ECM) relying on the electrochemical dissolution and deposition of active electrode metals. Both mechanisms play significant roles in resistive switching devices, and more studies are being carried out to achieve a deeper understanding of the mechanisms. Beyond those active metals, semiconductors are being used as a buffer layer between the metal electrode and the insulating layer in the memory devices, leading to interesting switching performance. The performance of such complicated heterostructures significantly change the memory characteristics such as operation voltage, resistance ratio, and multilevel storage performance etc., especially when choosing unconventional materials such as perovskite oxides SrTiO3 (STO) and $BaTiO_3$ (BTO) as switching layers. In this review, we try to understand the multilayer memristive devices using conventional perovskite heterostructures such as $BaTiO_3$, $SrTiO_3$, $CaTiO_3$ as they are cheap to fabricate and easily integrable in industrial CMOS processes. Through this review, we aim to understand the origin and dynamic behavior of migration of oxygen vacancies within these materials.

D 034

Gd Dopped BTO Thin Films Fabrication by Reactive Sputtering Technique for Electronic Applications

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ABSTRACT

$BaTiO_3$ is an oxide material used in electronic industry used in a variety of applications such as memory devices, microwave transduces, resonators and filters, energy storage in high frequency systems, waveguides and modulators, and photonic switching applications. By sufficiently doping of rare earth materials will significantly enhances the characteristics of energy storage of these materials. In this work the Gadolinium (Gd) doped $BaTiO_3$ (BTO) thin films were fabricated using reactive sputtering technique on different base substrate of silicon. The XRD pattern confirms the pure phase formation of BTO films, further the structural properties was studies by Raman spectra. The optical properties were investigated by UV-VIS measurements. The morphology of fabricated thin films was validated by SEM, AFM microscopy techniques. The P-E loop measurement support that the fabricated thin films exhibit capacitor like properties. The thin films material of energy storage applications has been examined. The fabricated Gd-dopped BTO thin films has promising applications in electronics and energy storage.

D 035

New Double Perovskite (La_2FeCoO_6): Flexible Thin Film Based on Polymer Composite with Dielectric and Ferroelectric Properties

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ABSTRACT

The application of a double perovskite ceramic phase in polymer-ceramic nanocomposite films is an exciting possibility for the development of flexible films featuring many functions in general and energy storage devices in particular. Using the sol-gel combustion process, double perovskite nanostructures were produced, leading to the formation of a single-phase monoclinic system with the space group P21/n. X-ray diffraction (XRD) analysis was used to confirm the structure of the system. Using full-prof software, Rietveld's refinement of XRD data reveals detailed structural information. The flexible nanocomposite films with double perovskite La_2FeCoO_6 (LFCO) nanostructures and polyvinylidene fluoride (PVDF) polymer were fabricated by the solution casting method. To create flexible nanocomposite films, various volume percentages (10%, 20%, 30%, 40%, and 50%) of LFCO ceramic nanoparticles are incorporated as fliers in the PVDF polymer matrix. The structural properties of the developed nanocomposite films are investigated using XRD and FTIR studies, while microstructural features are investigated through SEM analysis. Dielectric properties of nanocomposite thin film are studied at different frequency ranges (1–200 kHz) using an LCR meter. Furthermore, the ferroelectric behavior of the nanocomposite thin film was systematically examined using a PE Loop Tracer. The double perovskite is emerging as a potential system for various functional applications. Remarkably, the nanocomposite thin film containing approximately 30 wt% of LFCO exhibited significantly higher dielectric permittivity, low dielectric loss, and increased remanent polarization, coercivity, and spontaneous polarization at room temperature. These findings highlight the potential of this nanocomposite film as a flexible energy storage system.

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D 036

Tuning Structural, Dielectric and Ferroelectric Properties of BTO-Based Ceramics by Ca^{2+} and Sn^{4+} Substitution

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ABSTRACT

Different strategies for tuning the properties of ferroelectric materials are of decisive importance for advancing electromechanical applications. Among several material synthesis techniques explored, site substitution is most promising and effective approach. The present work focuses on $Ba_{1-x}Ca_xSn_yTi_{1-y}O_3$ (BCST) ceramics prepared by solid-state sintering route with different substitution levels (x = 0, 0.05 and y = 0, 0.09). The impact of site substitution on the properties of Barium Titanate (BTO), considering phase purity, structural analysis, chemical composition, dielectric, and ferroelectric properties is studied. An ionic radii difference at A-site and B-site substitution is the key factor for significant change in properties. X-ray diffraction patterns ensure the formation of pure phase perovskite structure in all the compositions. Raman spectroscopy indicates Ca substitution not only occurs at the A-site but also within the oxygen octahedra, adversely affecting the properties. Ca and Sn act as strong grain growth inhibitors, leading to a fine-grained and dense microstructure in BCST. While Ca substitution has a limited impact on the Curie temperature (T_C), Sn substitution lowers T_C in BST (54°C) and BCST (50°C) compared to BTO (126°C). The Sn substitution results in the co-existence of multiple phases (rhombohedral, tetragonal and orthorhombic) in BST, enhancing its properties (ε' = 6118 at RT, P_r = 5.50 μC/cm^2, Q_{11} = 0.060 m^4/C^2, d*$_{33}$ = 526 pm/V) in comparison to BTO, making it a potential candidate for actuator applications.

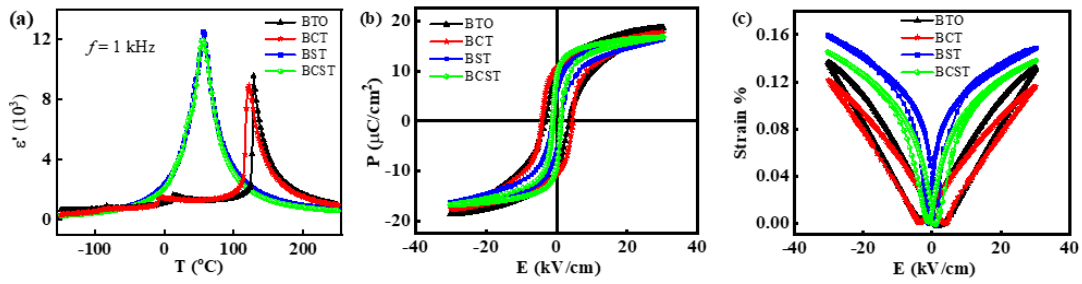

Figure 1. (a) Temperature dependent dielectric data (b) Room temperature PE and (c) Room temperature SE hysteresis loops for the BTO, BCT, BST, and BCST ceramics recorded at 10 Hz.

D 037

Lead-Free Magnetoelectric Poly(Vinylidene Fluoride) (PVDF)/$CoFe_2O_4$ Electrospun Fibers for Advanced Magneto-Mechano-Electric Nanogenerators

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ABSTRACT

Recently, polymer-based flexible nanocomposites are in great demand for design and development of energy harvesting devices. In this work, a high aspect ratio flexible PVDF/$CoFe_2O_4$ composite fibers were synthesised by electrospinning technique. Structural and morphological properties of PVDF/$CoFe_2O_4$ composite fibers were examined by XRD and SEM. The functional groups and percentage of electroactive β-phase were analysed using FTIR studies and achieved 67% of β-phase in the composite fibers with 10 wt % loading of $CoFe_2O_4$. The enhancement in dielectric and ferroelectric properties of the composite mats were observed with the incorporation of $CoFe_2O_4$. The magnetoelectric behavior of the composite fibers was confirmed by examining the ME coefficient values. The composite fibers were used to fabricate a biomechanical nanogenerator, which was capable of generating up to 12 V as a maximum voltage for a 10 wt% $CoFe_2O_4$-loaded fibers under finger tapping. Further, to harvest the stray magnetic energy, a magneto-mechano-electrical (MME) nanogenerator was built. When exposed to a weak AC magnetic field of 10 Oe at a frequency of 50 Hz, this MME generator produces a maximum peak-to-peak voltage of 13V and practical demonstrations with electrical home appliances were also performed.

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D 038

Magnetic and Antibacterial Properties of Ti^{4+} and Ag^{1+} Doped Cobalt Ferrites

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ABSTRACT

The spinel ferrites of AFe_2O_4 (A=Co, Zn, etc.) compositions have drawn attention because of their role in fabricating different electronic and magnetic devices, including microwave devices, data storage units, etc [1]. The materials also have different biomedical applications, such as antibacterial activity, drug delivery, hyperthermia, etc. In this paper, the magnetic and antibacterial properties of the parent and Ag^{1+} and Ti^{4+} doped cobalt ferrite (CFO, CAFO, and CTFO) samples, prepared using the sol-gel combustion technique, have been reported. The samples were found to have *Fd3m* space group with grain size in the range of 160-170 nm. The room temperature hysteresis loops of these samples studied using a maximum magnetic field of 15 kOe, are shown in Fig. 1. The values of the saturation magnetization (M_s), remanent magnetization, coercivity, experimental and theoretical magnetic moments, squareness ratio, and magneto crystalline anisotropy constant have been estimated. The doping of Ti^{4+} causes a significant enhancement in the value of M_s. We have studied the antibacterial activity of these materials using *S. aureus* and *E. coli* bacterial strains. Our findings show that the doped $CoFe_2O_4$ samples efficiently inhibited the growth of the microbes, and 200 mg/ml of Ti^{4+} doped cobalt ferrite is the most active material against *S. aureus* bacteria, with an 18 mm diameter of the zone of inhibition. We also find that this activity increases with increasing concentration, and the samples have shown better responses for Gram-positive bacteria than Gram-negative bacteria.

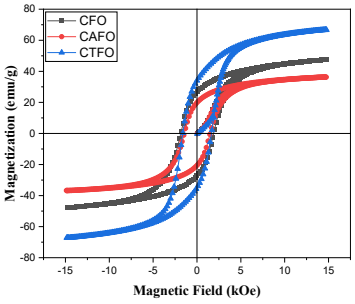

Fig.1. Room temperature magnetic hysteresis loops of the samples

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D 039

Effect of Doping on the Multiferroicity of Delafossite-Structured $CuCrO_2$

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ABSTRACT

A magneto-electric multiferroic material, $CuFeO_2$ is a member of the delafossite mineral group (ABO_2) has garnered a lot of interest because of its possible use in microwave frequency transducers, memory devices, sensors and also in photonic and spintronics systems. $CuCrO_2$ exhibits both ferroelectric and antiferromagnetic behavior having Neel temperature $T_N \approx 25$ K. M. Frontzek et al. reported that there are two magnetic phase transitions at 24.2K and 23.6K [1]. However, the transition temperature reported by L.Shijun et al. is at 23K. Doping $CuCrO_2$ with Ni, Co, Fe, Mn, and other elements may cause the material to exhibit ferromagnetic behavior with an elevated curie temperature. Table 1 shows the variation of some electric and magnetic properties of doped $CuCrO_2$. For Ni doped $CuCrO_2$, the transition temperature reduced to T~20.5 K with elevated magnetization [2]. However, Al doping results in the regain of its transition temperature to 23K. It should be noted that not only magnetic ordering, but also ferroelectric ordering is greatly affected by doping. It is argued that the Ni^{3+}-doping destabilizes the antiferromagnetic order of Cr^{3+} ions and modulates the spin configuration, leading to the weak ferromagnetism and enhanced ferroelectric polarization.

(**Table 1**: Variation of the electric and magnetic properties of $CuCrO_2$ on doping)

Material	Fabrication Method	Neel Temperature T_N (K)	Electric Polarisation P ($\mu C/m^2$)	Magnetization M(emu/g)
$CuCrO_2$	-	24.2, 23.6	24	0.0225(50K)
Ni doped $CuCrO_2$	Solid State Reaction	20.5	26	0.023(50K)
Al doped $CuCrO_2$	Solid State Reaction	23	NA	0.033(50K)

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D 040

2D Materials & Quantum Dots Based Photonic Synaptic Transistor (PST) for the Enhancement of Memory Operation in Artificial Visual System

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ABSTRACT

Information sensing, processing and memory operation are the building blocks of Artificial Visual System. Photonic Synapse is a promising component that can enhance the visual processing efficiency owing to the fast responsivity, low power consumption and large bandwidth. Herein, a Photonic Synaptic Transistor architecture has been developed having heterostructure configuration between Quantum dots and 2D materials layer. The chosen materials are Reduced Graphene Oxide (rGO) & Molybdenum Disulfide (MoS_2) as 2D layers and Carbon Quantum Dot (CQD) & Graphene Quantum Dot (GQD) as Quantum Dots which have been synthesized with a simple hydrothermal procedure. By the interfacial effect of high photosensitive characteristic of CQD & GQD and large surface area, enhanced semiconducting bandgap and high charge carrier mobility performance of rGO & MoS_2 2D layers show fundamental synaptic behaviors like excitory post-synaptic current, pair pulsed facilitation, plasticity i.e. transitions from short term to long term memory etc. This study mainly focused on the change in memory function with the different combinations of the above-mentioned materials, change in number of layers and change in thickness of the layers within the channel region; i.e. the device exhibits active layer dependent memory operation.

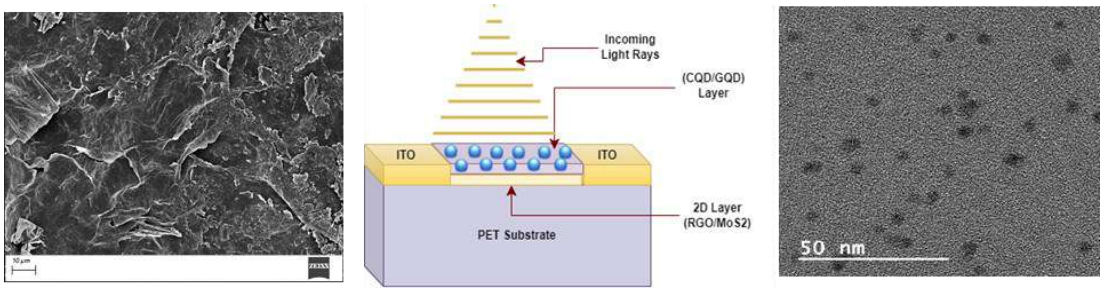

Fig. (left to right): FESEM image of rGO, Schematic Device Structure rGO/MoS2 and CQD/GQD heterostructure based Optoelectronic Synaptic Transistor, HRTEM image of CQDs

D 041

Effect of 3D Transition Metal Ion Doping on the Multiferroic Properties of $BaTiO_3$

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ABSTRACT

$BaTiO_3$, a renowned ferroelectric material, is explored extensively for its exceptional properties across various applications. This study investigates $BaTi_{1-x}M_xO_3$ (M = Fe, Cr, Mn, Ni) and the impact of transition metal ion doping concentrations. The findings reveal distinct structural stabilizations: Mn and Ni induce a singular, robust 6H-type hexagonal structure, while Fe and Cr induce double (Tetragonal and 6H) and triple phases (Tetragonal, cubic, and 6H) respectively [1]. In Figure 1(a), an intriguing linear correlation emerges between dopant concentration and maximum magnetization, attributed to increased dipolar interactions among magnetic ions [2]. Notably, unlike the behavior of other ion doping, Mn-doped $BaTiO_3$ exhibits decrease in magnetization with increase in concentration of dopant. Figure 1(b) demonstrates a concentration-dependent exponential decline in ferroelectric polarization due to high leakage current [3]. The coexistence of ferroelectricity, ferromagnetism, and piezoelectricity at room temperature in metal-doped barium titanate nanostructures underscores their intriguing multiferroic nature.

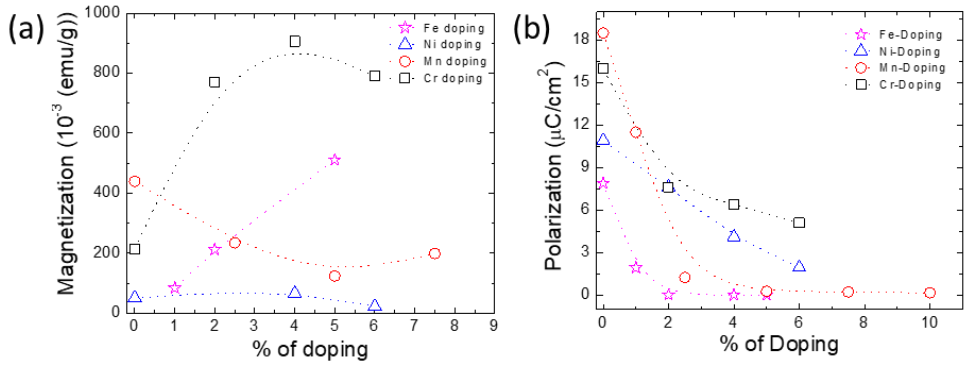

Fig.1 Doping concentration dependent (a) magnetization and (b) polarization of $BaTi_{1-x}M_xO_3$ at room temperature.

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D 042

Next Generation Lead-Free Ultra-High Ferroelectric Tunable Capacitors

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ABSTRACT

The past decade has witnessed remarkable advancements in wireless communication research. Nevertheless, the design and fabrication of environmentally friendly, low-cost, low-power, yet highly stable and tunable capacitors pose significant challenges. Perovskite complex oxides based ferroelectric materials possess the remarkable ability to alter their dielectric properties in response to the electric field, rendering them highly attractive for a wide range of applications, including tunable filters, sensors, actuators, and transducers. In our pursuit of advancing technology, we have successfully integrated high quality tunable capacitors, utilizing $Ba_xSr_{1-x}TiO_3$ (Sr-doped BTO) as the ferroelectric material, with $SrRuO_3$ serving as top-bottom metallic electrode on a $SrTiO_3$ and Silicon substrate. Our research has yielded impressive results identifying the underlying scientific issues- we achieved a maximum tunability of ~91% by varying the Sr concentration in $Ba_xSr_{1-x}TiO_3$ and carefully adjusting the film thickness to ensure minimal leakage while withstanding an electric field of 800 kV/cm. Building upon this success, we have also developed tunable filters with ~ 71% tunability on Silicon, and we are actively working to further improve this value. This achievement holds tremendous potential for the integration of ferroelectric-based capacitors into various industries.

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D 043

Influence of Particle Shape on the Surface Multiferroicity in Nanoscale Y_2NiMnO_6

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ABSTRACT

Magnetoelectric multiferroicity in surface and interface regions of nanostructured systems and thin film heterostructures and also in two-dimensional (2D) and van der Waals systems have started attracting the attention of the researchers [1] because of applications in novel spintronic devices and also for magnetic and electrical skyrmions [2]. In this work, we examined the room-temperature surface magnetism and ferroelectricity in nanocuboids and nanorods of Y_2NiMnO_6 – which in bulk form exhibits multiferroicity below TN ~70 K. The surface area to volume ratio is higher in the former case. The nanoparticles were synthesized by hydrothermal process and characterized by powder x-ray diffraction, field-emission scanning and transmission electron microscopy, and x-ray photoelectron spectroscopy. While crystallographic structure is monoclinic (P21/n) in both the cases with lattice parameters a = 5.222 Å, b = 5.550 Å, c = 7.477 Å, β = 89.865o, the average size of the particles is ~100 nm. Mapping of compositional homogeneity by energy dispersive x-ray spectra yields variation of surface defects (oxygen vacancies within a region of ~10 nm at the surface) in particles of different shape. Surface Mn^{3+}/Mn^{4+} ratio varies from ~75%:25% (nanocuboid) to 70%:30% (nanorod). This variation results in magnetic coercivity to be ~20 (nanocuboids) and ~30 Oe (nanorods). The magnetic domain size, probed by magnetic force microscopy, varies within 0.5-1.5 µm. The remanent polarization varies within ~2 to ~10 nC/cm2. In spite of weak surface magnetization and polarization, the magnetoelectric coupling – decrease in remanent polarization under a magnetic field (0-20 kOe) – is quite large as the surface ferroelectricity is induced by surface ferromagnetism via antisymmetric Dzyaloshinskii-Moriya exchange interaction driven by large spin-orbit coupling [3]. These results show that, along with 2D and van der Waals systems, even the surface of the nanostructured particles harness room-temperature surface multiferroicity.

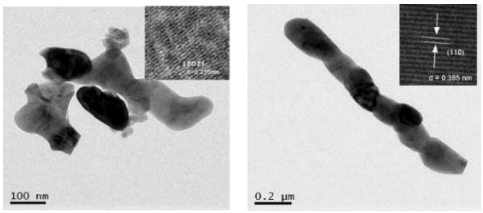

Fig. The TEM and HRTEM images for the (left) nanocuboids and (right) nanorods.

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D 044

Structural and Electrical Studies of Manganese Nickel Ferrite Prepared by Ceramic Technique Using High Energy Ball Milling

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ABSTRACT

In this study, a series of nickel substituted manganese ferrites of the compositional formula $Mn_{1-x}Ni_xFe_2O_4$ (x=0, 0.05, 0.15, 0.25, 0.35, 0.45) were synthesised via the ceramic technique using high energy ball milling. The prepared samples were calcined at 900°C for 1h. The calcined powders were pressed into pellets and sintered at 1200°C for 2h. The sintered samples were used for various characterizations. X-ray diffraction (XRD) and FTIR was done for structural and phase analysis. The XRD spectral analysis confirmed the single phase with spinel structure and the diffraction peaks are found to be improved in the higher nickel containing samples. The calculation of the structural parameter like crystallite size and lattice constant of samples were carried out using XRD data and studied for the varying nickel content. The room temperature electrical measurement such as dielectric constant, dielectric losses, ac conductivity and impedance were measured with variation of frequency for the different ferrites. The electrical parameters showed dispersion behaviour with variation in frequencies and using the impedance data the Nyquist plot obtained determined the conduction mechanisms in the samples. The results obtained have been discussed and reported in the paper.

Keywords: *manganese ferrite; X- ray diffraction; FTIR; dielectric constant; Nyquist plot.*

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D 045

Room Temperature Dielectric Mechanism in $Ni_{1-x}Zn_xFe_2O_4$ system

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ABSTRACT

Spinel Ferrites is a potential aspirant in the ferrite family due to its unique structural, optical, electrical and magnetic properties. $NiFe_2O_4$ is well renowned spinel ferrite material exhibiting ferrimagnetism with low tangent loss and high electrical resistivity[1,2]. The materials having high dielectric properties combined with magnetic properties is an asset for manufacturing efficient microwave application devices[3]. The presence of tetrahedral and octahedral sites is the reason behind the unique magnetic and electrical properties of $NiFe_2O_4$. Incorporation of foreign elements in these sites alters the magnetic and electrical properties of $NiFe_2O_4$. The incorporation of foreign elements in tetrahedral or octahedral sites induces a strain in the system which affects the movement of charge carriers in the system and it affects the optical and dielectric properties of the system. The present work elucidates the structural, optical and dielectric properties of the $Ni_{1-x}Zn_xFe_2O_4$. Zn substituted $NiFe_2O_4$ ($Ni_{1-x}Zn_xFe_2O_4$, x = 0.00, 0.25, 0.50, 0.75 and 1.00) are successfully synthesized by modified combustion technique. Rietveld refined XRD patterns reveal that inverse spinel structure of $NiFe_2O_4$ is turned into a normal spinel structure having space group Fd-3m with Zn substitution. FE-SEM analysis reveals that the grains of $Ni_{1-x}Zn_xFe_2O_4$ are arranged in a honeycomb structure and the grain size increases with Zn substitution. It is found that band gap increases with Zn substitution which is due to the decrease in localized states in the system, as confirmed by the variation of Urbach energy. The variation of band gap and Urbach energy influences the formation of space charge and free charge carriers which affects the dielectric properties of the system. Dielectric measurement reveals that the dielectric permittivity and dielectric loss decreases with Zn substitution. This variation in dielectric properties is mainly due to the space charge polarization, dipolar polarization and atomic polarization occurred in the system caused by the movement of free charge and space charge carriers in between the grains through grain boundaries. The polarization is originated by induced strain in the lattice, influence of localized states and nature of grain and grain boundary effect in the system and it will be discussed in detail.

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D 046

Synthesis and Investigations on Structural, Microstructural and Electrical Properties of Lithium Copper Ferrite Prepared by Ceramic Technique Using High Energy Ball Milling.

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ABSTRACT

Polycrystalline lithium copper ferrite ceramics with the compositional formula $Li_{0.5-0.5x}Cu_xFe_{2.5-0.5x}O_4$ where $0.1 \leq x \leq 0.5$ in steps of 0.1 have been synthesized by the conventional ceramic technique using ball milling technique. The prepared powder of lithium copper ferrite was calcined at of 900°C for 3h and sintered at 1000°C for 3h. Structural, morphological and electrical properties were studied by XRD, SEM and Impedance analyzer. XRD analysis confirmed the single phase spinal structure of the samples. SEM microphotographs revealed the grain size and grain size distribution of the ceramics prepared. The frequency dependence of the electrical properties were studied using an impedance analyzer and the dispersion behavior has been observed. The results have been discussed in the paper.

Keywords: *Lithium Copper ferrite, XRD, SEM, spinel.*

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D 047

Synthesis and Investigation on Structural, Electrical and Permeability Properties of Nickel Substituted Co-Zn Ferrites by Ball Milling Technique

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ABSTRACT

Nickel substituted Cobalt Zinc Ferrite with the compositional formula $Co_{0.8-x}Zn_{0.2}NixFe_2O_4$ (x=0.0, 0.05, 0.1, 0.15, 0.2, 0.25) have been synthesized by the conventional ceramic technique using ball milling technique. The prepared powder of cobalt zinc nickel ferrite was calcinated at 900°C for 3h and sintered at 1100°C for 3h. Structural, morphological, electrical properties were studied by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Impedance Analyzer. XRD analysis confirmed the single-phase spinel structure of the samples. The structural properties such as lattice constant, crystallite size, x-ray density was evaluated from the XRD data. SEM microphotographs revealed the grain size and grain size distribution of the ceramics prepared. The frequency dependence of the electric and permeability properties were studied using an impedance analyzer and the dispersion behavior has been observed. The results pertaining to the results are reported in the paper.

Keywords: *Nickel substituted cobalt zinc ferrite, XRD, SEM.*

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D 048

Modulation of dielectric and ferroelectric behavior of Sodium Niobate ($NaNbO_3$) by partial substitution of Na by Li in view of Energy harvesting system

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ABSTRACT

Piezoelectric materials are extensively exploring in energy harvesting as they can generate electricity from surrounding vibrations and strain. In the search for the lead free piezoceramics to replace Pb-based perovskites, sodium Niobate is gaining attention due to increased interest in environment protection. With this objective we have synthesised lithium doped $NaNbO_3$ system ($Na_{1-x}Li_xNbO_3$ where x = 0.02 to 1) by hydrothermal synthesis route. Structure is confirmed by X-ray diffraction techniques and Rietveld refinement has been carried out to extract the structural information. To validate its suitability for energy harvesting Electrical performance is revealed by measuring dielectric and ferroelectric behaviour with the help of impedance spectroscopy using potentiostat Auto lab 204, from temperature range 450^0C to room temperature from frequency range 1 Hz to 1MHz. The dopant induced ferroelectric behaviour has been systematically studied by P-E loop tracer. Energy harvesting ability is demonstrated.

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D 049

Tailoring the Switching Performance of Tantalum oxide-based Memristive devices by Interface Engineering

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ABSTRACT

Utilizing resistive switching properties, memristive devices have emerged as promising options for applications in non-volatile memory and neuromorphic computing[1], [2]. This study focuses on enhancing the switching performance of Ta_2O_5 memristive devices through the application of interface engineering[3], [4]. The research presents a demonstration of a Ta_2O_5 -based bipolar resistive switching device achieved via interface engineering. This involved the introduction of an ultra-thin interfacial layer (SiO_2)[5] and (HfO_2/SiO_2) with distinct features, such as a large band gap and a specific level of negative heat of oxide formation, positioned between the top electrode (TiN) and the resistive layer (Ta_2O_5). The investigation also delves into the role of defects and charge trapping at the interface, providing a more profound understanding of the fundamental mechanisms governing resistive switching in Ta_2O_5-based devices. The devices exhibit exceptional nonlinear properties under both positive and negative bias. Furthermore, the study explores the potential implications of the refined switching performance for practical applications like non-volatile memory and neuromorphic computing. The ability to control and enhance resistive switching behavior through interface engineering opens up new avenues for developing and deploying efficient and reliable memristive devices.

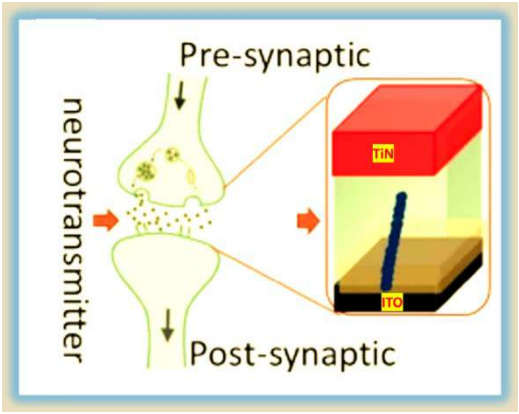

Figure 1: A simplified diagram of a biological synapses based on TiN/SiO_2/Ta_2O_5/ITO memristor with two terminal structures.

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D 050

Frequency dependence Dielectric behavior of lead free (1-x)BZT-xBCT (BCZT) ceramics

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ABSTRACT

We report the perovskite type (1-x)BZT-xBCT (BCZT) (x=0.4, 0.5 and 0.6) lead free composite ceramics prepared by solid state reaction process. A highly dense microstructure of nearly 95% of theoretical density was achieved for the ceramic sample sintered at 1450^0C for 5 hr. The XRD analysis revealed a pure perovskite structure with coexistence of tetragonal and rhombohedral phases at morphotropic phase boundary (MPB). The lossy behavior of ceramic sample may be corroborated to non-infinite resistance was perceptible from *P-E* hysteresis loop. The dielectric constant value (ε_r) of 540 and 1.0 tangent loss (*Tan*δ) at 500^o C was achieved in the ceramic sample. Both the (ε and *Tan*δ) value decrease with increasing frequency at different temperature (25^0C-500^0C) over a frequency range 1kHz to 1MHz. The exotic dielectric response may be attributed the involvement of different polarization, approaches towards a relaxor type of ferroelectric. Further

Keywords: *ceramic sample, composite, relaxor, lossy, polarization;*

D 051

Investigation of half-metallic ferromagnetism in Transition-Metal-Doped Calcium Oxides using mBJ-GGA Approach

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ABSTRACT

The present study investigated the structural, electronic, and magnetic properties of Ca1-xTMxO (TM= Ti, V) at x = 0.125 and 0.25 using Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method based on the density functional theory (DFT). The resultant compounds were found to exhibit half-metallicity with 100% spin polarization at the Fermi level (EF). The electronic and magnetic properties were calculated using the mBJ-GGA approach. The total magnetic moments of Ca1-xTixO and Ca1-xVxO at x = 0.125 and 0.25, were found to have integer values of ~2 μB and 3 μB, respectively, which indicated the half-metallic ferromagnetism (HMF) in these compounds. The p-d hybridization between O-p states and TM-d states is responsible primarily for the HMF. Additionally, the half-metallic (HM) gaps were calculated for the reported compounds. The predicted HM gap suggests that these compounds can be utilized as effective materials for spintronic applications.

D 052

Exploring magnetic properties of Cu-doped in Itinerant Ferromagnet $SrRuO_3$

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Tuning the magnetic properties in 4d-based perovskite oxide $SrRuO_3$ has garnered much interest owing to their complex interplay between structural, transport and magnetism, and their potential applications in spintronics device. Herein, we present a detailed investigation of the structural, microstructural, chemical composition and magnetic properties of Cudoped: $SrRu_{x-1}Cu_xO_3$ (x= 0 – 0.25) samples, which were synthesized using conventional solid-state technique. Room temperature X-ray diffraction patterns of these prepared samples revealed only pure phase of orthorhombic structure with space group P*nma*. Moreover, the magnetic investigations of these $SrRu_{x-1}Cu_xO_3$ samples showed several interesting magnetic features. For instance, the temperature-dependent magnetization (M vs. T) measurements exhibited the ferromagnetic behaviour below their Curie temperature (T_C), while the T_C is found to be intriguingly decreased from 163 to 128 K with doping of Cu^{2+} from x = 0 to 0.25 % at the Ru-site in $SrRu_{1-x}Cu_xO_3$ (see Fig. 1). Moreover, the 5-K field-dependent magnetization (M vs. H) curves exhibited the hysteric characteristics, and the obtained magnetization value at 6 T is uncovered to be reduce from 1.45 to 0.69 μ_B/Ru with x = 0 to 0.25 doping of Cu^{2+} (see Fig. 1). Furthermore, the remanent magnetization and coercive field were assessed from the measurement of M vs. H curves at different temperatures, and it followed the same characteristic as M vs. T. Interestingly, the magnetic dynamics from the AC-χ measurements on these samples showed that these samples were not belong to the spinglass magnetic behavior. The present study unveils the understanding of the magnetism and tuning the magnetic properties in Cu^{2+} doped in 4d-based perovskite oxide $SrRuO_3$.

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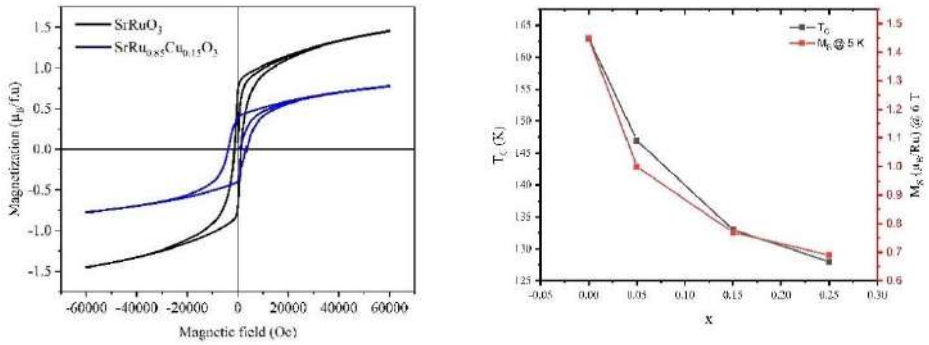

Figure 1: Field-dependent magnetization (M vs H) curve of $SrRu_{x-1}Cu_xO_3$ samples (Left panel), and the Curie temperature (Tc) and saturation magnetization (Ms) with the function of Cu-doping in SrRu1-xCuxO3 (right panel).

D 053

Spark Plasma Sintering characteristics of Li:ZnO and comparison to Flash and Conventional sintering

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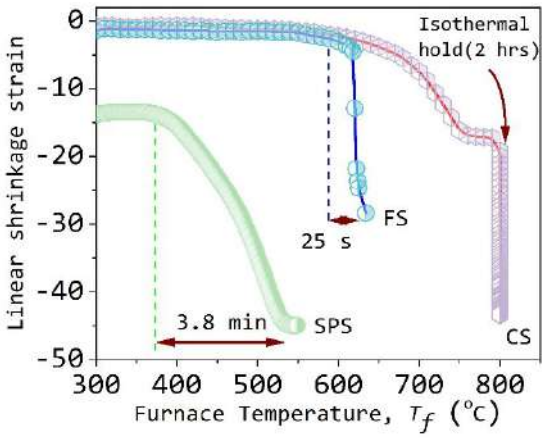
ABSTRACT

Zinc oxide is an archetypal *n*-type wide bandgap (3.3 eV) semiconductor, the electronic conduction originating from native point defects such as oxygen vacancies and zinc interstitials. Doping ZnO 'amphoterically' (both at substitutional and/or interstitial sites), especially with Li, produces *p*-type conductivity (Null↔ $Li_{Zn}^{'} + h^{\bullet}$), and may also induce ferromagnetism by stabilizing cation vacancies (Null↔ $2Li_i^{\cdot} + V_{Zn}^{''}$). The Li:ZnO system thus poses scientific and practical interest, and obtaining dense sintered (Conventional Sintering-CS) compacts have been attempted since 1978 [1]. Recently, electric field assisted sintering methods (Flash Sintering-FS and Spark Plasma Sintering-SPS) have evolved as major advancements reducing the sintering time and temperature considerably [2]. In this work we demonstrate the synthesis of Li:ZnO powders and study their structural changes; we subsequently compare the sintering behaviour and microstructures of the powders under FS and SPS. The addition of Li reduces the sintering temperature in both SPS and FS. The shrinkage strain rate, $\dot{\epsilon}$ in SPS was swift ~0.11-0.16/s and increasing with Li addition but was many orders higher in FS. SPS samples show uniform microstructures with an optimal Li content of 0.14 showing improved toughness. In contrast, FS samples show clear evidence of ion migration and electrochemical reactions near electrodes. Ac impedance measurements are also presented.



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D 054

Controlling tungsten structural phases via sputtering process parameters for spintronic applications

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ABSTRACT

Spin-orbit coupling (SOC) plays a crucial role in spin-to-charge interconversion [1]. Here, we report a systematic investigation of the growth of tungsten (W) by tuning sputtering process parameters and its influence on spin Hall angle ( ). The structure zone model explains the observed surface topography for a constant thickness which follows the VolmerWeber growth mechanism [2]. The X-ray diffraction and resistivity results reveal that W exhibits a structural phase transition from + -W to -W as a function of Ar deposition pressure ( ). The kinetic energy of sputtered atoms and the adatom's surface mobility determines the phase formation. W deposited with different deposition rates ( ) at constant suggests that the relative phase fraction of -W is tunable by where the observed resistivity further supports the observations. Thickness-dependent XRD and resistivity results manifest that the W phase is controllable via sputtering process parameters than its thickness. Ferromagnetic resonance-based spin pumping reveals that the enhanced linewidth broadening for (Permalloy or Py)/ + -W is due to spin transport across the interface. The maximum spin-mixing conductance is 10.1× 10 , with no magnetic dead layer. The estimated spin diffusion length is 0.98 (±0.01) nm. The estimated spin transparency is 0.74. Inverse spin hall effect (ISHE) is demonstrated for Py (20)/ + -W (10). The majority contribution for the voltage drop is owing to ISHE contributions. The estimated is found to be −0.24 (± 0.08). Our systematic study can give a guideline for choosing optimum sputtering process parameters for low-power-driven spintronic devices.

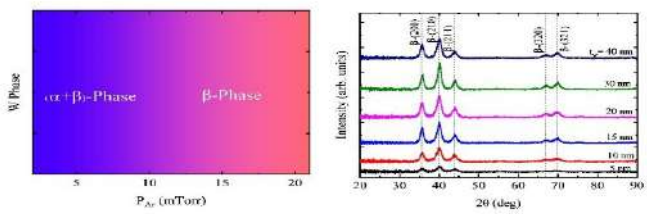

Fig 1: (a) Structural phase transition mapping from + -W to -W as a function of Ar deposition pressure. (b) Grazing incidence X-ray diffraction (GIXRD) result of 40 nm W as a function of Ar deposition pressure.

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D 055

Structural and Dielectric studies of $La_2Ni_{0.5}Cr_{0.5}MnO_6$ Double Perovskite

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ABSTRACT

$A_2BB'O_6$ based ceramic double perovskite sample $La_2Ni_{0.5}Cr_{0.5}MnO_6$ was developed using sol-gel method. X-ray diffraction peak profile confirmed the purity phases in the prepared double perovskite sample. Rietveld refinement performed using recorded XRD pattern suggested that ordered monoclinic ($P2_1/n$) phase exist along with disordered orthorhombic (*Pbnm*) and rhombohedral (*R3c*) structural phases. FESEM revealed the densely packed grains possessing well-defined grain boundaries with random distribution. Both dielectric constant and tangent loss (tanδ) exhibited dispersion at high temperature and low frequency. Dielectric constant showed a continuous decreasing trend with increase in frequency. The cation ordering at B/B′ octahedral sites have significantly influenced the dielectric constant due to individually strong localized polarizations [1]. Cole-Cole plots proposed a non-Debye type relaxation and indicated NTCR (negative temperature coefficient of resistance) behaviour for the synthesized sample [2]. The large dielectric constant and small tanδ at room temperature suggests its suitability in energy storage capacitor application.

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D 056

Synthesis and Characterisation of Cadmium Manganese Ferrite using Sol-gel Method

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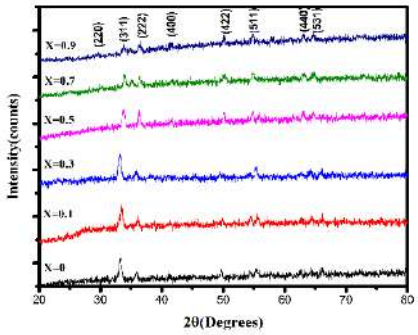
ABSTRACT

Utilizing the sol-gel technique, cadmium doped manganese (Mn- Cd) ferrite ($Mn_{1-x}Cd_xFe_2O_4$) nanopowders were synthesized. Pure spinel phase ($Mn_{1-x}Cd_xFe_2O_4$) with bigger crystallite size was obtained through X-ray diffraction (XRD) examinations. Fourier transform infrared spectroscopy (FTIR) research is used to identify the possible stretching and functional groups of title compound. The optical properties of the sample studied with UV visible ultraviolet (UV) spectrometer. The magnetic properties of after-calcined nanoparticles were measured at room temperature using a vibrating sample magnetometer (VSM). The electrical conductivity of the samples was analyzed by using current voltage (IV) technique. The dielectric constant and dielectric loss dependence on doping level and frequency at room temperature were also studied. The obtained data are extensively examined and understood



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D 057

Synthesis of ferrite and garnet nanoparticles for spintronics applications

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ABSTRACT

Ferrite and garnet nanoparticles have great importance in fundamental science, due to their unique chemical, electrical, mechanical, magnetic properties as well as their applications in high-density recording devices, spintronics, magnetic separation and drug delivery etc. [1-4]. Nanopowders of different spinel ferrites ($ZnFe_2O_4$, $MnFe_2O_4$ and mixed Mn-Zn ferrites), as well as Yttrium iron garnet (YIG) nanoparticles were prepared by the citrate combustion method [4-6]. Single-phase spinel and garnet structure were confirmed from the X-ray diffractograms. The particle sizes estimated from the XRD peaks were in a range 15-30 nm for powders calcined at 600°C/5 hours, whereas it varies from 50 -100 nm with the increase in the calcination temperatures (800-1000°C/3 hours). Particle sizes were also confirmed from the scanning electron micrographs (SEM). Saturation magnetization was low, whereas Curie temperatures were found to be higher for the nanopowders as compared to corresponding sintered bulk samples, due to particle size effects. The structural and magnetic studies on spinel ferrite as well as garnet nanoparticles will be discussed and presented in this paper.

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D 058

Nanomaterials for Energy Applications Relaxor Behavior of perovskite material

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ABSTRACT

Pellets composed of gadolinium-doped lead zirconate perovskite were prepared. The crystallization of perovskite was analyzed via XRD at 300 K, which confirmed the singlephase (tetragonal) system with the desired cation stoichiometry. The material under investigation follows the specific formula $Pb_{1-x}Gd_x(Zr_{0.50}Ti_{0.50})_{1-x/4}O_3$, (x = 0.03, 0.06, and 0.09). The incorporation of gadolinium, a soft dopant, enhances the ferroelectric and dielectric properties compared to undoped perovskite material. A noticeable variation in the critical temperature was observed with changes in composition, with the transition temperature decreasing as Gd^{3+} concentration increases. Confirmation of the tetragonal shape prepared perovskite was also confirmed by calculating the tolerance factor. Furthermore, the real and complex parts of dielectric permittivity were determined, along with the dielectric constant, Tangent loss, and Quality factor. Material under investigation exhibited characteristic Relaxor behavior and a Diffuse Phase Transition (DPT) with diffusivity falling within the range of 1-2. This distinctive relaxor behavior holds significant commercial potential for applications such as actuators and multilayer capacitors.

Keywords: *PGZT; XRD; Relaxor; tan δ; DPT*

D 059

Solution-Processed $ZnFe_2O_4$-based Heterostructure Thin Film for Multilevel Resistive Switching Memory

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ABSTRACT

World digitalization and technological modifications require further improvement in data storage memory devices to fulfill future needs.[1,2] Over the past decade, resistive switching (RS) memory has acted as one of the promising candidates for non-volatile memory devices because of its low power consumption, scalability, and simple metal-insulator-metal structure.[3] Integrating the multifunctionality in a single device further enhances the device's applicability and tunability.[4] Here, we have studied the spinel-structured $ZnFe_2O_4$ (ZFO) thin film potential for multilevel RS in a heterojunction with n-type TiO_2 prepared simply by a sol-gel spin coating method, making our device a cost-effective solution. The simple bilayer device structure of FTO/TiO_2/ZFO/Ag shows bipolar RS behavior with stable endurance performance for >500 cycles and retention stability for up to 10^4 s with an ON/OFF ratio of ~100. The study of the charge transport mechanism further explores the TiO_2/ZFO interface responsible for multilevel RS arising due to negative differential resistance (NDR) effect during the RESET process for highly stable memory devices.

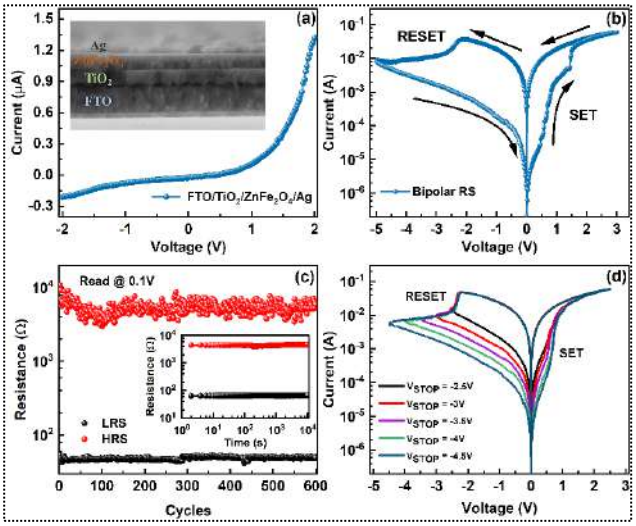

Figure 1. (a) Pristine state I-V for TiO_2/ZFO heterostructre (Inset shows cross-section FESEM). (b) Bipolar RS behavior, (c) endurance (inset: retention) data, and (d) multilevel RS performance for FTO/TiO_2/ZFO/Ag device.

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D 060

Micromagnetic Study of Exchange Bias in Co_2MnSi/IrMn-Based Heterostructures

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ABSTRACT

Recently, the exchange bias (EB) phenomenon, discovered in Co/CoO core-shell nanoparticles, has sparked enormous research interest in several ferromagnetic (FM) and antiferromagnetic (AFM) bilayers due to its intrinsic crucial role in spintronics devices. In this study, using micromagnetic simulation Mumax[3], we first report the emergence of negative Exchange Bias (EB) in the Co_2MnSi (CMS) Heusler alloy interfacing with an uncompensated AFM, exhibiting anisotropy phenomena likewise in IrMn-based exchange-coupled multilayers. Relatively to the higher pinning and AFM anisotropy values, we observe strong enough EB in such heterostructures. Our investigation suggests that while coercivity displays a non-monotonic increment with the increase in CMS layer thickness, however, EB reveals an inverse relationship. The analysis of spin canting angles suggests the presence of a maximum canting angle for the small number of spins in the CMS layer, which is close to the interface. We thoroughly analyze the spin configurations at the interface as well as away from it in the CMS (25 nm)/IrMn (5 nm) bilayer (a square shaped nanodot of dimension 128 nm × 128 nm) to better understand the mechanism of magnetization reversal. In cases of small AFM thickness (t_{AFM}), the exchange field proportionately increases with the t_{AFM}, whereas for large t_{AFM} (~ 25 nm), it scales as $1/t_{AFM}$. On the other hand, in addition, coercivity increases for all thickness of t_{AFM}. Interestingly, the angular dependence of the coercivity of the Co_2MnSi Heusler alloy exhibits a four-fold symmetry, thereby indicating cubic anisotropy, and a two-fold symmetry, representative of uniaxial anisotropy. Furthermore, the angular dependence study of EB revealed identical clockwise and counterclockwise rotations, with cos (θ) unidirectional dependence. Additionally, through the manipulation of the Meiklejohn-Bean parameter (R), we can adjust the magnitude of the coercive field and EB. All these results are crucial for the utilization of the Co_2MnSi/IrMn heterostructures for various applications in spintronics-based devices.

D 061

Design of Low Power Sense Amplifier for Enhanced Memory Performance

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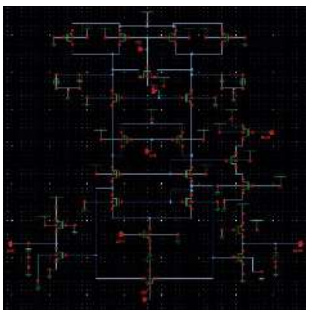
ABSTRACT:

VLSI plays a crucial role in the modern IT industry by allowing us to increase the power, size, speed, and efficiency of electronic equipment through the integration of millions of tiny switches onto a single computer chip. The performance and effectiveness of contemporary digital systems, such as DSPs, microprocessors, microcontrollers, and other computing devices, are heavily influenced by the design of their memory components. This paper highlights the critical importance of memory blocks, specifically sense amplifiers, in these systems and their role in achieving high-speed operation, low power consumption, and improved data storage quality for various forms of data, including audio, video, and images. This research presents innovative sense amplifiers that reduce sensing latency and increase power efficiency, as demonstrated by simulation results using 90nm technology.



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D 062

Structural, Magnetic and Ferroelectric Properties of ($0.7BiFeO_3$-$0.3BaTiO_3$) -(1-*x*) $NiFe_2O_4$ (*x* = 0.00 and 0.10) Ceramics

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ABSTRACT

Polycrystalline ($0.7BiFeO_3$-$0.3BaTiO_3$) -(1-x) $NiFe_2O_4$ (x = 0.00 and 0.10) ceramic compounds were prepared using solid-state reaction method and investigated the structural, magnetic, and ferroelectric properties of the compounds. Structural analysis revealed that the compound exhibited a rhombohedral structure with the *R3c* space group. The magnetic properties of the compounds show a decrease in saturation magnetization with the increase of x. The ferroelectric measurements indicated that remanent polarization increases with the increase of x.

Keywords: *Multiferroics, G-type antiferromagnetism, ferroelectric, band energy gap*

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D 063

Influence of Rare Earth Ion Substitution on Structural, Optical Properties of $Bi_{0.9}R_{0.1}Fe_{0.9}Sc_{0.1}O_3$ (R = La and Ho) Ceramics

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ABSTRACT

Polycrystalline $BiFeO_3$, and $Bi_{0.9}R_{0.1}Fe_{0.9}Sc_{0.1}O_3$ (R = Ho and La) compounds were prepared using solid-state reaction method and investigated the structural, microstructural, and optical properties of the compounds. Structural analysis revealed that the compound exhibited rhombohedral structure with *R3c* space group. Scanning electron micrographs confirmed the formation of dense, well-connected grains exhibiting a reduction in size in the substituted compounds. The optical absorption measurements indicated an increase in the energy band gap of $BiFeO_3$. The band gap of $BiFeO_3$, $Bi_{0.9}La_{0.1}Fe_{0.9}Sc_{0.1}O_3$, and $Bi_{0.9}Ho_{0.1}Fe_{0.9}Sc_{0.1}O_3$ compounds are 2.03 eV, 2.04 eV, and 2.06 eV, respectively.

Keywords: *Multiferroics, G-type antiferromagnetism, ferroelectric, band energy gap.*

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1. W. W. Eerenstein, N. D. Mathur and J. F. Scott, Nature, **442**, 759-765 (2006)
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E 001

Carbon Quantum Dot Sensitized Nanocrystalline ZnO Thin Films for Efficient Photoelectrochemical Hydrogen Generation

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ABSTRACT

Addressing future energy crisis, in an efficient way, is the prime concern of today's scientific community. One of the solutions to address the global energy crisis is the utilization of Solar energy but this being an intermittent source of energy, there is an urgent need for an efficient and environmental friendly method to store the solar energy in the useful form. Among the methods of solar energy harvesting, photoelectrochemical (PEC) splitting of water is an environment friendly method which utilizes the abundantly available solar energy to produce green and clean hydrogen fuel. Metal oxide semiconductors are the most researched materials for the purpose, due to their photocatalytic nature. Among them, Zinc Oxide (ZnO) is being explored for the purpose due to its excellent characteristic features such as relative abundance, low cost, non-toxicity, and high electron mobility but since its absorption lies in the ultraviolet range, it leaves a major part of solar energy unutilised. To overcome this drawback of ZnO, current research work focuses on the utilization of Quantum dots (QDs) as photosensitizer to make an efficient PEC system. Visible energy absorbing and hydrothermally prepared carbon quantum dots (CQDs)has been used to enhance the PEC water splitting efficiency of ZnO thin films synthesised by Sol-gel Method. ZnO thin films have been sensitized by CQDs for various time to have the optimized photo response. Enhanced photocurrent density and solar to hydrogen conversion efficiency was observed for all the sensitized samples. Highest photocurrent density of 3.08 mA cm^{-2} at 0.95V versus SCE was exhibited by the 48 hours CQDs sensitized ZnO thin film. Systematic investigation of structural, optical and morphological properties has been carried out. Photoelectrochemical (PEC) response viz., photocurrent density, Mott-Schottkey analysis, charge carrier concentration, barrier potential etc. has also been explored to understand and explain the enhanced photo response of CQDs sensitized ZnO thin films.

E 002

Facile Synthesis Methods and Electrical Transport Properties of Bismuth (Bi) Doped $SnSe_2$ Nanoparticles

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ABSTRACT

Pure Tin diselenide ($SnSe_2$) and Bismuth doped Tin diselenide $Sn_{1-x}Bi_xSe_2$ (x=0.5) nanoparticles were successfully synthesized using a facile hydrothermal method and co-precipitation method respectively. Subsequently, a comprehensive investigation was carried out to analyze their thermoelectric transport properties. The prepared samples are analyzed by XRD, SEM, EDX, UV-Visible and FTIR techniques. From charge transport studies thermoelectric parameters such as electrical resistivity, Seebeck coefficient and power factor were determined. The hexagonal crystal structure of $SnSe_2$ and $Sn_{1-x}Bi_xSe_2$ (x=0.5) is confirmed from XRD. From the Scherrer formula the estimated particle size of $SnSe_2$and $Sn_{1-x}Bi_xSe_2$ (x=0.5) are 21.6 nm and 15.96 nm respectively. The SEM image reveals the flower like surface morphology of for $Sn_{1-x}Bi_xSe_2$ (x=0.5). The chemical compositions are confirmed by EDX. From the UV-vis spectrum, a broad absorption peak is found at 619 nm with a band gap value of 1.35 eV from the Taue plot. The presence of different vibrational frequencies confirms the functional group in FTIR. Charge transport studies show that doping of Bi in $SnSe_2$ boosts the electrical conductivity by raising the charge carrier concentration while still preserving high carrier mobility, resulting in increased power factor of 19.63 $\mu Wm^1 K^{-2}$ at 573 K compared to the pure $SnSe_2$ (1.5 $\mu Wm^{-1} K^{-2}$ at 573 K) nanoparticle. Comparing the results of pure $SnSe_2$ and $Sn_{1-x}Bi_xSe_2$ (x=0.5), it is revealed that the annealing process and addition of Bi are essential for improving the thermoelectric performance of $SnSe_2$. $Sn_{1-x}Bi_xSe_2$ (x=0.5) nanoparticles and has the potential to be a good thermoelectric material. Further the Bi doped studies are to be extended to other concentrations.

Keywords: *Thermoelectric; Bi doping $SnSe_2$, Transport properties, hydrothermal method*

E 003

Hematite Thin Films Sensitized by Quantum Dots for Solar Hydrogen Generation by Photoelectrochemical Splitting of Water

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ABSTRACT

For widespread use of hydrogen as a fuel, burning need is to develop a clean, economical and sustainable method for its large-scale production. In this regard, photoelectrochemical (PEC) based system for hydrogen production via splitting of water using solar energy is considered to be the most promising, being non-polluting, wasteless and renewable. The method utilizes water and solar energy, both of which are abundantly available. Major impediments in the commercial viability of PEC system are the low efficiency and corrosion of semiconductor electrodes in existing systems. Recent research in the area is to develop suitable semiconductor by modifying their properties by newer technologies to get favourable properties for splitting of water in PEC cell. Recent advancement in nanotechnology has led to the development of quantum dots (QDs), which has applications in various fields due to their size tunable properties. Exploiting the properties of QDs, research work being presented here is on the design and development of QDs sensitized metal oxide (MOS) photoelectrodes for efficient generation of hydrogen using solar energy. Thin films of nanoporous undoped hematite prepared by spray pyrolysis were sensitized by CdSe QDs using chemical bath deposition method. Loading time of sensitizer to hematite thin films was found to be crucial in affecting its PEC properties. Film having sensitizer loading time as 42 h exhibited best photocurrent density of 553 $\mu A/cm^2$ at 1.0 V versus the reference electrode; SCE (Saturated Calomel Electrode). As a next step, sensitization on Zr doped hematite thin films has also been investigated for their PEC response. Highest photocurrent density of ~1.12 mA/cm^2 at 0.8 V/SCE electrode potential was observed for 48 h CdSe QDs sensitized hematite thin film. The novelty of the current study lies in the fact that it has explored the possibility of using narrow band gap QDs (CdSe) sensitization on a narrow band gap film (hematite) in PEC splitting of water. Sensitization of α-Fe_2O_3 thin films with other QDs e.g. ZnO and Carbon has also been investigated for their PEC performance. ZnO QDs and CQDs sensitization in α-Fe_2O_3 thin film exhibited remarkable enhancement in the photocurrent density, highest being ~2.80 mA/cm^2 at 0.75 V/SCE. As a next step sensitization of hematite thin films with graphene oxide is also being explored. Overall, improved photoelectrochemical performances of sensitized hematite films have been discussed thoroughly with supporting characterizations.

E 004

Design and Development of Indoor Energy Harvesting Circuit with OPV and Supercapacitor as Storage Module for Microelectronics Applications

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ABSTRACT

This research article explores the development of an indoor energy harvesting circuit that includes a supercapacitor storage module. Specifically designed for microelectronics applications, the system utilizes organic photovoltaic (OPV) technology to collect ambient light energy effectively. This study covers the entire development process, including the selection of OPV materials, the design of circuit architecture, and the integration of a supercapacitor module to ensure efficient energy management and storage. Using organic photovoltaics allows for flexibility and adaptability, making it a suitable system for various indoor applications. By integrating a supercapacitor storage module, energy fluctuations are addressed and a stable power supply is ensured without the use of batteries for connected microelectronics. After conducting extensive experiments, it has been concluded that our circuit design showed high effectiveness in converting and storing indoor light energy. We conduct a thorough analysis of the system's performance metrics, which include energy conversion efficiency and power output stability. The findings demonstrate that the indoor energy harvesting circuit and supercapacitor storage module are both feasible and practical. This paves the way for sustainable power solutions across various indoor microelectronics applications. The research aims to connect energy harvesting technologies with indoor microelectronics, providing a potential solution for creating self-powered and energy-efficient devices in different indoor environments.

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E 005

Exploring Spin Torque Diode Effect in Composite Spin Valve Pillar for Efficient Energy Conversion

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ABSTRACT

The global pursuit of sustainable energy sources has fueled significant interest in novel technologies capable of efficiently harnessing and converting the electromagnetic energy such as radiofrequency energy (RF energy) into DC power. In this context, spintronics has emerged as an innovative domain that combines the principles of electronics and magnetism, opening up new avenues for energy conversion. At the forefront of this objective, we come across the phenomenon known as Spin Torque Diode (STD) effect characterized by the interaction between spin currents and magnetization dynamics, offering possibilities for energy conversion applications. Our study explores STD effect in the composite spin valve pillar, a structure with distinct magnetic and non-magnetic layers. The magnetic multilayer system considered for study is represented as AF/F_0/NM1/F_1/NM2/F_2. The composite spin valve pillar serves as a dynamic platform to explain the underlying mechanism that governs the STD effect and its potential as an efficient energy harvesting tool. The theoretical investigation delves into the intricate interplay between spin dependent charge transport and magnetic fields. Notably, we extend our enquiry to find the frequency response of our device, to explore the operating frequencies, thereby enabling optimal utilization of the device across a wide range of operating condition. Furthermore, our study includes the detection of sensitivity, which is quantified by calculating the ratio of its output voltage to the applied input power. As the world moves towards a more sustainable future, the STD effect emerges as a promising guiding light illuminating the way to effective energy conversion technologies.

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E 006

Synthesis, Structural and Optical Properties Of P-Type SnSe Material for Potential Thermoelectric Application

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ABSTRACT

Tin Selenide (SnSe) is a very promising thermoelectric material and several approaches to enhance its thermoelectric performance have been emerged including power factor through modifying the electronic structure, reducing the thermal conductivity through all small phonon scattering. [1,2] In this regard, researchers have focused their attention on polycrystalline SnSe because of its properties. In this paper we have reported the synthesis, structural and optical properties of p-type SnSe material with molecular formula $Zn_xSn_{1-x}Se$ have been synthesized with varying concentration of Zn from 0.02 to 0.08 using a vacuum sealed quartz ampule and hot press sintering method and annealed at 950°C. Their structural and elemental studies is carried out by XRD and SEM-EDS. The crystallite size of $Zn_xSn_{1-x}Se$ is increased from 47.01 nm to 53.04 nm as increases the Zn concentration from 0.00 to 0.08. From microstructural and composition analysis the confirmation of synthesized material has been reconfirmed. The optical properties were carried by UV-VIS spectroscopy and energy band gap was calculated by Tauc's plot and estimated energy band gap (E_g) from 1.2eV to 1.3eV. The detailed results will be presented and discussed.

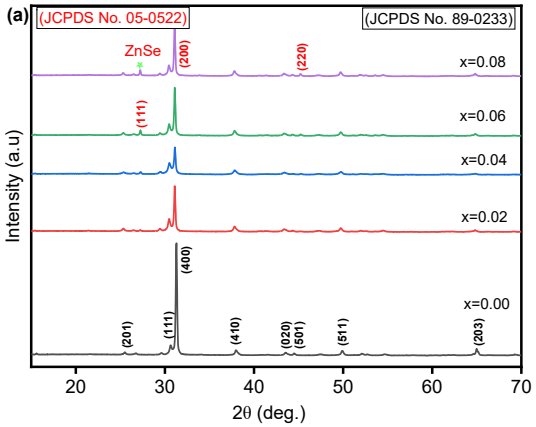

Fig.1. shows the XRD pattern for $Zn_xSn_{1-x}Se$ samples (x = 0, 0.02, 0.04, 0.06, 0.08)

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E 007

Electron Transport Properties Analysis of Titanium Dioxide Dye-Sensitized Solar Cells (TiO_2-DSSCS) Based on Ratio (TiO_2 Powder-P25) Using Dye Gambier as Sensitizer

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ABSTRACT

The depletion of fossil fuel supplies and their impact on climate change has led to an energy crisis. Scientists have developed a third-generation solar cell technology called dye-sensitized solar cells (DSSCs) to address this issue. DSSCs have many advantages, including low cost, simple production, good performance in low illumination levels, and the ability to use multi-color dye options. However, the efficiency of DSSCs is still low compared to thin film-based solar cells. The two components that have a significant impact on DSSC performance are the semiconductor (as the working electrode) and the dye (as the sensitizer). For the semiconductor, titanium dioxide (TiO_2) is used because it has a band gap of 3-3.2 eV, which allows electrons to be transferred from the HOMO to the LUMO. Meanwhile, the dye is one of the primary components influencing cell performance. The use of natural dyes is a promising strategy since natural sources are plentiful, and the extraction process is simple and non-polluting. For this investigation, Gambier dye was chosen because it has numerous capabilities that can be used to increase the performance of DSSCs. The optimal ratio of TiO_2 was determined based on the electron transfer and dye absorption, which can be examined electrically and optically.

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E 008

Investigation of Thermoelectric Properties of Alkali Metal Doped Zinc Ferric Oxide for High Temperature Applications

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ABSTRACT

In view of increased energy demand in every aspect of modern life and the depletion of non-renewable energy resources, it is necessary to utilize conventional sources of energy more efficiently. Thermoelectric energy conversion is very promising for harnessing waste heat by converting heat energy to electrical power with high reliability in the automotive and energy industries, which otherwise will contribute to global warming. However, oxide materials attracted more attention because of their abundance, non-toxicity, and chemical stability at high temperatures. Spinel ferrites have attracted the attention of the scientific community because of their excellent combination of structural, electrical, and magnetic properties, as well as their easy, inexpensive, and stable formation. This research aims to investigate alkali metal-doped $ZnFe_2O_4$ prepared through the sol-gel method, and sintered pellets were subjected to high-temperature electrical resistivity and Seebeck measurement analysis. The enhancement in electrical conductivity could be due to the collective contribution of several factors, like electron hopping due to the exchange of electrons between the cations in the octahedral site (B site) of the same element (Fe), which exhibits more than one valence state, and increased phonon scattering by doping alkali metals in the B site. $ZnFe_{1.975}Mg_{0.025}O_4$ shows the highest power factor of 20μW/mK^2 and an electrical conductivity of 525 S/m at 850 K. This opens up a new pathway for using spinel ferrite as a novel thermoelectric material to overcome the long-lasting challenge of developing high-performance thermoelectric materials.

Keywords: *Clean energy generation; Spinel composites; Thermoelectric properties; electron hopping*

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E 009

Synthesis And Performance of PTh/WO_3 Composite as Counter Electrode In Dye Sensitized Solar Cell

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ABSTRACT

In this study, Polythiophene-tungsten trioxide (PTh/WO_3) nanocomposite was synthesized at varying mass ratios (1:4 $(PTh/WO_3)_A$, 1:2 $(PTh/WO_3)_B$ and 1:1 $(PTh/WO_3)_C$) by in-situ polymerization and the nanocomposite's effectiveness as counter electrode (CE) in dye sensitized solar cell (DSSC) was evaluated. The electrochemical characterizations demonstrated that the DSSC with a CE composed of PTh/WO_3 nanocomposite at a 1:1 mass ratio exhibited superior electrocatalytic property with improved power conversion efficiency. The impedance parameters derived from Nyquist and Bode plots for this CE, showed the lowest values for charge transfer (R_{ct}) and solution resistance (R_s) measuring 11.01 Ω cm^2 and 13.81 Ω cm^2 with peak frequency (f_{max}) and electron lifetime (τ_e) of 11.9Hz and 13.4ms. Furthermore, the physiochemical analysis of the PTh/WO_3 nanocomposite, revealed a combination of particle and rod type morphologies with tungsten, oxygen and sulfur as predominant elements. The FTIR analysis also indicated the presence of functional groups of both PTh and WO_3 within the nanocomposite. The DSSC fabricated with $(PTh/WO_3)_C$ as CE generated a maximum open-circuit voltage(V_{OC}), short circuit current density (J_{SC}), fill factor (FF) and overall energy conversion efficiency(η) of 0.60V, 8.03mA.cm^{-2}, 0.57 and 2.75% under 100mW cm^{-2}, AM 1.5 G illumination. The facile synthesis procedure and attractive photo-electric properties benefits PTh/WO_3 composite to be used as a credible CE in DSSCs.

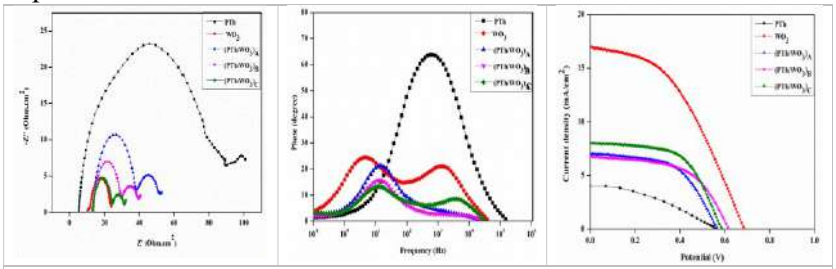

Fig 1: (a) Nyquist plots (b) Bode plot and (c) J-V characteristics of DSSCs fabricated with different CEs

Keywords: *Counter electrode; Dye sensitized solar cells; Hydrothermal method; PTh/WO_3 composite*

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E 010

Origin of Low Lattice Thermal Conductivity Through Micro-Structural Defects in Ni Substituted Bi_2S_3 for Enhanced Thermoelectric Performance

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ABSTRACT

Bismuth sulphide (Bi_2S_3) is a V-VI group semiconductor which are a prominent material in mid-temperature (303 K to 623 K) applications. In this work, $Bi_{2-x}Ni_xS_3$ (x = 0, 0.025, 0.05 and 0.075) were incorporated by hydrothermal along with the hot-press technique. Increasing the Ni concentration on Bi_2S_3 leads to achieving a high power factor for all the samples due to the significant increases in electrical conductivity. Notably, the x= 0.075 sample reached the highest electrical conductivity of 9835.98 Sm^{-1} at 623 K, owing to introducing Ni into the interstitial sites of the Bi_2S_3 lattice, thereby enhancing the carrier density. Furthermore, the phonon thermal conductivity of samples decreases through rising temperature. The x = 0.025 sample exhibited a remarkably low lattice thermal conductivity value of 0.432 Wm^{-1} K^{-1} at 623 K primarily due to the presence of various defects significantly enhancing the multiple phonon scattering. Consequently, the x = 0.025 sample demonstrated a good thermoelectric figure of merit (zT) value of 0.17 at 623 K, attained *via* the combination of reasonably high PF and low-slung phonon thermal conductivity.

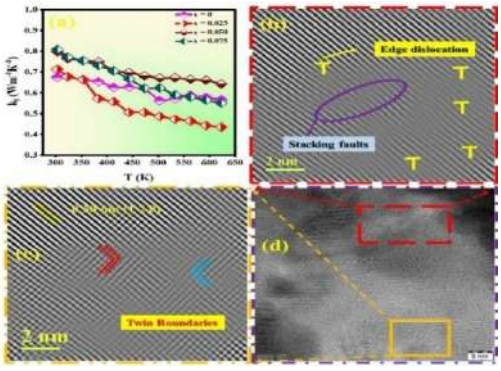

Figure (a) Temperature-dependent lattice thermal conductivity, (b and c) IFFT pattern images with stacking faults, edge-dislocation and twin boundaries, (d) High magnification HR-TEM image with marked area.

Keywords: *Dislocation, carrier mobility, phonons scattering and electrical conductivity.*

E 011

Sn Adatom as a Catalyst for Hydrogen Adsorption on Graphene: A DFT Study

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ABSTRACT

The hydrogen adsorption capacity of pristine graphene nanosheet (G_N) and tin (Sn) decorated adatom in the graphene nanosheet (SnG_N) system has been investigated using density functional theory calculations in this study. The binding of H_2 molecules to the clean G_N and SnG_N sheet ensues through physisorption. The average binding energy of H_2 molecules lies in the ideal range of -0.1 eV to -0.6 eV. Electronic property investigation reveals that before and after adsorption of H_2 molecules in G_N and SnG_N confirms that the interaction between H_2 and SnG_N substrate is of electrostatic nature. This theoretical modelling suggests Sn acts as a catalyst to enhance the hydrogen adsorption in pristine sheet G_N. Resulting in SnG_N substrate with better affinity and stability towards hydrogen molecule interaction.

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E 012

Modelling and Analysis of Bi Based Perovskite Solar Cell Using SCAPS-1D

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ABSTRACT

In present work, a lead-free structure of configurations FTO/TiO_2/$(FA)_2BiCuI_6$/Spiro-OMETAD/Au has been numerically investigated using one dimensional simulator i.e., SCAPS-1D. Initially, the optimisation of absorber thickness, absorber defect density and incident intensity are performed and a remarkable efficiency 38.99% (V_{oc} = 1.15 V, J_{sc} = 40.31 mA/cm^2 and FF = 83.57%) is achieved. After that, two theoretical interfaces ETL/absorber and absorber/HTL are included for examining the impact of interface defects on optimised device performance. Further, we examine the effects of series resistance, shunt resistance, and temperature on cell performance. This study reveals that the cell performance of purposed structure increases with shunt resistance, which means it must keep at higher value. Moreover, the performance gets declined with increase of interface defect density, series resistance, and temperature. Therefore, for better performance, the value of these factors is maintained at their minimum values. The validity of simulated results are verified through comparison with previous reported results. This detailed analysis of Bi based perovskite solar cell will be helpful in synthesizing the lead-free device with broader application prospects.

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E 013

Investigation on Microstructural, Optical and Electrical Properties of Indium Tin Oxide Thin Films Prepared by Thermal Evaporation

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ABSTRACT

Improving the efficiency of thin film solar cells can be accomplished through the utilisation of thin transparent conducting oxide materials possessing low resistivity and high transmittance as the front contact. This work encompasses the fabrication of Indium Tin Oxide (ITO) thin films via thermal evaporation. Indium and Tin, both in their pure metallic forms, were blended in two distinct compositions using a mortar and pestle. This mixture of metals was subsequently deposited onto glass substrates through the process of thermal evaporation. To achieve a single-phase Indium Tin Oxide (ITO) material, the deposited metal films underwent oxidation through air annealing at different temperatures and for varying durations. This work focused on investigating the effect of oxidation temperature and annealing duration on the structural, optical, morphological, and electrical characteristics of the produced films. A range of techniques was employed to study these properties comprehensively. X-ray diffraction analysis confirmed the presence of the crystalline cubic ITO thin film phase, while X-ray photoelectron spectroscopy validated the oxidation states. Raman spectroscopy was employed to ascertain the chemical structure of the prepared films. Optical assessments conducted with a UV-visible spectrophotometer demonstrated that the film possesses high transmittance of 80% within the visible spectrum and the optical band gap of these films was determined by tauc plot and subsequently compared. Moreover, atomic force microscopy was utilised to investigate surface properties, including particle size, shape, and roughness, which revealed a consistently smooth texture on the film's surface. The I-V characteristics of the films indicated the conductive nature with low resistance.

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E 014

Engineering Enhanced Energy Storage and Energy Harvesting Performance in $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ Ceramics through Dopant-Controlled Structure and Sintering Techniques

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ABSTRACT

This investigation delves into the influence of dopants on $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (BCZT) ceramics, utilizing Sr^{2+} ions as donor dopants at the A-site, Zn^{2+} ions as acceptor dopants at the B-site, and Pr^{3+} or Pr^{4+} as amphoteric dopants at either A- or B-site through the solid-state reaction (SSR) method. The introduction of dopants has a significant effect on the crystal structure, microstructure, and chemical defects of BCZT ceramics, leading to notable changes in their tetragonality [1]. Sintering processes have been carried out using both conventional and rapidly cooled techniques at 1350 ºC for 4 hours, unveiling superior electrical properties with the latter method. Rapidly cooled sintering resulted in a decrease in the transition temperature (T_c) of doped BCZT ceramics compared to conventional method. The microscopic heterogeneity observed in doped BCZT compositions played a crucial role in diffused dielectric behavior. The dopants caused a substantial disruption in the long-range ferroelectric (FE) order, inducing a transition from a ferroelectric to a relaxor ferroelectric phase. This transition is attributed to the presence of locally polar nano regions (PNRs), leading to stable temperature-viable dielectric properties [2]. The optimization of the energy storage density, in terms of recoverable energy density value (W_{rec}) and the efficiency, and mechanical energy harvesting performance of the BCZT ceramics, has been achieved by carefully controlling both the dopants and the sintering process [3].

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E 015

Highly Strained Pd-Coated Au-Ag Nanoprism as An Efficient Electrocatalyst for Formic Acid Oxidation

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ABSTRACT

Finding an alternative source of energy became the major focus of human civilization as people worldwide are trying to build a relationship between modern-day life being in harmony with nature. Direct formic acid fuel cell (DFAFC) represents one of the most effective candidates for clean energy production with their high-power density, fast electrooxidation, low fuel crossover, and ease of handling. Pd is a good alternative to Pt-based material for the electrooxidation of formic acid as Pd catalysts present better CO tolerance and higher power density. From our previous experience, we have seen that moving from monometallic to bimetallic nanoparticle enhances the catalytic activity due to increased lattice strain. Keeping this fact in mind we have synthesized a trimetallic plasmonic nanoparticle using Au, Ag, and Pd. We have developed a facile synthetic protocol for the fabrication of Pd-deposited Au-Ag bimetallic nano prism which acts as an effective catalyst for formic acid oxidation in 0.5 M H_2SO4 medium. We have deposited Pd layers of different thicknesses (14 nm, 30 nm, and 40 nm) over the bimetallic Au-Ag prism and 30 nm Pd deposited prism shows the best catalytic activity. To our surprise, Elemental mapping shows that Pd is deposited only at the edges of the bimetallic prism and most interestingly forms an alloy with Ag which increases strain in the particle. 30 nm Pd-Prism shows the highest ECSA, mass-specific activity, and better durability. Our best catalyst shows 4 times greater ECSA and 6.5 times better mass activity than commercial 10 wt% Pd/C. Recently we have developed a prototype of a formic acid fuel cell in which we will use our catalyst as anode catalyst.

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E 016

Novel Configuration of 1D-Photonic Crystal for Realizing Colored Photovoltaic Devices

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ABSTRACT

Photonic Crystals (PCs), which are fabricated by controlling the passage of light, have attracted much interest due to their appealing aesthetic qualities and visual attributes. Thus, following an approach combining optical modeling studies and experimental techniques, we report the design and fabrication of highly reflecting PCs and their implementation for making colored photovoltaic (c-PV) devices. High and low refractive index materials are utilized for realizing various color PCs. Prior to the in-hand experiments, we determine the optimal thickness of the different layers with optical modeling assistance. Usually, for realizing c-PV devices, the PC is deposited after the fabrication of the entire device, but here, in a novel approach, to realize a colored perovskite solar cell (c-PvSC), the fabricated PC is mechanically stacked to the back side of the bottom transparent substrate of the PvSC, which may aid in preventing any damage to the delicate or fragile layers in the PvSC device stack. In this way, we successfully fabricated highly efficient and stable blue and yellow-colored PvSCs. It is believed that the proposed method of incorporating a PC into any photovoltaic device can be of great use in providing a better aesthetic view of any PV technology.

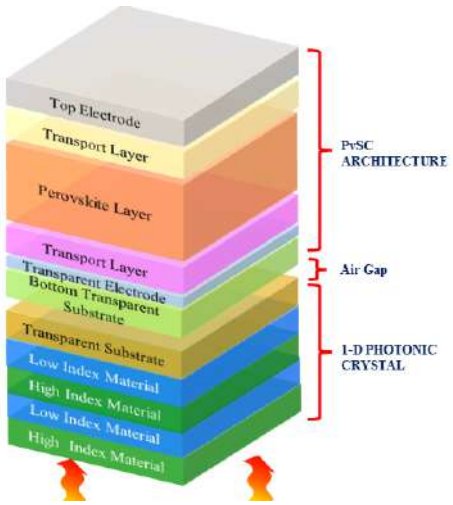

Figure 1: Device configuration of the mechanically stacked colored PV device.

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E 017

Fossil fuel derived GQD as a photosensitizer in Dye-Sensitized Solar Cells

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ABSTRACT

Solar energy is an abundantly available renewable source and for harnessing it several generations of photovoltaic cells has been developed. Dye sensitized solar cells are one among viable and potent solar energy harvesters[1]. Sensitizer being the heart of DSSC has been researched for years. Alternatively, fossil fuel-coal is one of the world's best-known energy sources. Lignite coal is a naturally occurring heterogeneous macromolecule having a three-dimensional cross-linked structure with multiple functional groups[2]. Unfortunately, it's been used as a fuel for power generation and tagged as a pollutant. Therefore, in this study we manifest the usage of lignite derived GQD as a sensitizer for DSSC and attempt to provide value addition to coal. GQDs with varied bandgap were obtained and used as sensitizer and a maximum PCE of 2.87% was obtained. Additionally, GQD sensitizers were exposed to UV light for 48 hours and the fabricated device exhibited 2.90% efficiency, showing the photostability of GQDs. Furthermore, device showed a higher R_{rec} of 166.57 Ω that verifies the reason for better performance. Thus, sensitizers derived from lignite showed a novel use for feedstock that had previously been used for combustion.

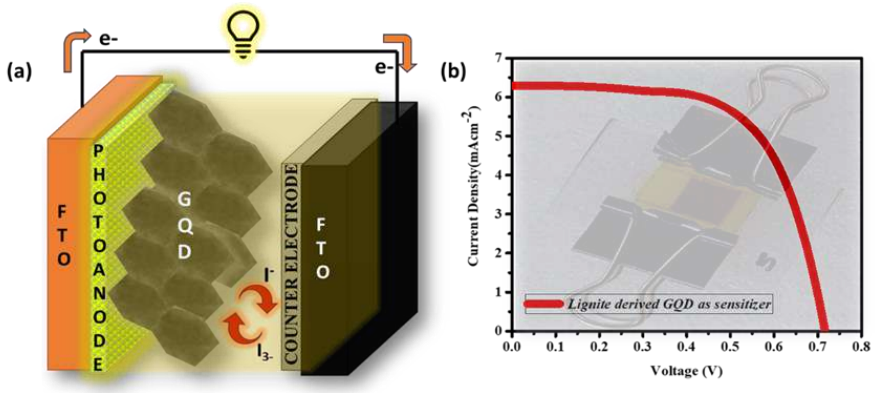

Figure 1.(a) Schematic representation of DSSC (b) J-V curve

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E 18

Ultra-High Power Factor of In And Ga Co-Doped n-Type Thermoelectric Material for Mid-Temperature Applications

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ABSTRACT

Bismuth Selenide (Bi_2Se_3) is a potential *n*-type Te-free thermoelectric (TE) candidate for room temperature application owing to its dominant intrinsic Se vacancy and alternative for Bi_2Te_3. Here, we demonstrate an isovalent co-doping of Indium (In) and Gallium (Ga) in polycrystalline Bi_2Se_3. The phase purity of the as-prepared samples is confirmed by the crystallographic planes while, highly textured grains were captured using HR-SEM. Co-doping strategy has significantly improved the electrical properties, resulting in an increased power factor of 1220 μW/mK^2 at 303 K. Also, the low lattice thermal conductivity of 0.28 W/mK was measured at 573 K due to the influence of interstitial-phonon scattering, lattice strain and mass-fluctuation phonon scattering.

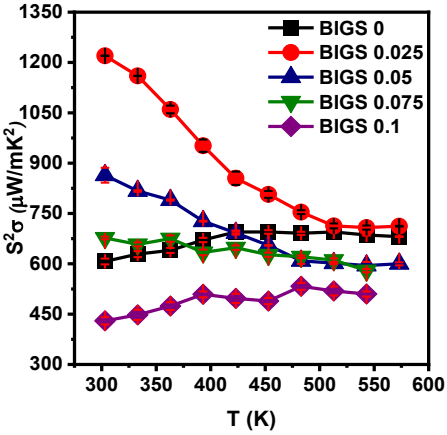

Figure: Temperature dependent power factor of In and Ga co-doped Bi_2Se_3.

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E 019

Lead-Free Piezoelectric KNN-Natural Rubber Composites for Energy Harvesting Applications

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ABSTRACT

In past years, different techniques have been introduced for the development of piezoelectric materials with enhanced properties. Furthermore, recent studies in the area of self-powered piezoelectric technology have shown the potential of using piezoelectric materials in securing a sustainable powering source for sensor networks. This work aims in the development of novel series of flexible and biocompatible integrated mechanical energy harvester for self-powered sensor applications that require microwatts of power, based on lead-free potassium sodium niobate (KNN) piezoelectric ceramics incorporated in natural rubber (NR) matrix. Piezoelectric composites based on NR matrix is less explored, which is highly flexible, water resistant, durable, eco-friendly. KNN ceramic particles are prepared via conventional mixed oxide method. Composites with 0-50 volume percent of KNN ceramic particles in NR matrix is prepared and is subjected to piezoelectric, dielectric, mechanical and thermal characterization. Piezoelectric coefficient of 6pC/N is obtained for composite with 30% KNN filler percentage. The same was repeated for 40 and 50 volume percent of KNN in the composite system. Thus prepared composite was used for fabricating a workable method as energy harvester for sensor networks.

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E 020

Transition metal Doped ZnO Quantum dot Solar Cells (QDSC): A Collection of Recent Advances and Future Scope

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ABSTRACT

The world has an abundance of renewable energy sources such as solar energy, wind, water and many more. Yet, coal, oil and natural gas still make up over 75% of the total energy production worldwide. A rapidly increasing global population and ever-growing demand for energy supplies forces the scientific community to manipulate and design materials that can be used as efficient energy converters. Quantum dots are one among such materials which offers distinct optoelectronic attributes due to quantum confinement. Numerous amounts of QDs have been discovered in the past few years, over which ZnO quantum dots have bagged the weightage of exhibiting magnetic, mechanic, optoelectronic and other properties while exist in the quantum state. Gathering all the remarkable properties like high absorption coefficient, tunable band gaps and large surface area to volume ratio, ZnO QD have extensively used in solar cells and making it as a replacement to the organic dye sensitized solar cells. Creation of more surface charge carriers in ZnO QDs allows wide range of doping and hence enhances the physicochemical and photochemical properties. In this review paper, synthesis, materials used and variation of power conversion efficiency (PCE) of doped ZnO QDSCs have been presented. A brief description of quantum confinement effect based on size reduction also have been included. A part of this article focuses on the applications of transition metals doped ZnO QDSCs in different industries.

Keywords: Renewable Energy, Solar cell, ZnO Quantum dots, Doping

E 021

Solvothermal Synthesis of SnS Nanoparticles Using Different Sulphur Sources: Structural, Morphological, Optical and Electrical Properties

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ABSTRACT

Tin (II) sulphide has high potential as an absorber layer in thin film solar cells due to its promising properties which will help to reduce the material cost and increase the cell efficiency. This work investigates the influence of different sulphur precursors such as sodium sulphide (SS), thioacetamide (TA) and thiourea (TU) on the chemical and crystal structure, surface morphology, optical and electrical properties of SnS nanoparticles synthesized solvothermally at a reaction temperature of 170 °C. Here, $SnCl_2\,2H_2O$ is used as the tin precursor and ethylene glycol is used as the reducing agent. The single phase formation of SnS is optimized through varying the Sn:S source concentration ratio (1:1 to 1:15 M) and reaction time (Rt) (1.5 to 12 hr). The phase purity of the prepared samples are studied using Raman, XRD, XPS and EDAX analyses which showed the formation of single phase of SnS for SS (1:12 M with Rt 1.5, 3, 6 and 12 hr), TA (1:12 M with Rt 3 hr) and TU (1:15 M with Rt 3 and 6 hr) precursors. Whereas in all other cases secondary phases (SnS_2 and Sn_2S_3) are formed along with SnS due to its low formation energy. FE-SEM and HR-TEM analyses revealed the formation of nanorods, spherical flower and peony-dahlia like morphology for SS, TA and TU sulphur precursors respectively. The observed variations in the direct energy band gap can be well correlated with (a) the formation of different phases and (b) the variation in size and shape of the nanoparticles.

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E 022

Plasma-Engineered Zeolite Material for Enhanced Activity Towards Hydrogen Evolution

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ABSTRACT

The world is currently going through an energy crisis, and the hunt for cleaner fuels is important for the environment.H_2 is one of the cleanest fuels available, producing enormous energy when combined with oxygen. The hydrogen production is carried out using a reforming process, which requires enormous energy input. Thus, a lot of efforts are focused on producing H_2 in a clean and environmentally friendly way. Electrochemical water splitting is one of the fascinating domains researchers have stumbled upon, and it is the only way for the net neutral carbon footprint to exist. Thus, in our current work, we have tested the impact of thermal reduction of zeolites and plasma-reduced zeolite surface for hydrogen evolution reactions. For this purpose, the FAU zeolite with Si/Al ratio 1 is thermally reduced in an H_2 atmosphere at various temperatures from 300ºC to 600ºC in a split tubular furnace. Later, the FAU zeolite sample is also treated in plasma at ambient conditions (30ºC 1 atm), and the activity is compared with the thermally treated sample. The sample activity is tested using a 3-electrode setup where a glassy carbon electrode acts as a working electrode, platinum as the counter and Ag/AgCl as the reference electrode. The cyclic voltammetry was run in various electrolytes (KOH and H_2SO_4) in a potential window of 0.8 to -0.8 V. The cyclic voltammetry reveals excellent stability of plasma-treated Zeolite compared to thermally-treated zeolite. The Linear sweep voltammetry studies revealed that plasma-activated/treated zeolite surface exhibits excellent stability for 1000 cycles and the lowest overpotential than the commercial reference of 5% Pd/C.

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E 023

Fabrication of Self-biased Piezoelectric Nanogenerator Based on KNN/PDMS Flexible Piezoelectric Nanocomposite

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ABSTRACT

Recently, there has been a lot of focus on creating improved material composites for energy harvesting and sensing applications. Piezoelectric materials are the potential materials which can be utilized as an energy harvester. The exponential rise in flexible piezoelectric nanogenerators (PENGs) has drawn significant interest in alkali niobates, which are seen as an environmentally acceptable replacement for lead-based piezoelectric devices, which are not as sustainable. Here in, efforts have been made to develop lead free flexible PENG using Potassium Sodium Niobate (KNN) as a nanofiller with Polydimethylsiloxane (PDMS) matrix using solution casting technique. KNN nanoparticles were synthesized using a simple wet ball milling method and then incorporated into PDMS matrix together. KNN nanoparticles powder was evenly distributed throughout the PDMS matrix, improving the dielectric and piezoelectric properties of the prepared composite. A piece of 2 cm x 2 cm was cut from the flexible sheet and silver (Ag) was coated as the electrode on both sides. The open circuit output voltage generated from the fabricated PENG was found to be ~10 V at zero biasing. The results show the potential of flexible KNN-PDMS composite to be used as large-scale, eco-friendly self-biased PENGs.

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E 024

Enhanced Energy Harvesting with a Flexible Pedot: Pss based Photo-Thermoelectric Generator

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ABSTRACT

In recent years, flexible hybrid generators have gained attention as a highly promising option for powering wearable electronic devices. They offer a solution to the limitations associated with traditional batteries, including the need for frequent recharging, environmental concerns, and their inherent physical rigidity. Thus, in the present work efforts have been made to develop a flexible photo-thermoelectric generator (PTEG) with the simple structure composed of a thermoelectric generator and light to thermal conversion layer to harvest both thermal and radiation energies based on a single platform. The simple drop-cast technique is used to prepare poly (3, 4-ethylenedioxythiophene) polystyrene sulfonate (Pedot: pss)/Ag thermocouple chain with the silver as metal contact over a flexible polyamide substrate. The light to thermal conversion layer consists of a light absorbing film and a light reflecting film to solar radiation harvesting. The light-absorbing layer is composed of graphite combined with Polydimethylsiloxane (PDMS), while the reflecting layer is made up of TiO_2 in conjunction with PDMS. The resultant PTEG features seven pairs of thermoelectric (TE) legs. When exposed to one-sun (100 mW/cm_2) solar radiation, the light-absorbing layer and the light-reflecting layer quickly generated a temperature difference of 20°C in just 2 minutes, resulting in an open-circuit output voltage exceeding 25 mV. Meanwhile, during the flexibility test, the internal resistance remained consistently stable, demonstrating the outstanding ability of the created PTEG to recover from bending. This reveals that the proposed PTEG can indeed be regarded as a dependable power supply for wearable electronic devices.

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E 25

Charge Transport Nd Spin State Blockade in Electron (Hf) Doped Strongly Correlated Mott Insulator $LaCoO_3$

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ABSTRACT

In this work, we have measured the electrical resistivity and thermopower of hole (Sr) and electron (Hf) doped $LaCoO_3$ in the temperature of 303 – 753 K. With the increasing temperature, the insulating behaviour (303 – 503 K) with dominance of small polaron hopping to metallic transition (> 503 K) is observed. The electron doped sample shows an insulating behaviour (19.5 Ωcm) and positive thermopower (139 μVK^{-1}) value due to the spin state blockade mechanism that an electron hopping from high spin Co^{2+} to low spin Co^{3+} is strongly inhibited whereas the hole doped one shows the ferromagnetic metallic behaviour (0.03 Ωcm). The calculated weighted mobility (μ_W) of 0.01 to 0.96 $cm^2V^{-1}s^{-1}$ validates the proposed concept of spin blockade in electron doped sample. The fluctuation of spin/orbital ordering and point defect scattering results in the low thermal conductivity of 0.5 $Wm^{-1}K^{-1}$ for electron doped sample. It is obvious that diverse spin/orbital configuration along with the spin state transitions prevailing in $LaCoO_3$ provides a new route for exploring and designing new thermoelectric oxides.

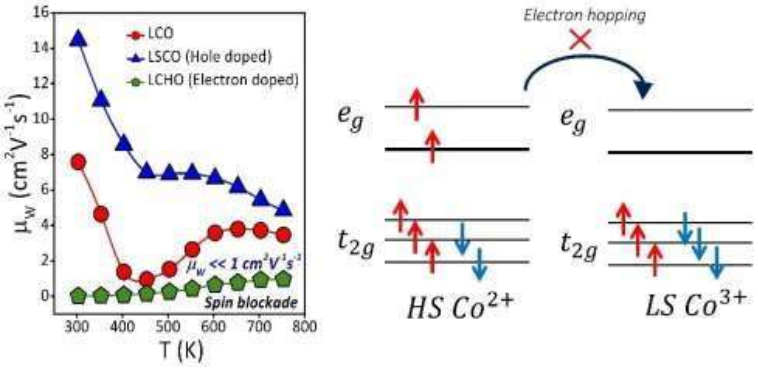

Figure 1. Weighted mobility and schematic representation of spin blockade mechanism

E 026

Effects of SnS/Cu_2Se Composites in Reducing the Thermal Conductivity of Polycrystalline SnS

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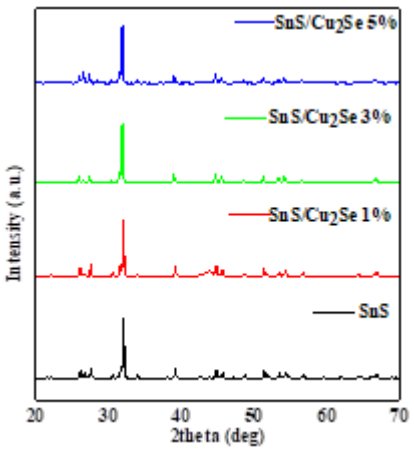
ABSTRACT

SnS is one of the most promising layered chalcogenide materials for thermoelectric applications[1], [2]. Novel SnS/Cu_2Se composites were prepared by the hydrothermal technique combined with the ultrasonication method. SnS has a high Seebeck coefficient but lacks good electrical properties, so the introduction of Cu_2Se to the SnS matrix can be a potential solution. The addition of Cu_2Se has resulted in the suppression of the intrinsic thermal conductivity of SnS from 0.891 W/mK to 0.447 W/mK at 753 K. Almost 50% reduction in thermal conductivity is observed due to enhanced scattering of Phonons from the grain boundaries, stacking faults and lattice distortions. The specific heat capacity, as well as diffusivity, shows a monotonic trend with respect to temperature as well. When we consider the crystallite size it is shown to decrease with respect to the increase in composite percentage while the dislocation density and microstrain increased with composite percentage.



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E 027

Flexible Polymer Thick Films Based on Room Temperature Multiferroic $Na_{0.5}Bi_{0.5}TiO_3$ –$BaFe_{12}O_{19}$ Composite for Mechanical Energy Harvesting

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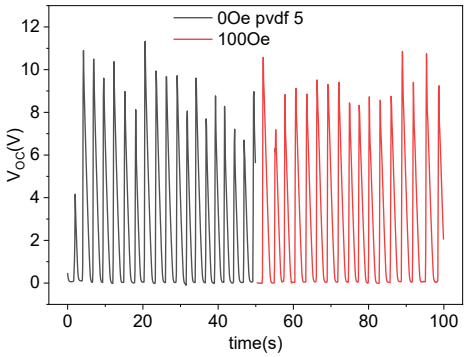
ABSTRACT

In this work, multiferroic $Na_{0.5}Bi_{0.5}TiO_3$ –$BaFe_{12}O_{19}$ composite was introduced in PVDF matrix as a filler material for the development of magnetoelectric mechanical energy harvester. Firstly, the structural, electrical and magnetic properties of the filler material was investigated which confirmed the successful formation of the multiferroic composite. The composite material was blended with PVDF by varying the filler percentage (5%, 10%, 15% and 20%) and flexible films were fabricated using solution casting method. The room temperature magnetoelectric coupling properties of the thick films were studied as a function of applied dc magnetic field up to 1000Oe with a constant ac magnetic field of 1Oe. The potential use of the films in magnetoelectric sensors was confirmed from the giant room temperature ME coupling coefficient of the films. Flexible and light weight nanogenerators were fabricated from the thick films which were able to generate a maximum open circuit voltage of 12.5V and a maximum output power of 178nW with finger tapping force. The continuity of the electrical output provided by the nanogenerator was checked by charging capacitors of 1μF and 4.7μF for 100 seconds. With proper design and engineering, these films can be used in the development of wearable self-powered electronics with hybrid magnetic or pressure sensing and energy harvesting properties.



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E 028

Flexible PDMS-BST Based Polymer Film for Piezoelectric Energy Harvesting Application

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ABSTRACT

A comprehensive study in the utilization of novel Polydimethylsiloxane (PDMS) filled with piezoelectric Barium strontium titanate ($Ba_{0.8}Sr_{0.2}TiO_3$/BST) nanocomposite has been discussed for the piezoelectric energy harvesting applications. The incoporation of piezoelectric BST nanopowder into the highly flexible PDMS make it suitable for the development of flexible piezoelectric nanogenerators. Sol gel derived BST nanopowder was blended uniformly into the PDMS solution and casted to form the flexible polymer thick film. The structural and microstructural properties of the PDMS-BST nanocomposite was investigated by using X-Ray Diffractometer (XRD), Scanning electron microscope (SEM), Fourier transformed infra-red (FTIR) spectroscopy etc. The observed results reveals a well dispersed BST phase within the PDMS matrix. The room temperature dielctric constant measured at 1KHz frequency was found to be 45. The saturation and remanent polarization of the prepared nanocomposite sample was found to 0.8μC cm^{-2} and 0.15μC cm^{-2}respectively. Moreover, the prepared flexible nanocomposite shows a notable energy storage capacity with 70% energy storage efficiency. The output voltage of the piezoelectric nanogenerator was measured by applying different mechanical force where a maximum open circuit, peak to peak voltage of 15V was observed. This paper shows the possibility of the PDMS-BST for the piezoelectric energy harvesting application.

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E 029

Study of the Impact of Mixed Phase of Manganese Sulfide Nano Photocatalyst on Waste Water Treatment

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ABSTRACT

A mixed phase of manganese sulfide (MnSs and γ-MnS) nanoparticles was fabricated, and their photocatalytic degradation ability in waste water has been investigated. These mixed-phase nanoparticles were fabricated using a simple chemical precipitation technique at room temperature. PEG was added drop-wise to the reaction solution during the ageing process to get a highly stable and perfect mixer of nanoparticles. The crystallite size and lattice strain of the synthesised particles were calculated from XRD. It also confirms the mixed crystal system in the prepared sample. The UV-visible analysis confirms a suitable band gap regime that is capable of absorbing visible light. Due to these desirable factors, the degradation ability of the waste water has been checked under sunlight at various dosages (mg/L) and various time durations under ambient temperature conditions. The degraded waste water samples were analysed using UV-visible spectroscopy, and the results are discussed.

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E 030

Stable and Efficient Hydrogen Evolution Activity of Tungsten-Incorporated $BaSnO_3$ Electrocatalyst

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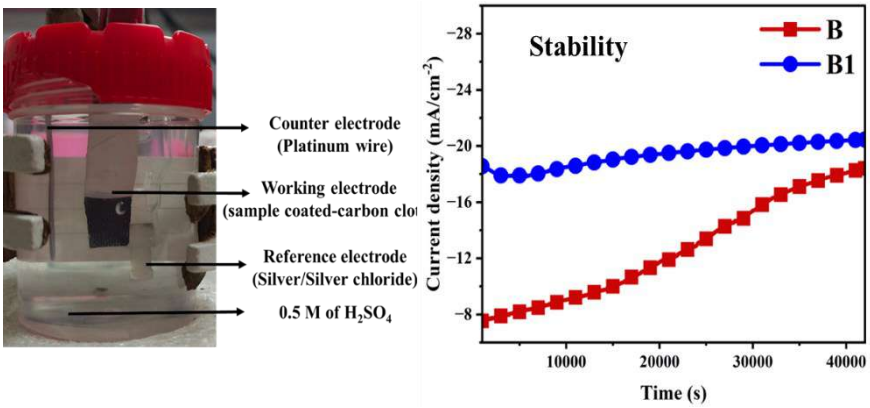
ABSTRACT

Hydrogen evolution reaction (HER) is a promising renewable energy conversion technique. Ternary perovskite barium stannate ($BaSnO_3$) (Sample code-B) has been not explored widely for water splitting and electrocatalysis. Tungsten (W) 1% incorporated $BaSnO_3$ (Sample code-B1) synthesized by facile hydrogen peroxide route is explored as an electrocatalyst for HER activity for the first time. The pure and W-incorporated $BaSnO_3$ exhibited promising HER activity with an overpotential of 233 and 295 mV at 10 mA/cm^2 in acidic medium with enhanced electrochemical surface area of 7.309 and 3.075 Fcm^{-2}, respectively. A 12-hour stability test not only concluded the durability and performance of hydrogen evolution but also confirmed the enhanced initial current density for the W-incorporated sample.



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E 031

Passivation of Interface for Improved Performance of All- Inorganic Perovskite Solar Cells Based on Carbon-Electrode in Ambient-Air

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ABSTRACT

Inorganic perovskite solar cells (IPSCs) that utilize $CsPbIBr_2$ absorbers are currently a subject of growing interest among researchers due to their outstanding thermal stability and opto-electronic properties. These IPSCs are manufactured through easy solution processing technique, making it feasible to achieve compositional optimization and uniformity of the perovskite film in normal laboratory conditions. However, the presence of unavoidable defects on the surface of the perovskite material undermines the quality of the interface and hampers the performance and stability of the devices. To address this issue, a passivation layer composed of a novel green deep eutectic solvent (DES) is applied to the low-temperature $CsPbIBr_2$ layer. This DES layer effectively interacts with interfacial charge defects due to its ionic nature, minimizing energy loss at the perovskite-carbon interface in carbon-based IPSCs (C-IPSCs) processed under open-air conditions (70% relative humidity) without the need for a hole-transport layer (HTL). Comprehensive analyses of the structural, morphological, optical, electrical, and photovoltaic properties of these C-IPSCs have been conducted using various techniques, including XRD, FTIR, FESEM, XPS, UV-*Vis* spectroscopy, PL, UPS, current-voltage (J-V) characteristics, and electrochemical impedance spectroscopy. These analyses are then compared to the characteristics of pristine C-IPSCs. The findings from these studies reveal that the optimal concentration of DES effectively passivates uncoordinated ions and halide vacancies present on the surface of $CsPbIBr_2$ when processed in ambient air. This treatment resulted in enhanced morphology, crystallinity, and alignment of energy levels. Consequently, there is an increase in charge transfer and efficiency for HTL-free C-IPSCs by 49% with higher photovoltage, current density, fill factor, and reduced hysteresis. Additionally, the optimized devices demonstrate significantly improved resistance to heat and humidity. Hence, this work presents a simple approach for achieving enhanced photovoltaic performance and stability of C-IPSCs in realistic ambient conditions, facilitating their potential commercialization.

E 032

Effect of Carbon Electrode Annealing Temperature on Perovskite Solar Cells

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ABSTRACT

Perovskite solar cells (PSCs) have shown an outstanding performance improvement since their first introduction[1]. Currently, high-performing PSCs still utilize gold, silver, or platinum as their counter electrode which can hinder the path of commercialization. Thus, carbon is introduced as an alternative counter electrode for PSC. Usually, to utilize a carbon counter electrode, carbon powder was made into a paste and then deposited onto the substrate. The substrate is then heated to evaporate the solvent and become a solid carbon layer. Research related to carbon annealing temperature was already conducted by another researcher, but their structure was mesoscopic where the carbon layer was deposited before the perovskite layer[2]. In this research, we investigate the effect of the annealing temperature of carbon counter electrode in PSC. The PSC was constructed on a fluoride-doped tin oxide (FTO) glass substrate. The FTO/compact TiO_2/mesoporous TiO_2/Perovskite/CuSCN/carbon structure was used. Carbon annealing temperature was varied to 80ºC, 100ºC, and 120ºC.

It was found that as the annealing temperature was increased, the PSC's performance decreased. The notable decrease factor was from the open-circuit voltage (V_{OC}) parameter where it was 0.90 V at the annealing temperature of 80ºC, then steadily decreases to 0.81 V and 0.71 V at 100ºC and 120ºC, respectively. Short circuit current density (J_{SC}) also gives a similar decreasing trend. This might be caused by the change in perovskite crystal[3]. Even though the perovskite crystal formation was completed since its deposition process, exposing it to high temperatures during carbon layer deposition changed its characteristics and decomposed the perovskite material. It also noticed that the hysteresis of the PSC increases when exposed to high temperatures. Until now, the hysteresis issue in PSCs is under debate, but one factor is from defect in perovskite material which induced trap-assisted charge recombination[4]. High annealing temperature might induce a defect in the perovskite material. From the experiment, a carbon annealing temperature of 80ºC gives the best PSC performance with V_{OC} of 0.90 V, J_{SC} of 9.44 mA/cm^2, fill factor of 0.40, and efficiency of 3.36%. These results provide consideration on the preference of annealing temperature of a layer that deposited after perovskite, especially for carbon counter electrode.

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E 033

Impedance Spectroscopy Analysis of Low-Cost mixed halide MAPbI1-xClx, Highly Efficient $FAPbI_3$ and Non-Toxic Lead-free $CsBi3I10$ Perovskite Solar Cells: A Comparative Numerical Analysis using SCAPS-1D

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ABSTRACT

Rapid development of Perovskite solar cells (PSCs) over the past few years, with significant improvement in efficiency from 3.8% to above 25% extended its research prospects in the emerging field of photovoltaics. Impedance Spectroscopy when applied to emerging photovoltaics presents new challenges towards potential device applications to the complex device structures of PSCs. In this work a comparative numerical analysis of 3 PSCs with ETL –TiO_2 , HTL- Cu_2O and 3 different perovskites such as $FAPbI_3$, $CsBi_3I_{10}$ and MA Pb (I_{1-x} Cl_x) are studied using SCAPS-1D, a solar capacitance simulator that investigates performances of planar perovskite solar cells. The simulation studies by optimising the transport and active layer thickness, defect density and dopant concentrations are done along with Impedance Spectroscopy analysis of all 3 PSC structures. The simulation results prove that the mixed halide perovskite MAPb(I_{1-x} Cl_x) outperforms the other active layers $FAPbI_3$ and $CsBi_3I_{10}$, despite the fact that the power conversion efficiency (PCE) of $FAPbI_3$ is achieved as 22.04% when compared to 16.65 % for $CsBi_3I_{10}$ and 19.71% for MAPb(I_{1-x} Cl_x). This is due to the fact that large diameter of Nyquist plot for $FAPbI_3$ and $CsBi_3I_{10}$, indicates a high resistance value of approximate 40K Ohm and 6K Ohm respectively, which corresponds to the processes like charge transfers at the interface, recombination and bulk internal material resistance. The Nyquist plot of MAPb(I_{1-x} Cl_x), gives a more focussed and narrower spectrum of impedance values of the range 2K Ohm. From the above simulation results MAPb(I_{1-x} Cl_x), proves to be one of the best perovskite absorber layer that can be utilized for perovskite solar cells.

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E 034

Bicyclopentadithiophene-based Organic Semiconductor for Stable and High-Performance Perovskite Solar Cells Exceeding 22%

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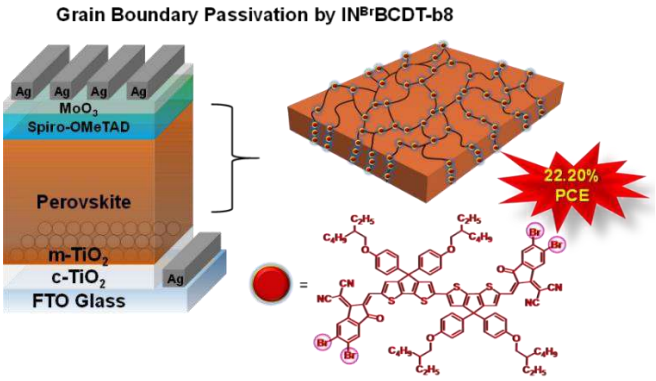
ABSTRACT

Well-performing organic-inorganic halide perovskites are susceptible to poor efficiency and instability due to their various defects at the interphases, grain boundaries, and surfaces. Here, we report an in-situ method to effectively passivate the under-coordinated Pb^{2+} defects of perovskite with new non-fullerene acceptors (NFAs) (IN^{X}BCDT; X = H, Cl, and Br) through their carbonyl and cyano functional groups, during the anti-solvent dripping process. This effective defect passivation decreases the trap density to increase the carrier recombination lifetime of the perovskite film. It reveals that bicyclopentadithiophene (BCDT) core with highly electron-withdrawing end-capping groups passivate grain boundaries and boosts perovskite grain growth. As a result, bromo-substituted dicyanomethylene indanone (IN^{Br})-end-capped BCDT (IN^{Br}BCDT-b8; 3a)-passivated devices achieve the best power conversion efficiency (PCE) of 22.20% in Pb-PSCs. To the best of our knowledge, this is the first example of the simplest high conjugation additive for perovskite film to achieve a PCE greater than 22%, maintaining ~90% of their initial PCE in a longterm stability test for 63 days. This simple treatment, by adding new brominated NFAs in the anti-solvent for crystallization of perovskite film, improves the efficiency and stability of the PSC by defect passivation.



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E 035

A Detailed Study on Capacitance Spectroscopy of Hybrid Perovskite Solar Cells

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ABSTRACT

In recent years, perovskite solar cell gained more attention due to outstanding photovoltaics efficiency. To design high performance and stable device it is essential to understand static and dynamical characteristics of the photovoltaics. In this work, both experimental and simulation capacitance spectroscopy, static characteristics, of methylammonium lead iodide perovskite solar cells are carried out. Specifically, capacitance-voltage (C-V), capacitance-frequency (C-*f*) measurements were carried out and from these results various associated parameters were derived. C-V characteristics was investigated to study the variation in space charge depletion property, with respect to varying ac voltage (10 - 100 mV) and applied *ac* frequency. Further, built-in potential (V_{bi}) and charge carrier concentration (N) were calculated from Mott-Schottky relation. Capacitance-frequency (C-*f*) characteristics of the device was obtained and from these measurement, distribution of trap states in the depletion region was calculated. Similar investigation was performed under illuminated condition and the obtained results were discussed. The forward and reverse bias photovoltaics characteristics are also reported. Finally, the experimental results were compared with the simulated results and reported.

Keywords: *Indoor photovoltaics; Indoor Light Harvesting; Capacitance; Doping Density; Perovskite Solar Cells.*

E 036

Piezoelectric Nanogenerators for Energy Harvesting Applications

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ABSTRACT

In view of the rapid growth of the Internet of Thing (IoT), enormous low power consuming (micro watt or milli watt) electronics devices such as sensors, actuators, and wireless transmitters have been integrated into every corner of this world for a variety of applications. Traditional batteries have issues with low life time and environmentally toxic end materials. In this context, technologies to develop small scale nano energy harvesting devices are very much demanding. Instead of the conventional energy generation approaches, we uses a technology which can harvest mechanical energies from human body motions in electrochemical energies. For this purpose we developed composite piezo electric nano fibers with very high energy conversion efficiency. The Ba-$SrTiO_3$ nanoparticles were synthesized via single step combustion method and low temperature annealing. The structure of the nanoparticles was estimated using powder X-ray diffraction analyses and also by measuring FWHM of the XRD peaks Ba-$SrTiO_3$/PVDF nano fibers of optimised diameter has been fabricated through electrospinning technique. Morphological properties of PVDF/ZnO nanofibers were examined by scanning electron microscopy (FESEM).

Key words: *Nano fibers, polymers, nano generators, piezo electricity*

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E 037

Synthesis and Characterization of TiO_2, Sn and Sr Doped TiO_2 and Co-Doped with TiO_2 nanoparticles for Dye Sensitized Solar Cell Applications

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ABSTRACT

In this work, undoped TiO_2, alkaline earth metal (Tin), and transition metal (Strontium) doped TiO_2 and co-doped TiO_2 nanoparticles were synthesized using the sol-gel method for DSSC applications. The structural analysis indicates the formation of a mixed phase of TiO_2 (anatase and rutile), and the doped samples show nanocomposites of TiO_2, SrO_2, and SnO_2. From the microstructural analysis, the crystallite size was in the range of 6.4 – 22.8 nm. The vibrational modes of TiO_2 are confirmed by micro-Raman spectrometry. The functional groups were analyzed by FTIR spectroscopy, and the bands observed at 458 cm^{-1}, 546 cm^{-1}, and 654 cm^{-1}, confirming the symmetric and asymmetric vibrational modes of O-Ti-O, Ti-O-Sn, Sn-O, Ti-O-Sr, and Sr-O. From the FESEM analysis, the spherical morphology was observed. The PL analysis shows doped samples with less intensity than un-doped samples, indicating the decrease in the recombination of electron-hole pairs. UV-DRS analysis shows the transitions are direct allowed with a band gap in the range of 3.28 to 2.38 eV. The optical absorption was redshifted, with increased Sn concentration. DSSC devices were fabricated using synthesized samples as photoanode, Platinum counter electrode, N719 dye, and iodine/tri-iodide electrolyte. J-V characteristics were tested for all samples, and the sample with equimolar concentration of Sn, Sr co-doped TiO_2 showed a PCE (η) of 3.35% with a fill factor of 42.0%, short circuit current (Jsc) of 10.29mA/cm^2 and open circuit voltage (Voc) of 0.76V.

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Mesocrystals- A New Material Design for Thermoelectric Applications

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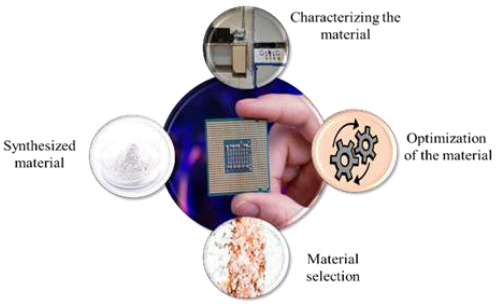
ABSTRACT

Waste to wealth approach is highly demanding sustainable approach in energy sector. Thermoelectric materials (TEMs) are promising candidates to convert waste heat into electricity, which have received much attention as it is solid-state device and approaches green energy conversion.,The TEMs are semiconducting nanoparticles with tunable energy gap and nominal figure of merit (zT). Different materials were attempted to obtain high zT however achieving high zT is still challenging due to toxicity of material, high thermal and poor electrical conductivity. Mesocrystals are new design strategy can improve the materials property due to its unique crystallographic features and micron in size. They find wide applications in optical, electrical and biomedical fields. ZnO is wide-band semiconducting material which have been widely investigated for different applications including TEs due to its optical and chemical properties. Our aim is to prepare ZnO mesocrystals by hydrothermal route and investigate the impact of this new materials design for TE properties. We also used Cobalt as dopant with ZnO at different concentrations. by following the same synthesis method. NaOH and citric acid were added to zinc acetate dihydrate precursor to control the pH and as a capping agent. The TE properties of pristine ZnO results were compared with cobalt doped ZnO to study the effect of dopants on the mesocrystals formation and zT. The synthesized materials were characterized using SEM and XRD to confirm the phase and mesocrystal structure and we successfully applied new materials design for TE application. Optimizing mesocrystals for the TE properties are in progress to investigate and confirm the role of mesocrystals in TE application.



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E 039

Electrochemical Incorporation of Cobalt Nanoparticles in WS_x for Energy Efficient Hydrogen Production

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ABSTRACT

Non precious metal/metal composites show significant electrocatalytic activity towards Hydrogen evolution reaction (HER) when exposed to alkali. Tungsten sulphide (WS_x) is one of the predominant catalysts for electrochemical HER process, but its stability for prolonged reaction is not reliable. In this work, we report an enthralling finding of electrodeposition of Cobalt nanoparticles on Tungsten sulphide (Co@WS_x), a well-known HER electrocatalyst using a simple voltammetric technique. As a result, improved HER kinetics and better charge transfer were achieved, reducing the overpotential for HER to 87 mV, much better than pristine WS_x at 10 mA cm^{-2}. Besides, it also showed a lower Tafel slope of 167.5 mV/dec explaining that water dissociation process on the catalyst's surface is predominant and higher ECSA in terms of C_{dl}, which further explains the enrichment of HER activity of the composite. The Cobalt incorporated tungsten sulphide also exhibited excellent stability upon potentiostatic electrolysis for over 40 hours, which depicts the successful and stable incorporation of cobalt in tungsten sulphide. Thus, this work opens up new avenues for studying other non-precious metal/metal composites modified with other transition metal nanoparticles in alkaline HER towards better hydrogen production.

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E 040

Boosting photofixation of nitrogen by using oxygen-vacant Ni-ZrO_2/Bi_2O_3 visible light photocatalyst with p-n heterojunction

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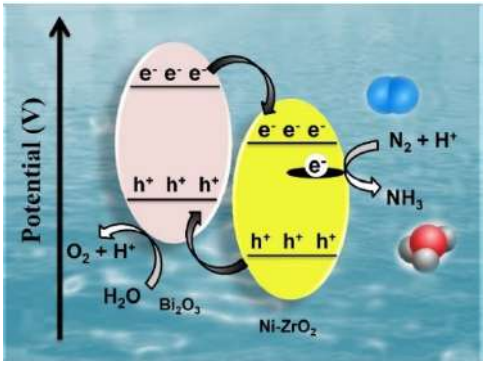
ABSTRACT

About 2% of the energy consumed annually is used for ammonia production due to its extensive use in various sectors, including hydrogen storage. Traditionally, ammonia is synthesised by the energy-intensive Haber-Bosch process, which releases carbon dioxide as an undesired byproduct. To diminish the energy input and carbon footprint, there is a paramount need to produce ammonia in ambient conditions. Photocatalytic nitrogen fixation is, therefore, one of the promising strategies for synthesising ammonia in mild conditions using sunlight, water, N_2 and a semiconductor photocatalyst[1-2]. Tailoring a visible-light photocatalyst that adsorbs and activates the triply bonded, chemically stable N_2 with high charge separation efficiency is imperative for efficient photofixation of nitrogen. Herein, a visible-light absorbing Ni-ZrO_2/Bi_2O_3 is engineered with p-n heterojunction and oxygen vacancies to remarkably enhance ammonia generation (9668.2 µmol h^{-1} g^{-1})[1,3-4]. Furthermore, the formation of the desired photocatalyst is confirmed by systematic characterisation studies. This work presents a promising strategy to design appropriate visible light-responsive photocatalysts that efficiently reduce nitrogen.



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E 041

State of the Art in Plasmonic Metal Nanoparticles for Hydrogen Evolution

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ABSTRACT

In the wide-range usage of low-dimensional materials, plasmonic nanoparticles (PNPs) exhibit higher internal and external quantum efficiencies when interacting with electromagnetic radiation. Increased confinement of plasmon excitations on the surface of PNPs gives a longer lifetime and a more significant number of high-energy hot charge carriers on extended metal surfaces, allowing selective surface chemical reactions for generating solar fuels without any unwanted by-products. One notable application of PNPs has been their integration into the field of solar hydrogen evolution through water splitting. Over the past two decades, research in photocatalytic (PC) water-splitting has been actively driven to split water and improve hydrogen evolution rates. Tailoring an antenna-reactor system with PNPs (antenna) and photocatalysts (reactor) as hybrid photocatalysts to a specific chemical reaction (here, water-splitting) increases the quantum efficiency and the overall reaction rate, as this would provide a more efficient means of producing hydrogen, a vital component in the quest for clean energy sources and sustainable fuel production. This research review not only contributes to the advancement of renewable energy technologies but also holds the potential to play a pivotal role in mitigating climate change and reducing our reliance on fossil fuels

E 042

Electrodeposition of Ni_xWO_yRu@NF for Alkaline HER Applications

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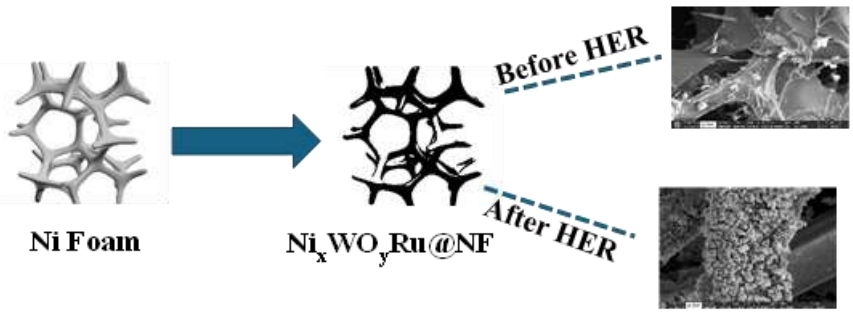
ABSTRACT

Metal hydroxide/metal oxide/metal in the trimetallic catalyst are electrodeposited on nickel foam using chronoamperometry technique to undergo hydrogen evolution reaction in alkaline water electrolysis. the electrodeposition of a Ni_xWO_yRu@NF trimetallic catalyst on a nickel foam substrate, followed by the evaluation of its catalytic performance for the Hydrogen Evolution Reaction (HER) in a 1.0 M potassium hydroxide (KOH) solution. This trimetallic catalytic electrode system is designed to efficiently promote the dissociation of water into protons and hydroxide ions using the Ni component and then efficiently discharge protons to generate hydrogen gas using the Ru component. Tungsten is being used as a co-catalyst or as a part of the catalytic system to optimize the bonding of hydrogen and prevent deactivation of Ruthenium by certain reaction intermediates. Ni_xWO_yRu@NF are performed excellent activity with low over potential (-48.8mV) to deliver a current density of -10mA/cm^2 and it showed the low tafel slope values (-134.2mV) due to the presence of nickel and tungsten along with Ruthenium in a catalytic system is likely aimed at improving the kinetics of the hydrogen-evolving reaction.



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E 043

Enhancing Charge Carrier Transport in High-Efficiency Organic Solar Cells with Perovskite Metal Oxide (M= Co, Ni, Mn) Electron Transport Layers

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ABSTRACT

In this study, new ferroelectric materials based on $MTiO_3$ (M = Co, Ni, Mn) were synthesized using the hydrothermal method as charge transport layers (CTLs). The metal oxide electron transport layers (CTLs) were found to boost the performance of PSCs due to their ability to improve the optical and electronic properties. The metal oxide-based perovskite structure influences the enhanced optical behavior of the charge transport layer (CTLs) and plays a role in reducing the band gap energy, promoting charge carrier mobility, and enhancing charge carrier transport and charge collection efficiency in OSCs. In particular, the use of perovskite metal oxides with oxygen vacancies has been shown to enhance charge carrier transport and improve charge collection efficiency in OSCs. The use of perovskite metal oxides with oxygen vacancies has been shown to optimize the PL properties of organic solar cells, resulting in enhanced light emission and reduced recombination losses. As a result, meticulously designed approach was used to attain a high photocurrent density (JSC), enhance open circuit voltage (VOC), and achieve a notably high-power conversion efficiency (PCE) in highly efficient devices employing the FTO/TiO_2/CTLs/P_3HT: PC71BM/MoO_3/Ag architecture. The effectiveness of these design modifications was confirmed through electrochemical impedance spectroscopy (EIS) analysis, which confirmed the presence of high charge recombination resistance, fast charge transport, prolonged electron lifetime, improved charge collection efficiency, and longer carrier lifetime.

Keywords: *Enhance photoabsorbing ability, Superior charge carrier mobility, Charge transport layer, High efficiency, Organic solar cells*

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E 044

Hydrazine -Functionalized Perylene Diimide Integrated Ti^{3+} Self-Doped TiO_2 Heterostructure for Visible Light-Driven Photocatalytic H_2 Evolution

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ABSTRACT

Solar light-powered photocatalytic reactions for highly efficient hydrogen evolution remain a formidable challenge. Herein, a hydrazine-functionalized perylene diimide derivative (HPDI) supramolecular aggregates were incorporated into a Ti^{3+} self-doped TiO_2 (Ti^{3+}-TiO_2) by solvent mixing method for highly efficient photocatalytic hydrogen production. The integration of HPDI effectively minimized the electron transfer path and improved the photoelectrochemical activity through π–π stacking of perylene core and hydrogen bonding of the terminal moiety with the Ti^{3+}-TiO_2. Further, the Ti^{3+}-TiO_2 formed by the partial hydrolysis of titanium isopropoxide (TTIP) followed by calcination also introduces Ti^{3+} bound states in TiO_2 forming oxygen vacancies. It is demonstrated that HPDI with π–π stacking structure along with j-aggregation effectively improve the light absorption in the visible region. The photocatalytic studies for hydrogen production showed a successful formation of the step scheme mechanism in HPDI incorporated Ti^{3+}-TiO_2 system and it exhibited a superior hydrogen production efficiency of 1390 µmol/g, which is four-folds higher than bare TiO_2. Thus, this work paves the way to design molecular structures as efficient photocatalysts for hydrogen production.

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E 045

$La_{1-x}Ce_xCoO_3$ Based Oxide Perovskites for Mid Temperature Thermoelectric Applications

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ABSTRACT

Due to the capability of thermoelectric (TE) generators and coolers to facilitate a direct conversion between heat and electricity without any emissions or moving parts, TE materials play a pivotal role as one of the solutions for redeeming the global energy crisis. The energy conversion efficiency of TE devise depends on the thermoelectric performance of constituent materials. A good thermoelectric material is judged by its dimensionless figure of merit ZT ($ZT=\sigma S^2T/(\kappa_{el}+\kappa_{lat})$) which needs high electrical conductivity σ, Seebeck coefficient S and low thermal conductivity κ to attain a high value. Traditionally, Bi_2Te_3 and its alloys are the primarily used thermoelectric materials in commercial applications, but its optimal operation has been limited to only around room temperature which urges researchers to look for new efficient and eco-friendly thermoelectric materials for applications at elevated temperatures. Hole-doped eco-friendly perovskite cobaltite- $La_{1-x}A_xCoO_3$ (A=divalent alkaline-earth element) have attracted a lot of attention due to their interesting electric and magnetic properties [1, 2]. In contrast, the investigations on TE properties of electron-doped $LaCoO_3$ (e.g., tetravalent Ce^{4+} doped $LaCoO_3$) are still scarce. The present work investigates the effect of electron doping on the structural and thermoelectric properties of perovskite based $La_{1-x}Ce_xCoO_3$ with a wider doping range ($0 \leq x \geq 0.2$).

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E 046

Hydrogen evolution via Photoelectrochemical Water splitting by using Hematite Photoanode

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ABSTRACT

As an ideal photoelectrochemical (PEC) water oxidation area, hematite (α-Fe_2O_3) has received much attention from scientists on account of its favorable band gap and excellent stability in alkaline media. However, the practical photocurrent yield of α-Fe_2O_3 is much less than the theoretical value because of the high charge recombination and the low charge transport. Here, the photoanode is fabricated by two different types of methods: precipitation and hydrothermal. The nanoparticles' size, structural, optical, and magnetic properties were determined and compared using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FT-IR), and ultraviolet-visible (UV-Vis) analysis. Hematite (α-Fe_2O_3) has emerged as a promising photo-electrode material due to its significant light absorption, chemical stability in aqueous environments, and sample abundance. However, its performance as a water-oxidizing photoanode has been crucially limited by poor optoelectronic properties that lead to both low light harvesting efficiencies and a large requisite overpotential for photo-assisted water oxidation. This research presents a novel route to enhance the efficiency of charge separation and affords theoretical guidance for preparing the high-efficiency PEC photoanodes and the switchable control of the photoelectrochemical response.

Keywords: *α-Fe_2O_3, precipitation and hydrothermal, PEC water splitting*

E 047

Single Charge Carrier Mobility Measurement of High-Performance Organic-Inorganic Hybrid Conducting Polymer Nanocomposite for Indoor Photovoltaics

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ABSTRACT

Indoor photovoltaics is a promising tool to power smart wireless electronic devices in the branch of the Internet of Things (IoT). The ternary blend-based organic photovoltaic improves optoelectronic properties and enhances the power conversion efficiency (PCE). In this work, PTB7:$PC_{70}BM$ binary system was investigated along with the molybdenum disulfide nano-sheet (MoS_2N) and the mobility of the hole and electron were calculated using a modified SCLC equation. The MoS_2N having a high mobility value of 200-500 $cm^2 V^{-1}s^{-2}$ and exhibits a direct bandgap of 1.9 eV. Due to the above properties of MoS_2N, the charge carrier mobility value was increased. The modified SCLC studies were carried out for ITO/ZnO/PTB7:$PC_{70}BM$/Ca/Al (binary) and ITO/ZnO/PTB7:$PC_{70}BM$:MoS_2N /Ca/Al (ternary) design was used for the electron only device. ITO/PEDOT:PSS/PTB7:$PC_{70}BM$/Au (binary) and ITO/PEDOT:PSS/PTB7:$PC_{70}BM$:MoS_2N/Au (ternary) device design was used for hole-only measurement. The ternary blend showed balanced electron-to-hole mobility along with enhancement in the mobility. Further, the electron-only and hole only device simulation was carried out and the obtained results were compared with the experimental results and reported.

Keywords: *Indoor photovoltaics, Mobility, 2D materials.*

E 048

Study of synthesis and characterization of Praseodymium doped Nickel Zinc Ferrite for Photovoltaic Application

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ABSTRACT

Ferrites are one such type of ceramic-like material that possesses super magnetism. Spinel-structured Nickel Zinc Praseodymium ferrite ($NiZnPr_yFe_{2-y}O_4$) was successfully synthesized by the sol-gel auto-combustion method. The above ferrite was synthesized by using pure double distilled water, Nickel nitrate,Zinc Nitrate, Praseodymium Nitrate, Ferric Nitrate, and Citric acid as a fuel with y=0, 0.025, 0.050, 0.075, 0.1, 0.125. Saturation Magnetization Ms, CoercivityHc, MagneticremanenceMr, and Squareness Ratio are obtained by M-H plots confirming super magnetic behaviour of $NiZnPr_yFe_{2-y}O_4$samples.The X-ray diffraction (XRD) pattern $NiZnPr_yFe_{(2-Y)}O_4$ was recorded with an X-ray diffractometer. The average crystallite size and other structural parameters were calculated by using XRD analysis. FTIR analysis confirmed the formation of spinel structure. The crystallite size of $NiZnPr_yFe_{(2-y)}O_4$ was decreased on Pr doping. The effect of Pr doping on the band gap of zinc ferrite was studied by UV-vis analysis.

Keywords: Nanoparticles, Spinel ferrite, Coercivity, Magnetic remanence.

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E 049

$SrTiO_3$/rGO Heterojunction Photoanode with Improved Pore Diameter Synthesized by Facile Hydrothermal Route for DSSCs Applications

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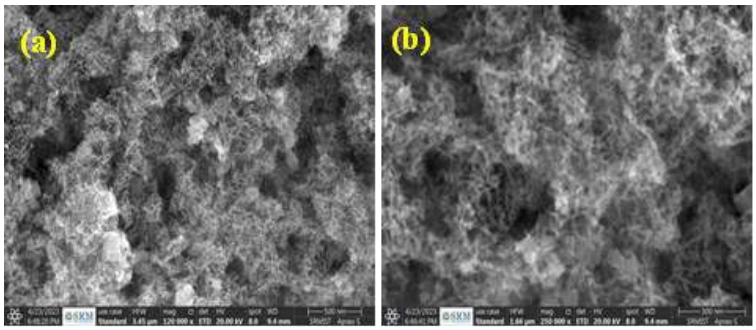
ABSTRACT

In this work, we present a novel type of $SrTiO_3$/rGO hybrid structure synthesized by facile hydrothermal route, with a tunable, phase component and surface area by adjusting the molar ratio of Sr and rGO precursors. The substitution doping with rGO 1%, 5%, and 10% into $SrTiO_3$- nanowire, among all the samples of 10% $SrTiO_3$ of the synthesized $SrTiO_3$/rGO hybrid structure nanostructures can provide a high surface area and porous structure. It is noteworthy to improve dye loading capacity and the amount of photo-generated charges contributing to the dye-sensitized solar cells (DSSCs). The formation of hybrid structures between $SrTiO_3$ and rGO with a uniquely matched band gap energy structure can efficiently separate photo-generated charge carriers. The structure and surface morphology of the $SrTiO_3$/rGO hybrid structure were carried out by SEM, TEM, and XRD characterization techniques. The heterojunction of $SrTiO_3$/rGO low photoluminescence intensity (PL) indicating reduce the charge recombination deliver an enhanced efficiency (DSSCs) and electrochemical impedance spectroscopy (EIS), (I-V) measurements reveal a lower recombination rate of photo-generated electrons and holes and a longer electron lifetime for the DSSCs based on the $SrTiO_3$/rGO hybrid structures. The photoelectric conversion efficiency and shortcircuit current density of DSSCs based on $SrTiO_3$/rGO hybrid structures show a higher short-circuit current density of 12.55 $mAcm^{-2}$ and a maximal photoelectric conversion efficiency of 2.35% under one direct sunlight illumination.



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E 050

Improved Thermoelectric Performance in Polypyrrole/Polyaniline/Carbon Black (PPy/PANI/CB) Polymer Ternary Composite for Room-Temperature Application

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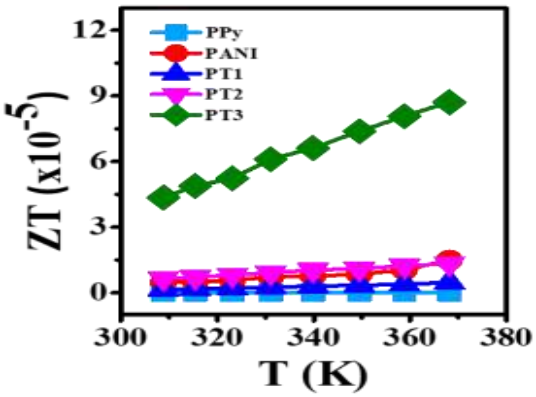
ABSTRACT

Recently, conducting polymers (CPs) have drawn more interest as potential thermoelectric materials due to their low cost, low toxicity, environmental stability, low thermal conductivity, and flexibility. In this work, Polypyrrole (PPy) with high electrical conductivity, good environmental stability, and low thermal conductivity than other CPs, is regarded as the TE material whose performance has been enhanced by the inclusion of polyaniline (PANI) and carbon black (CB). Initially, PPy/PANI binary composite was prepared through chemical polymerization and then CB was added in varying amount (10, 20, and 30 wt.%) to create PPy/PANI/CB ternary composite. The XRD, FTIR, XPS, and FESEM results demonstrated the successful formation of composite and the good interaction among PPy, PANI, and CB. The thermoelectric results demonstrated that both electrical conductivity and Seebeck coefficient increased with increasing CB content from 10 to 30 wt.% within the PPy P/PANI/CB composite. Finally, the composite possessing maximum CB content (30 wt.%) demonstrated higher electrical conductivity (55 S/m), higher Seebeck coefficient (29.4 μV/K), and lower thermal conductivity (0.21 W/mK), which resulted in a high ZT of 8.7×10^{-5} at 370 K (Fig.1). The obtained high ZT of the PPy/PANI/CB composite is 609 times greater than that of pure PPy particle. The improved TE performance in the PPy/PANI/CB ternary composite was attributed to the strong non-covalent interaction and the increased carrier scattering.



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E 051

Evaluating the Enhancement in Thermoelectric Properties of Co-doped MoS_2 for Mid Temperature Applications

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ABSTRACT

Thermoelectric (TE) materials play a crucial role in directly converting waste heat into electricity, making a significant contribution to mitigating the global energy crisis. The research community has exhibited considerable interest in two-dimensional transition metal dichalcogenides (2D-TMDCs) for thermoelectric applications, with MoS_2 emerging as a particularly promising material. This study demonstrates the synthesis of Co-doped MoS_2 using the hydrothermal method, aimed at exploring its potential for thermoelectric applications. The phase purity and crystal structure of the synthesized samples were confirmed by X-ray diffraction studies. A systematic investigation was conducted on the thermal and electronic transport properties of Co-doped MoS_2 to understand its influence on thermoelectric properties. The reduction in thermal conductivity to 0.447 $Wm^{-1}K^{-1}$ for the 5% Co-doped sample is lower than that of pristine MoS_2. Co-doping into the hexagonal crystal lattice of MoS_2 promotes mass fluctuation, grain boundary and point defect phonon scattering. The significant enhancement in electrical conductivity and a satisfactory Seebeck coefficient result in an improved power factor of 18.08 $\mu Wm^{-1}K^{-2}$. The improved phonon scattering and carrier transport contribute to enhancing the zT value of 3% Co-doped MoS_2 to 0.017.

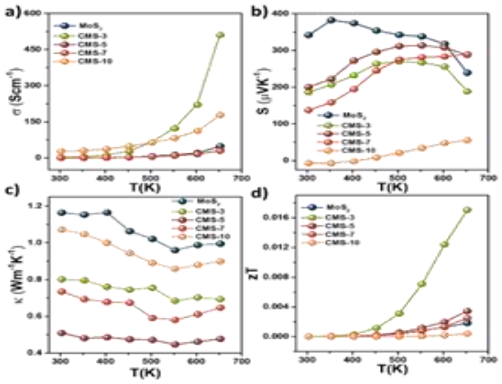

Fig. Temperature dependent a) electrical conductivity, b)Seebeck coefficient, c) thermal conductivity and d) figureof-merit (zT) of Co-doped MoS_2

E 052

Enhanced Electrical Conductivity and Seebeck Coefficient Synergistically Boost the Thermoelectric Performance of Bi Substituted Ag_2Se

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ABSTRACT

Thermoelectricity is a process that enables the direct conversion of heat energy into electrical energy, and vice versa, without any harmful emissions, thereby making it an eco-friendly technology. The pursuit of finding a thermoelectric material with exceptional efficiency at ambient temperature has been high demand. Transition metal chalcogenides have emerged as a promising group of materials. Among them, Ag_2Se has been identified as a top contender due to its remarkable thermoelectric performance at near-room temperature. This property has generated a lot of interest as a potential alternative to n-type Bi_2Te_3. Ag_2Se is categorized as a typical "phonon-glass electron-crystal" material, exhibiting an extremely low κ_l value. Here we synthesized Bi substituted Ag_2Se by solvothermal method followed by hot press densification technique. Bi substituted sample shows an exceptionally high mobility of 2983 $cm^2V^{-1}S^{-1}$ at room temperature and a maximum power factor of 2077 $\mu Wm^{-1}K^{-2}$ at 393 K. The maximum zT of 0.5 is obtained at 383 K for Bi substituted sample. The electric transport properties of the material were improved and the thermal conductivity is reduced for Bi substituted Ag_2Se samples resulting in enhanced thermoelectric properties.

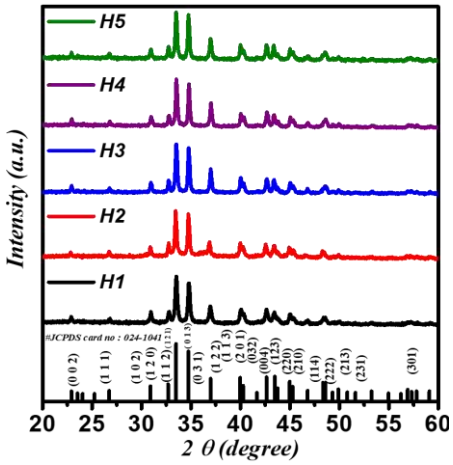

Fig.1. XRD spectrum of Bi substituted Ag_2Se

Key words: *Electrical conductivity; Hall measurement; Solvothermal method; hot press*

E 053

Investigation of Rare Earth Element Substitution Y^{3+}/Sr^{2+} On Ba Site of Barium Stannate for High Performance DSSC Application

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ABSTRACT

The construction of a high performance DSSC device with appropriate photoanode material can effectively transfer the maximum charge carrier that leads to production in large-scale commercial applications. Recently, n-type ternary perovskite ABO_3 structured metal oxide has been proposed as an alternative photoanode in DSSC. Here, we have chosen two rare earth elements (Y^{3+}/Sr^{2+}) that were partially substituted on the higher ionic radius of the cationic 'Ba' site. The pure and doped samples (1%, 3% & 5%) were prepared by the co-precipitation method. The structural, optical and morphological studies were analyzed with XRD, UV-DRS, SEM and TEM respectively. Here, the mesoporous TiO_2 is used as a compact layer. The fabricated device will show high transportation of electrons at the BSO/m-TiO_2 interface because [1] it prevents the recombination of electron-hole pairs and [2] limits the back scattering of electrons. The photovoltaic I-V measurements for all devices were examined by a solar simulator with an input power of 100mW/cm^2. The interfacial charge transfer resistance of iodide electrolyte/dye/BSO/m-TiO_2 devices and their electron lifetime were analyzed by using the electrochemical workstation.

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E 054

Ionovoltaics with Lead-free Perovskite

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ABSTRACT

In the realm of harnessing solar power, the challenge of ion migration looms large. However, when it comes to humidity sensors, ion migration takes center stage in boosting their capabilities. Water, a highly, polar liquid, possesses a unique ability to stabilize charged species like salt, acids, and bases. The separation of solvated cations and anions creates electric fields. Achieving a macroscopic asymmetric ion distribution result in an electromotive force, generating voltage between two electrodes in a device. This voltage, when connected to an external circuit, drives a current. In this study, we successfully developed a lead-free perovskite using a solution-based approach. Our focus was on exploring its humidity sensing capabilities for applications in both humidity sensors and ionovoltaic electricity generators. The research highlights the reliable performance of these devices, demonstrating their ability to generate open-circuit voltage and short-circuit current even at high moisture levels. The $Cs_3(SbBi)_2Br_9$ sensor stood out for its consistent performance during extensive testing, a long-term stability tests confirmed its resilience to high humidity conditions. Beyond its role as a humidity sensor, the sheet-like mixed alloy $Cs_3(SbBi)_2Br_9$ perovskite material also served as an ionovoltaic achieving an impressive power density of 3.06 mW/cm^2. The study delves into the influence of anions in lead-free antimony-based perovskite materials, such as $Cs_3Sb_2X_9$ (X=Cl/Br/I), on their versatility of applications such as humidity sensing, and ionovoltaics. At 85 % RH, $Cs_3Bi_2Br_9$ perovskite achieved a peak open circuit voltage of 0.267 V and a short circuit current of 25 µA.

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E 055

Enhanced catalytic performance of NiO nanosheets by the substitution of Co^{2+} ions for dye-sensitized solar cells application

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ABSTRACT

Dye-sensitized solar cells (DSSCs) show significant promise as an emerging technology, particularly in overcoming the hurdle of replacing the expensive platinum (Pt) counter electrode (CE) with cost-effective and chemically stable materials [1,2]. In this work, the DSSCs fabricated with two-dimensional hexagonal mesoporous (2D-HM) NiO and different mol% of Co^{2+} (1, 3, and 5%) substituted NiO (Co (1-5%)-NiO) nanosheets (NSs) based CEs. The 2D-HM NiO and Co (1-5%)-NiO NSs were prepared by a facile hydrothermal method. The BET result of NiO and Co (15%)-NiO reveals that the specific surface area of 2D-HM NiO NSs increased with the increase of Co^{2+} ions concentration in Ni^{2+} sites which resulted in a higher number of exposed electrocatalytic sites, thereby accelerating the reduction rate of I_3^- ions. The cyclic voltammetry (CV) result of 5 mol% of Co substituted NiO (5-CNO) shows outstanding electrocatalytic activity towards the redox reaction of I_3^-/I^- redox mediator. The DSSCs fabricated with 5-CNO CE exhibit excellent photovoltaic performance because of their high active surface area and enhanced electrical conductivity resulting by the substitution of Co^{2+} ions in Ni^{2+} sites. The 5-CNO CE has low cost, excellent electrocatalytic activity, and superior photovoltaic performance than NiO and other Co (1-3%)-NiO which makes it a suitable candidate for Pt-free DSSCs application.

Keywords: DSSCs, counter electrode, catalyst, specific surface area, EIS, NiO, nanosheets

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E 056

Topological Insulator/Carbon Nanotube Hybrid Composites as Novel Counter Electrode Materials for Dye-Sensitized Solar Cells and Near-Infrared Photodetector Applications

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ABSTRACT

Two-dimensional layered bismuth telluride (Bi_2Te_3), a prominent topological insulator, has garnered global scientific attention for its unique properties and potential applications in optoelectronics and electrochemical devices. Notably, there is a growing emphasis on improving photon-to-electron conversion efficiency in dye-sensitized solar cells (DSSCs), prompting the exploration of alternatives to noble metal catalysts like platinum (Pt). This study presents the synthesis of Bi_2Te_3 and its hybrid nanostructure with single-wall carbon nanotubes (SWCNT) via a straightforward hydrothermal process. The research unveils a novel application for the Bi_2Te_3-SWCNT hybrid structure, serving as a counter electrode in platinum-free DSSCs, facilitating the conversion of triiodide (I_3-) to iodide (I-) and functioning as an active electrode material in a photodetector (n-Bi_2Te_3-SWCNT/p-Si).The resulting DSSC employing the Bi_2Te_3-SWCNT hybrid counter electrode achieves a power conversion efficiency (PCE) of 4.2%, a photocurrent density of 10.5 mA/cm^2, a fill factor (FF) of 62%, and superior charge transfer kinetics compared to pristine Bi_2Te_3-based counter electrodes (PCE 2.1%, FF 34%). Additionally, a spin coating technique enhances the performance of the n-Bi_2Te_3-SWCNT/p-Si photodetector, yielding a responsivity of 2.2 AW^1, detectivity of 1.2 x 10^{-3}, and enhanced external quantum efficiency. These findings demonstrate that the newly developed Bi_2Te_3-SWCNT heterostructure enhances interfacial charge transport, electrocatalytic performance in DSSCs, and overall photodetector performance.

Keywords: *Topological insulator, DSSC, SWCNT, photodetector, heterostructure*

E 057

$AgBiS_2/g\text{-}C_3N_4$ hybrid composite: Synthesis, characterization and counter electrode performance in DSSC

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ABSTRACT

In this work, $AgBiS_2$ was produced utilising the solvothermal approach and $g\text{-}C_3N_4$ was produced by heating melamine to 500 °C, and composition was carried out via sonication. Agglomerated flakes formed on the surface of the $g\text{-}C_3N_4$'s multilayer structure. The bandgap expanded to 1 eV and the absorption spectra revealed a red shift. The stretching modes of C-N heterocycles and the robust interaction between the two materials were confirmed by functional groups. The improved cathodic current density and low charge transfer resistance implied improved catalytic activity by adding $g\text{-}C_3N_4$. Also, the photovoltaic performance increased to 1.42 %. The strong interaction between the $g\text{-}C_3N_4$ and $AgBiS_2$ contributes enhanced photovoltaic performance.

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E 058

A 920 MHz RF-to-DC Rectifier Circuit as Radio Frequency Energy Harvesting Module for Agriculture Applications

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ABSTRACT

Agriculture 4.0, which is the future of agricultural technology, symbolizes a revolution in farming through the integration of advanced technologies such as the Internet of Things (IoT), precision agriculture, and many more. One method for involving the next-generation IoT implementation in proactive energy replenishment and next-generation wireless network is Radio Frequency (RF) energy harvesting. As a tool for energy harvesting, a rectenna (rectifier and antenna) is proposed in LoRA frequency of 920 MHz, which consists of a receiver antenna, matching network, RF-to-DC Rectifier, storage element, and a load. By exclusively capturing the LoRa frequency characterized by narrowband features, the selectivity of RF signal energy targeting and extraction from particular sources is heightened. This optimization aims to maximize the potential for energy harvesting while minimizing vulnerability to interference from undesired noise sources. The two-stage voltage multiplier based on the Greinacher voltage doubler is adopted for rectifier and combined with dual-band E-shaped patch antenna. According to the simulation results, the proposed circuit has an output voltage of 3.3 V, an output current of 2.2 mA, and an efficiency level of 73.31%. This circuit is constructed in a PCB with a 4 x 2.4 cm dimension.

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E 059

Structural and Optical Study of Fe-doped ZnO Alloys

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ABSTRACT

In this work, Fe-doped Zn ($Zn_{1-x}Fe_xO$, x=0.0, 0.02, 0.03) alloys were synthesized by solution method. The prepared samples were characterized with different characterization methods. The structural investigation was performed with X-ray diffraction technique. It was observed that Fe-doping does not change the crystal structure of ZnO, but the geometrical parameters of prepared samples depend upon Fe concentration in ZnO. The optical properties were studied with UV-Visible and photoluminescence spectroscopy. It was found that Fe doping is responsible for blue shift and responsible for reducing the defect density in doped samples.

Keywords: *Fe-doped ZnO alloys, structural and optical study*

E 060

Design and Optimization of PVDF-AlN-Metglass Magnetoelectric Transducer for Magnetic Energy Harvesting

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ABSTRACT

Wireless sensor networks (WSNs) for IoT and remote monitoring have advanced significantly in recent years. Concurrently, energy harvesters are being developed to meet power needs, extending device runtime, and overcoming traditional power supply limitations, such as batteries. Among the various resources for energy harvesting, the magnetic noise could be converted into electricity by strain mediated flexible Magnetoelectric (ME) transducer with high efficiency energy conversion. The ME transducer integrates piezoelectric material and magnetostrictive material. ME-based energy harvester can harness energy from both mechanical vibrations and magnetic fields simultaneously. In this study we have prepared flexible PVDF-AlN polymer-ceramic fiber with different concentrations using electrospinning method. The structure and morphology of fabricated fiber was confirmed by using XRD, FTIR and FE-SEM techniques. It was found that the dielectric and ferroelectric properties of the fiber are strongly affected by the exposure of ultraviolet light. Subsequently, ME transducer were designed by integrating PVDF-AlN polymer-ceramic composite and metglas. Furthermore, we will study ME coupling coefficients of composite PVDF-AlN/Metglass, and optimal DC power density by exposing the device under weak magnetic field of 6 Oe at a frequency of 50 Hz.

E 061

Improvement of Electrical and Energy Harvesting Properties of Lead-Free Sb Modified $K_{0.5}Na_{0.5}NbO_3$ Ceramic

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ABSTRACT

Lead-free ferroelectric materials have attracted considerable attention due to their potential application in mechanical energy harvesting. In this research, the properties of $K_{0.5}Na_{0.5}NbO_3$(KNN), a promising lead-free ferroelectric material, were enhanced by introducing 3.5% Antimony (Sb) doping on the B-site (KNNS) using the solid-state reaction method. The crystal structure analysis conducted through X-ray diffraction (XRD) confirmed that both the KNN sample and KNNS ceramic and lattice parameters were calculated by Rietveld refinement using *fullprof* software. Raman spectroscopy revealed shifts towards lower frequencies in various stretching and bending modes of KNNS ceramic, suggesting modifications in the lattice dynamics and phonon behaviour of the material. Dielectric measurements carried out at room temperature demonstrated an increase in the dielectric constant of the Sb-doped sample. Although the tangent loss showed a slight reduction, it implied a potential decrease in energy dissipation. Temperature-dependent dielectric measurements exhibited two phase transitions such as orthogonal to the tetragonal phase (T_{O-T}) and the tetragonal phase to the cubic phase (T_{T-C}) for both ceramics. Hysteresis loop studies revealed a better-defined ferroelectric loop with a slimmer shape in the KNNS ceramic compared to the undoped ceramic. Further, the energy is harvested through finger tapping for both KNN and KNNS ceramics. The results demonstrate the successful incorporation of 3.5% Sb doping in KNN while maintaining its orthorhombic crystal structure. UV-visible spectroscopy indicated that the band gap of both ceramics remains the same. The KNNS ceramic exhibited modified lattice dynamics, improved dielectric properties, enhanced ferroelectric behaviour, and increased breakdown electric strength. These findings underscore the potential of Sb doping in enhancing the properties of lead-free ferroelectric KNN for applications in mechanical energy harvesting.

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E 062

Catalytic Hydrogenation of CO_2 using Metal doped Mesoporous Hydroxyapatite

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ABSTRACT

Global warming and the mitigation of the important greenhouse gas, CO_2 is a vital problem encountered in the recent days. Scientists are working towards carbon capture, utilization and storage process from large point sources, where fossil fuels are used to generate power. Instead of storage, utilizing CO_2 by converting into value added chemicals and feedstocks by several electrochemical, photochemical, photo electrochemical pathways and hydrogenation is a promising approach. Catalytic hydrogenation of CO_2 has tremendous scope in converting CO_2 into high carbon energy sources such as methanol, ethanol, gasoline and even jet fuels, with proper selection of catalysts. The most challenging part lies in the activation of CO_2 because of high energy involved in the highly stable C=O bond. Both homogeneous and heterogeneous catalysts are used as reducing agents. However, heterogeneous catalysts can be tuned to achieve high selectivity towards a specific product. Mesoporous supports are proved to have high surface area with thermal and hydrothermal stability, and can be tuned to improve the selectivity of a product. Hydroxyapatite is a naturally occurring calcium phosphate mineral, which has high adsorption towards CO_2. In this study, mesoporous hydroxyapatite was synthesized by template method using cetyltrimethylammonium bromide as a surfactant and the ratio of Ca/P was maintained as 1:67. Active metals such as Zn, Mn and Fe were loaded on Meso-HAP by incipient wetness impregnation method. All the catalysts were characterized by XRD, BET, HR-TEM, HR-SEM, FT-IR, and UV-Visible DRS to study their physico-chemical properties. The catalysts were tested for catalytic hydrogenation of CO_2 in a fixed bed reactor. All the products were analyzed by Gas Chromatography using FID and TCD detectors. The parameters such as time, temperature, GHSV and ratio of CO_2/H_2, loading of active metal were optimized. The catalysts were found to be highly active towards hydrogenation of CO_2.

Keywords: *Hydroxyapatite, Mesoporous material, Microwave method, CTAB, CO_2 Hydrogenation.*

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E 063

A Study on The Potential Thermal Regulation Effects of Micro Granules of Lauric Acid @Alginate PCM Implemented in Green Geopolymeric Cement

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ABSTRACT

Organic Phase Change Materials (PCM), are latent heat storage material, and their efficiency is enhanced while they are encapsulated in a shell. This way, we can avoid the leakage of PCM during phase transition. The most widely used PCM is paraffin with a working temperature range of 35-40 C but dependency on fossil fuel for production and non-biodegradability restrict their implementation. To find alternate green PCM, Lauric Acid (LA) from natural sources working in the temperature 35-40°C aimed for to develop microcapsules using calcium alginate. The LA beads are optimized in the ratio of core to shell as 1.0 by cross-linking the alginate, a biopolymer using calcium chloride. The prepared microcapsules are integrated into the ambient cured alkali excited fly ash - Ground granulated Blast Furnace slag, in the ratio of 4:1. In-depth study was conducted to elucidate the microstructure and functional properties relation (GP – LA and GP – LA@ Alg) using multiple characterization techniques. Phase assemblages by powder X-ray diffraction and chemical structure by Fourier Transform Infrared spectroscopy showed the distinguishable assignments for GP, LA, and Alginate, proving that no chemical reaction occurs between beads and geopolymer. Morphological analysis from SEM micrographs reveals that the spherical alginate beads act as a microcapsule, encapsulating LA, thereby preventing their leakage during heating. Thermal stability was ascertained from Thermogravimetric analysis and Differential scanning calorimetry results. The latent heat capacity of the LA @Alg and GP – LA@ Alg. The liquid migration test results showed the tightness of LA@ Alg and GP – LA@ Alg and remained stable until 100 thermal cycles. The incorporated LA@ Alg effectively reduced heat transfer with improved thermal energy storage (TES) capacity without affecting the mechanical property.

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E 064

Breaking of Phonon Bottleneck in $CsPbI_3$ Nanocrystals

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ABSTRACT

Inorganics lead halide perovskite (LHP) have been shown their supremacy in optoelectronic application due to their flexible bandgap tunability, defect tolerance and high photoluminescence quantum yield nature. Although, LHPs have many hallmark properties which can support highly efficient photovoltaic devices, but faster thermalization time of hot carriers support electron and hole recombination at band-edge which obstruct in carrier extraction and emit the light which preferable for light emitting devices. To increase their efficiency in solar energy harvesting, we must extract the hot carriers before they recombine which can be possible when thermalization time will be longer. Recently, efficient photovoltaic and light emitting devices are immediate requirement for future technological development. Here, we have chosen $CsPbI_3$ and Cu doped $CsPbI_3$ nanocrystals (NCs) and addressed both issues simultaneously by using transient absorption spectroscopy. Our sample can be classified as an intermediate confined system as the size of NCs is 16 nm (32 nm) for $CsPbI_3$ (Cu-doped $CsPbI_3$) NCs which are higher than Bohr's radius (~12 nm), and give sharp excitonic peaks in ground state optical absorption with excitonic position at ~2.1 eV. Further, by femtosecond laser with central wavelength 800 nm and 120 fs pulse width, we have generated second harmonic, 400 nm (3.1 eV) and excited these NCs. The fluence-dependent excitation activated the many body interaction and reveals hot carriers dynamics. At higher fluence, say 150 $\mu J/cm^2$ and above, pristine $CsPbI_3$ NCs shows breaking of phonon bottleneck effect by fast decay while Cu-doped NCs showed slow thermalization. To get insight, we have calculated Auger recombination (non-radiative) lifetime measurement by subtractive method. The lifetime measurements clearly distinguished the appearance of contrast results due to efficient Auger process associated with pristine $CsPbI_3$ NCs. Thus, our results provide insight to incorporate metal doping and understanding about hot carrier dynamics for solar energy harvesting.

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E 065

Robust Magnetic Energy Harvesting of Self-Biased $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$-PVDF Composites through Solvent Casting Method

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ABSTRACT

Harvesting energy from ubiquitous stray magnetic fields through magneto-mechano-electric (MME) devices facilitates the autonomous powering of wireless sensor networks (WSNs). [1] In this study we proposed a lead-free, flexible MME generators incorporating $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$-PVDF composites through the solvent-casting method in different proportions and magnetostrictive Metglas layer was attached to the fabricated composite. The resultant MME generator with optimized composition generated a maximum ME voltage with zero DC bias field. [2] This significant result of magnetoelectric coupling coefficient was achieved for optimum composition ascribed due to the interfacial interactions between the inorganic nanoparticles and the polymer matrix of the resultant optimised composite. This developed MME generator has the ability to efficiently tap the magnetic field noise around the power cables which hold promising applications in powering sensor networks and miniature electronics applications. [3]

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E 066

Effect of Sn-Doping on the Thermoelectric Performance of Bi_2Se_3

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ABSTRCT

Bismuth Selenide (Bi_2Se_3) is a potential alternative to Bi_2Te_3 for room-temperature thermoelectric applications. For the past several decades, researchers work on Bi_2Se_3 but still it has not achieved zT more than unity. There are challenges and limitations to overcome. This work tries to overcome the interdependence of electrical and thermal transport properties of Bi_2Se_3. The carrier concentration of Bi_2Se_3 is optimized by the aliovalent Sn doping. $Bi_{2-x}Sn_xSe_3$ is synthesized by the hydrothermal method followed by cold-press densification. The Hall measurement affirm the n-type semiconducting behaviour of the samples. In addition, it was found that the carrier concentration increases with Sn content, which has a great influence on the electrical properties of Bi_2Se_3. Also, the presence of Sn in place of Bi leads to lattice shrinkage, due to mass fluctuation and ionic radius mismatch which decreases the thermal conductivity.

Key Words: *Bismuth Selenide, Aliovalent doping, Interdependency, Electrical Conductivity, Seebeck coefficient.*

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E 067

Improving DSSC Efficiency Using a Highly Active MoO_3/MoS_2-rGO Composite as a Pt-Free Counter Electrode

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ABSTRACT

The current study is directed towards advancing cost-effective electrocatalysis for Dye-Sensitized Solar Cells (DSSCs), focusing on the enhancement of counter electrode (CE) kinetics using less-explored MoO_3 rods. The approach involves the integration of two-dimensional materials, MoS_2 and reduced graphene oxide (rGO), with MoO_3 rods. This amalgamation of MoO_3 rods and a 2D layered network creates a high surface area for CE, facilitating interaction with the electrolyte, providing more active sites for redox reactions, and ensuring efficient charge transfer between the CE and electrolyte for dye regeneration. The optimized concentration of MoS_2 and rGO in the layered network demonstrates comparable performance to the conventional Pt CE. The presence of MoS_2-rGO reduces the charge transfer resistance of MoO_3/MoS_2-rGO by 2.6 times. Additionally, both limiting and exchange current densities experience significant increases of 2.2 and 2.9 times, respectively. The MoO_3/MoS_2-rGO CE with an optimized rGO concentration achieves a maximum power conversion efficiency of 5.0%, surpassing the efficiencies obtained by MoO_3 and Pt CEs by 2.9 and 1.1 times, respectively. This study establishes the MoO_3/MoS_2-rGO counter electrode as a promising alternative to Pt-based CEs, contributing to the reduction of DSSC costs and facilitating commercialization.

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E 068

Thermoelectric Performance of Pulsed Laser Deposited Sulphur Doped ZnO Thin Films

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ABSTRACT

In recent years, there is increasing interest in the study of low-dimensional zinc oxide thin films for thermoelectric applications. Combining low dimensionality with sulfur doping in ZnO has been found to enhance electrical conductivity while reducing phonon transport. These materials hold promise for improving thermoelectric performance. In this work, we present an analysis of the morphology, electrical transport, and thermoelectric performance of thin films of sulfur-doped ZnO. These films were processed using the pulsed laser deposition (PLD) technique. The structure and morphology of the films were examined using X-ray diffractometry and scanning electron microscopy. XRD analysis revealed that the films are primarily oriented along the (002) plane at 34.56 degrees. and, the thermoelectric properties were assessed using a Seebeck instrument. additionally, Additionally, we employed temperature-dependent Hall measurements to analyze the electrical properties of the sample.

Key Words: *Zinc Oxide, thin films, Pulsed Laser Deposition, Morphology and thermoelectric properties*

E 069

Integrating Dual Piezo Effect via Bi_2WO_6/ZnO to Improve Photocatalytic Activity

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ABSTRACT

In recent years, the piezo photocatalytic mechanism has been intensively recognized as a potential and promising route to sewage treatment. Here we report the Bi-piezoelectric effect improved heterogeneous photocatalysis of Bi_2WO_6/ZnO (BOW/Z) in organic pollutant removal. Initially, the nanomaterials were characterized for their physicochemical and optoelectronic properties using analytical techniques such as x-ray diffraction (XRD), scanning & transmission electron microscopes (SEM & TEM), UV–vis spectrophotometer and photoluminescence spectroscopy (PL). In addition, the photoelectrochemical activity of determining the photocurrent density and electrochemical impendence response were also been conducted. The catalytic properties of the composite, BWO/Z was studied with the degradation of RhB with visible photons irradiation and ultrasonication. In piezo photocatalysis, degradation up to 99% of norfloxacin was achieved with several folds than photocatalysis and piezo catalysis.

E 070

Performance Study of Albumen as a Positive Layer for Triboelectric Nanogenerators

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ABSTRACT

Triboelectric Nanogenerators (TENG) which works on triboelectrification over the years have proved to be an efficient, cost-effective, approach for generating electricity from mechanical motions over a wide range of frequencies. Utilising this technology with biodegradable materials in low-frequency applications presents a promising environmentally friendly alternative to traditional systems for energy harnessing. This study focuses on the viability of using Albumen TENG (Egg White TENG) paired with Polytetrafluoroethylene (PTFE) over a varying range of frequencies and surface area. The application of materials onto copper electrodes was accomplished through the spin coating method. A specifically designed arrangement was utilised to incorporate diverse frequencies and an electrometer was utilised to measure both the open-circuit voltage and short-circuit current. The maximum power density, output voltage and current obtained were 38.8706μW, 62.70038V, and 0.619942μA respectively at 1 Hz. The conclusion drawn is that the suggested pair demonstrates effective performance at low frequencies, making it a viable power source for various microelectronic devices designed for low-frequency applications.

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E 071

g-C_3N_4/CdS@ Reduced Graphene Oxide Nanocomposite for Hydrogen Evolution Reaction Through Electrocatalytic Water Splitting

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ABSTRACT

Electrocatalytic water splitting is a very promising method for producing clean hydrogen through the splitting of water. A nanocomposite of g-C_3N_4/CdS@ reduced graphene oxide (rGO) was selectively synthesized using a simple hydrothermal method. The resultant gC_3N_4/CdS@rGO nanocomposite was subjected to various analytical methods in order to confirm its structural, morphological, and electrochemical properties. As-prepared nanocomposite used in a three-electrode electrochemical cell as the working electrode (WE). Experimental measurements confirmed that the g-C_3N_4/ZnS heterojunction was uniformly embedded on the reduced graphene oxide (rGO), which enhanced the synergetic effect of the heterojunction and promoted the charge carriers. The g-C_3N_4/CdS@rGO nanocomposite demonstrated strong electrocatalytic performance, with an observed hydrogen evolution reaction (HER) overpotential of about 320 mV at a current density of 10 mA cm^{-2}. The g-C_3N_4/CdS@rGO nanocomposite exhibited outstanding electrochemical stability and significantly enhanced performance compared to the g-C_3N_4 and g-C_3N_4/CdS composite. Therefore, the results suggest that this material is more stable at the electrode-electrolyte interface to produce hydrogen by water splitting.

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E 072

Optimization of Layered Structure (PVDF-BZT)/(PVDF-Co) Flexible Nanocomposite for Magneto-Mechano-Electric Generator

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ABSTRACT

The magnetoelectric (ME) phenomenon in multiferroics describes the alteration of electric polarization or magnetization when exposed to a magnetic or electric field. This arises from the connection between a material's electric order and its magnetic properties, involving piezoelectric effects or magnetostriction. In the ME effect, a magnetic field causes mechanical strain in the magnetic layer via magnetostriction, which is then transmitted to the piezoelectric layer, generating electric displacement or dielectric polarization through the piezoelectric effect. An application utilizes the consistent low-frequency periodic magnetic field (50/60 Hz) surrounding current-carrying cables as an optimal ambient energy source for smart device power. This energy is effectively captured through a highly promising technology is called Magneto-Mechano-Electric (MME) generators. In this study, PVDF-BZT and PVDF-Co nanocomposite were synthesized using electrospinning method. Subsequently, we prepared layered structure MME generators (PVDF-BZT)/(PVDF-Co); (PVDF-BZT)/(PVDF-Co)/(PVDF-BZT) and (PVDF-Co)/(PVDF-BZT)/(PVDF-Co). The structural and morphological analysis were studied by using XRD, FTIR and FE-SEM techniques. We studied the details of magnetoelectric coupling coefficients of 2.78 mVcm $^{-1}$ Oe^{-1} for (PVDF-Co/PVDF-BZT/PVDF-Co) MME generators. This MME generator harvests a sinusoidal wave with a maximum output peak-to-peak voltage of 11.9 V when exposed to a weak AC magnetic field of 10 Oe at a frequency of 50 Hz. Additionally, the device demonstrates an exceptional optimal DC power density of 4.86 µW cm^{-3}. As a result, it holds great promise as an efficient autonomous power supply for various Internet of Things based applications.

E 073

Role of Defects in Lowering Thermal Conductivity for Enhanced Thermoelectric Properties in Zn Substituted SnS

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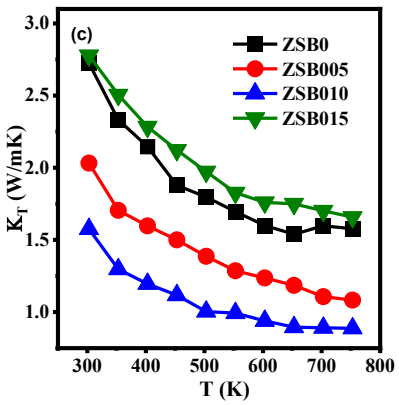
ABSTRACT

Tin Sulfide (SnS) is the most promising material for thermoelectrics owing to its layered structure, anharmonicity, earth abundance, and low toxicity in nature. Carrier concentration optimization plays a significant role in the enhancement of thermoelectric performance. In this work, the hole concentration of SnS has been enhanced by Zn substituting through the vacuum melting process. Further, the X-ray diffraction verifies the origination of a single phase with the orthorhombic structure for a pristine sample and examined the secondary phase for the Zn substituted samples. Point defect scattering due to mass fluctuation and strain field fluctuation arising from Zn substitution leads to low lattice thermal conductivity. The reduction in thermal conductivity is not only due to the presence of point defect scattering but also due to the influence of the various defects such as lattice dislocations, stacking faults, grain boundaries, etc., The synergy of multi-scale scattering results in low thermal conductivity of 0.47 W/mK at 803 K. Further, the hall measurement confirmed the p-type semiconducting nature of the sample and Zn substitution significantly improved the carrier concentration from 9.92 x 10^{15} cm^3 to 1.62 x 10^{17} cm^3 resulting in enhanced electrical conductivity and power factor.



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E 074

Carrier and Phonon Transport Properties of Ge and Ag co-Doped *p*-type Mg_3Sb_2 Nanostructure for Thermoelectric Application

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ABSTRACT

Zintl phase *p*-type magnesium antimonide (Mg_3Sb_2) have been extensively studied as promising mid-temperature thermoelectric materials due to their intrinsic low thermal conductivity, less toxicity, greater abundance, and compatibility. These compounds promote the modification of carrier concentration via chemical doping, improves the thermoelectric performance. In this present investigation, Ge and Ag co-doping strategy has followed at Mg site and interstitial site as $Mg_{3.4-x}Ge_xAg_{2x/3}Sb_2$ (x=0~0.1), which were prepared by solid-state techniques and investigated the thermoelectric transport properties. The X-ray diffraction (XRD) analysis confirms the phase formation. Further, thermoelectric properties are characterized by Seebeck coefficient, electrical conductivity, and thermal conductivity measurements from 303 K to 753 K. The presence of Ag can increase the hole carrier concentration, leading to enhancing the power factor of 158.5 $\mu W/mK^2$. Moreover, the contribution of germanium (Ge) strengthened the phonon scattering through point defect, which reducing the lattice thermal conductivity of 0.62 W/mK, resulting in a peak *zT* value of 0.13 at 753 K for $Mg_{3.3}Ge_{0.1}Ag_{0.06}Sb_2$.

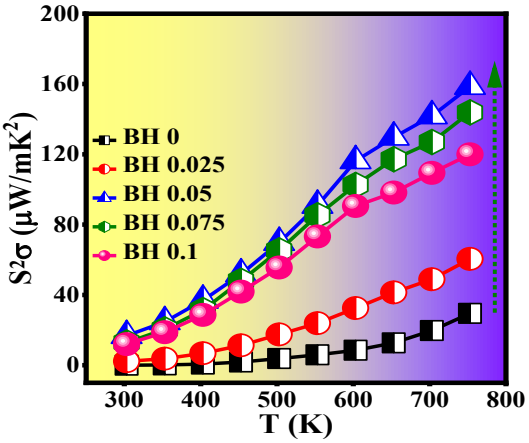

Fig. Power factor of $Mg_{3.4-x}Ge_xAg_{2x/3}Sb_2$ (x=0~0.1).

Keywords: Zintl phase, Mg_3Sb_2, co-doping, Nanostructuring, Power factor, Carrier mobility.

E 075

Tailored Ternary Nanohybrid Ag/TiO2/rGO for Efficient Light Harvesting in Plasmonic Dye Sensitized Solar Cells (PDSSC)

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ABSTRACT

In this work, we used a facile synthesis for ternary Ag/TiO_2/rGO nano-hybrid using a modified solgel-hydrothermal method. The as-synthesized ternary nanohybrid is utilized as a photoanode for highly efficient plasmonic hybrid dye-sensitized solar cells (PDSSC). The hybrid was synthesized using cetyltrimethylammonium bromide (CTAB) as the capping agent with 0.1wt% graphene content and two different Ag nanostructures than as-grown TiO_2. The addition of graphene and Ag to the TiO_2 system can improve its photovoltaic performance significantly because of the plasmonic property of Ag and graphene's conducting nature enhances charge separation at interfaces. Characterization of the synthesized hybrid photoelectrode was carried out utilizing XRD, Raman, SEM, TEM, XPS, and UV-Vis absorbance spectroscopy. The energy conversion efficiency of the plasmonic dye-sensitized solar cell (PDSSC) is significantly higher when utilizing a hybrid photoelectrode Ag/TiO_2/rGO, compared to the efficiency of a DSSC that only relies on a pure TiO_2 photoelectrode. The results suggest that the high photovoltaic performance of the PDSSC is due to the large specific area of Ag/TiO_2/rGO, which leads to high dye loading, the LSPR properties of Ag NPs and the enhanced electrical conductivity of the prepared ternary nanostructures. The proposed plasmonic hybrid nanostructures show a new approach to establishing solar energy conversion technologies large-scale applications.

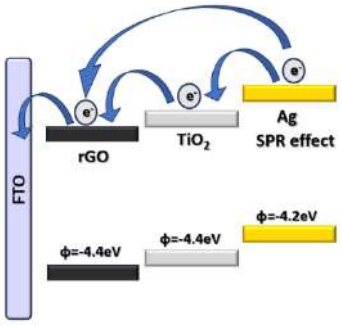

Fig1: Schematic representation of the charge transfer process influenced by a plasmonic hybrid nanostructure (Ag/TiO_2/rGO)-based DSSC device.

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E 076

Enhanced Photocatalytic Hydrogen Production from Metal Nanoparticle Decorated gC_3N_4/MoS_2 Heterojunction

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ABSTRACT

Limitations of pristine carbon nitride (gC_3N_4) reduce its effectiveness in photocatalytic hydrogen generation. Here, we overcame the constraints of pristine gC_3N_4 by creating an efficient heterojunction with molybdenum sulfide (MoS_2) by a simple co-calcination and hydrothermal procedure to boost its charge transfer efficiency. Additional metal nanoparticles were incorporated into gC_3N_4/MoS_2 to improve the hydrogen production. Characterization studies to analyse crystalline structure and morphology were done using X-ray diffraction (XRD), high-resolution TEM (HRTEM), and scanning electron microscopy (SEM). Using the photoluminescence (PL) spectrum and ultraviolet-visible diffusion reflection (UV-vis), the optical properties of the as-prepared nanocomposites were investigated on composite materials to understand the charge transfer mechanism. Photocatalysis and photoelectrochemical studies on composite materials demonstrated superior performance compared to bare materials.

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E 077

Actively Optimizing the Miscibility Gap of $Mg_2Si_{0.6}Sn_{0.4}$ Solid Solution for Mid-Temperature Thermoelectric Application

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ABSTRACT

Magnesium silicide–stannide (Mg_2Si-Sn) solid solutions are promising n-type leg for thermoelectric generators (TEG) due to their abundance and cost-effectiveness. Optimization of the thermoelectric (TE) properties of selective $Mg_2Si_{0.6}Sn_{0.4}$ compound can be accomplished by the precise control of miscibility gap (Mg_2Sn – rich) through the adjustment of the solid-state fabrication process of vacuum melting (923 K, 2 h – 24 h). The modified phase and structure of all material's solubility were followed by XRD, HR-SEM, and HR-TEM. A noteworthy phenomenon named band degeneracy has been observed in the pseudo-binary $Mg_2Si_{0.6}Sn_{0.4}$ compound due to the energy separation changes resulting from the Si^{4-}: Sn^{4-} ratio (60%: 40%). On this basis, optimized thermoelectric properties were systematically explored, including their electrical conductivity (σ), thermopower (S), and total thermal conductivity (κ_T). In addition to that improved power factor (PF) and 49% of reduced lattice thermal transportation (κ_L) were caused by the intrinsic solubility condition of alloying as a function of temperature. The established work is an essential foundation for further optimization of the thermal transportation for the performance of $Mg_2Si_{0.6}Sn_{0.4}$ composite at an intermediate temperature range (500-900 K).

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E 078

Empowering a Sustainable Future: Enhanced Triboelectric Nanogenerators using Dual-Surface Modified Ecoflex Polymer for Carbon-Neutral Technology in India

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ABSTRACT

After years of industrialization and advancements in globalization, the world has begun to realize the importance of sustainable technology. As global paradigms evolve towards sustainability, India, being a rapidly growing economy, is predicted to be at the fore-front of formulating and adopting green policies, thereby providing opportunities to innovate technologies for a carbon-neutral future. This study analyses the use of one such method that can hugely impact the way we power technological solutions. Triboelectric nanogenerators (TENGs), can harvest energy from low-frequency mechanical movements. This work suggests a straightforward and economical way to create a dual-surface modified Ecoflex polymer (SME Sponge) that has micro pyramidal projections on the surface and a porous interior structure. Pores and micro pyramidal projections' effects on triboelectric performance are examined by the construction of an Ecoflex-Aluminum-based contact separation triboelectric nanogenerator (EA-CS TENG). In order to confirm the powering and sensing applications of EA-CS TENG, a fully autonomous tally counter is demonstrated to function in a battery-free method. This work demonstrates that low-cost EA-CS TENG may be used as a sustainable energy source to power devices without requiring batteries and to generate electricity from mechanical motions.

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E 079

Effect of Post Selenization in Thermoelectric Properties of WS_2

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ABSTRACT

Tungsten disulfide (WS_2) has fascinated in recent decades because of its unique characteristics such as direct bandgap, anisotropy, low thermal conductivity, and high Seebeck coefficient is being widely researched on thermoelectric materials. The layered structure of this material possesses a large surface area that restricts phonon transportation and allows the carriers to con fine, which enhances thermoelectric properties. In this work, WS_2 is deposited on SiO_2/Si wafer through Atmospheric Pressure Chemical Vapor Deposition (APCVD) technique with Argon as a carrier gas. The effect of WS2 deposition on the substrate was analyzed by varying the growth parameters such as temperature, time and gas flow rate. As-deposited WS_2 thin film was characterized by Raman spectroscopy, HR-SEM and Seebeck measurement. The appearance of the in-plane and out-plane vibration modes $E^1{}_2g$ (351 cm^{-1}) and A_{1g} (420 cm^{-1}) corresponds to a lateral and vertical growth of WS_2. The high-resolution scanning electron microscope (HR-SEM) analysis revealed the controlled growth of WS_2. The effect of post selenization in thermoelectric properties of WS_2 and the results were studied in detail.

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E 080

Superior Thermoelectric Power Factor in BiCuSeO Enabled by Ferromagnetic Metallic Phase and Spin Entropy Effect

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ABSTRACT

Here, we investigated the influence of ferromagnetic metallic phase and spin entropy in thermoelectric properties of BiCuSeO. The magnetic characterization such as VSM and EPR confirms the presence of ferromagnetic phase $Bi_2Cu(SeO_3)_4$ in BiCuSeO. Over the temperature, the electrical conductivity (σ) decreases which confirms the metallic nature of the sample. Meanwhile, the deterioration of Seebeck coefficient was negligible compared with pure because of additional spin entropy effect confirmed from the g-factor value of 2.278. The occurrence of ferromagnetic metallic phase is effective in decoupling the thermopower and electrical conductivity with high power factor of 493.73 $\mu W\ m^{-1}K^{-2}$ at room temperature.

Key words: *Spin entropy, Ferromagnetic metallic phase*

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E 081

Effect of Heat Treatment on the Thermoelectric Performance in p-type Higher Manganese Silicide

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ABSTRACT

Higher Manganese Silicide (HMS) is a promising Te- ree p-type material with interesting functional properties. HMS is an incommensurate group of phases that crystallizes in the Nowotny chimney (Si subsystem) ladder (Mn subsystem). HMS is generally represented as $MnSi_{2-x}$ or $MnSi_{\gamma}$ ($\gamma = c_{Si}/c_{Mn}$) with 6364 at. -% of silicon than manganese (36-37%). Herein, the thermoelectric performance of $MnSi_{1.8}$ has been optimized by altering the melting periods (6h, 12h, 24h, and 36h) at (1100˚ C). The crystal structure and elemental composition have been examined by XRD and HR-SEM. Upon varying the heat treatment, the minor phases of Si and MnSi in the matrix has varied in presence. This resulted thermal conductivity of the 24-hour melted sample to be comparatively low ~ 2.09 W/mK due to the presence of the Si minor phase as meso-precipitates forming defects in the lattice. The PF of the 24-hour melted sample has achieved the highest throughout the trend 661μW/mK^2 at 803K compared to other samples. Owing to the highest power factor and lowest thermal conductivity, among all the melting periods, the 24-hour sample shows the highest zT ~ 0.25 at 803K.

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E 082

Energy Filtered Acceleration of Carrier Transport in Strongly Correlated Thermoelectric $La_{0.95}Sr_{0.05}CoO_3$/rGO Composite

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ABSTRACT

In the pursuit of developing eco-friendly, thermally stable and chalcogenide free thermoelectric material, we demonstrated the effect of incorporating 2D - rGO (reduced graphene oxide) on the thermoelectric properties of strongly correlated perovskite oxide $La_{0.95}Sr_{0.05}CoO_3$. Among the perovskite oxides, $LaCoO_3$ is a promising material due to its high Seebeck coefficient $500 - 550\ \mu VK^{-1}$ at room temperature arising from the strong correlation of $3d$ electrons and distinctive spin degeneracy. The Anderson localization (small polaron formation) is predominant in the hole transport of $LaCoO_3$ perovskites, which hinders from obtaining high thermoelectric power factor. In this work, it is shown that the incorporation of rGO facilitates the delocalization of carriers resulting in increased weighted mobility (μ_W) and power factor of $180\ \mu Wm^{-1}K^{-2}$ at 353 K. The enhancement in thermoelectric properties has been explained with the help of energy filtering effect and reduced carrier-phonon coupling strength. The low energy carriers are expected to scatter due to the increased Schottky barrier ($La_{0.95}Sr_{0.05}CoO_3$/rGO interface) height resulting in the simultaneous enhancement of Seebeck coefficient and electrical conductivity. Our strategy of incorporating 2D material in strongly correlated perovskite opens up the possibility of designing high performance thermoelectric oxides for low grade waste heat recovery.

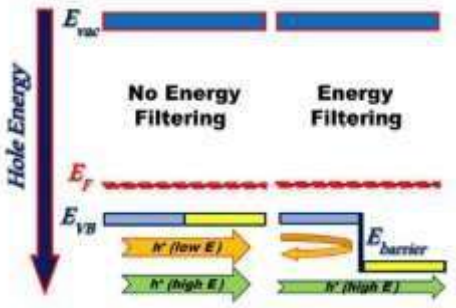

Figure 1 Schematic representation of energy filtering effect

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E 083

Investigation of Hot Carrier Cooling Dynamic in Lead Halide Perovskite Films Using Femtosecond Spectroscopy

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ABSTRACT

Photoexcitation of semiconductors above their band gap generates hot charge carriers, which later relaxes to the band edge in a few picoseconds. Investigation of the hot carriers and their relaxation dynamics is crucial, especially in the context of hot carrier solar cells. Further, a systematic investigation of the relaxation dynamics of these hot carriers and various factors that affect these dynamics is thus crucial. We employed femtosecond transient absorption (fs-TA) spectroscopy on hybrid perovskite films to uncover the mechanisms of photoexcited charge carriers immediately after photoexcitation. Results suggest that, the above bandgap photoexcitation of lead halide perovskite films generates a highly localized and bound hot carriers population immediately which dissociates to free carriers within 20 fs after photoexcitation. Further, the hot charge carriers cool down to the band edge with a time constant in the range of 250 – 350 fs in two-dimensional perovskites whereas in the case of three-dimensional perovskites the cooling time constant would be around 500 fs, depending on various factors such as no. of inorganic layers in the 2D perovskite materials, the pump excitation wavelength and the initial carrier density. Our investigation also reveals that the charge carriers in the perovskite films couple with the lattice motions via the Fröhlich mechanism. Careful analysis of the fs-TA data reveals a weak spectral modulation near the band edge of the materials which has been attributed to various optical phonon modes with frequencies ranging between 50 – 150 cm^{-1}. We believe that direct observation of the electron-phonon interaction in various materials will help in understanding the moderate charge carrier mobility and high power conversion efficiencies in perovskite-based solar cell devices.

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E 084

High-performance and Biodegradable HPMC-ZnObased TENGs for Advancing Medical Implant Technology

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ABSTRACT

Biodegradable and biocompatible Triboelectric Nanogenerators (TENGs) made from a composite of Hydroxypropyl Methylcellulose (HPMC) and Zinc Oxide (ZnO) nanostructures are fundamental in advancing medical implant technology, providing sustainable and environmentally friendly power source and sensing. Our research focuses on synthesizing and optimizing a novel biodegradable thin-film TENG layer composed of HPMC and ZnO composites. The sol-gel method is employed to fine-tune HPMC and ZnO at a concentration of 10%. Subsequently, a thin film is developed using the spin-coating technique. The surface and chemical compositions of the developed HPMC and ZnO composite thin films are confirmed through Field Emission Scanning Electron Microscopy (FeSEM), X-ray Diffraction (XRD), and Fourier Transform Infrared Spectroscopy (FTIR). The results obtained from FeSEM, XRD, and FTIR confirm the structural, compositional, and morphological characteristics of the HPMC and ZnO composites. The enhanced HPMC: ZnO composite film was utilized as the positive layer in TENGs and evaluated in conjunction with the silicon Eco flex tribo-negative layer, maintaining a constant frequency and force of 16N and 8Hz, respectively. The HPMC: ZnO composite film demonstrated a voltage that was 71.87% higher than that of the pure HPMC film, highlighting the remarkable potential of developed biodegradable thin films to not only offer sustainable alternatives but also substantially improve the efficiency of TENGs performance.

E 085

A Novel Mechano-synthesized Zeolitic Tetrazolate Framework for High-Performance Triboelectric Nanogenerator and Self-Powered Selective Neurochemical Detection

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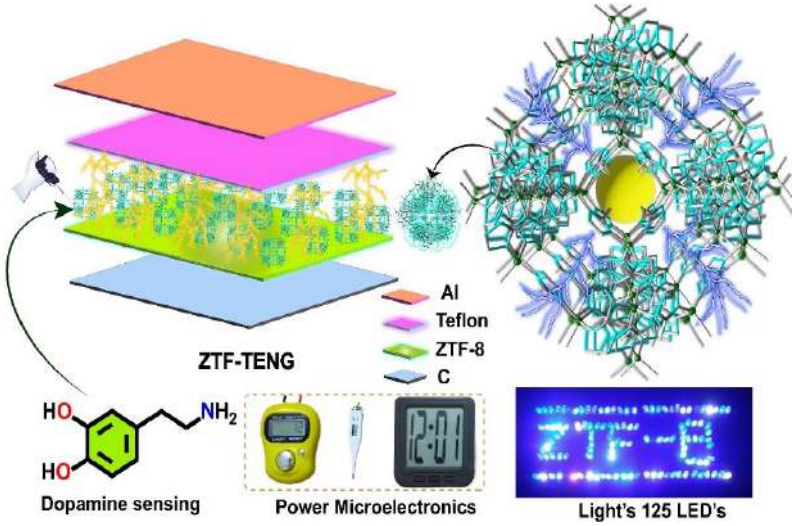
ABSTRACT

Designing a high-performing triboelectric novel material with eco-friendly, rapid, cost-effective synthesis is the future of material research in triboelectric nanogenerators (TENG). We report a mechanochemical ball mill synthesis of a Zeolitic Tetrazolate Framework (ZTF-8) which is isostructural with the well-known zeolitic imidazolate framework ZIF-8. ZTF-8 is extremely stable in water, 0.1 M aqueous acid and base solutions for 75 days at 25 °C and boiling water (100 °C) for 7 days. Kelvin probe force microscopy and Molecular Electrostatic Surface Potential computational analysis showed that ZTF-8 has very high positive surface potential. Three-Dimensional Digital Microscopy Analysis and Atomic Force Microscopy studies reveals the high roughness profile in the ZTF-8 film. The unique structure, exceptional acid/base stability, good dielectric property, high roughness profile combined with extreme electropositive nature of ZTF-8 makes it as a suitable candidate as a polymer free triboelectric positive material in TENG with outstanding performance (power density of 720 mW /m^2). This high triboelectric output was further validated using COMSOL Multiphysics simulation tool. Simple mechanical hand tapping of the ZTF based TENG (ZTF-TENG) device generates high electric output, which was practically used to power numerous low-powered devices like tally counter, clinical thermometer, digital clock and also illuminates 125 numbers of Light Emitting Diodes. In addition, the efficiency of ZTF-TENG was utilized as a self-powered device for selective dopamine (DA) sensor with good sensitivity (377.76 mV/µM/cm^2), wide range linearity (5-120 µM), and excellent limit of detection (0.42 µM). This report is extremely distinct and stand-out due to the fact that the developed TENG device's positive layer contains no polymer participation (low cost, scalable and eco-friendly approach) but still provides excellent performance and selective neurochemical sensing behavior.



E 086

Numerical Investigation on the Effect of Various ETLs and HTLs on the Performance of an Improved, Stable $MAPbI_3$ Perovskite Solar Cell with a PbS QD Layer: Using SETFOS 5.3

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ABSTRACT

Perovskite solar cells (PSC) can be considered potential competitors of silicon solar cells owing to their excellent photo conversion efficiency (PCE). However, this has not been possible so far in view of its poor environmental stability (1). A layer of quantum dot (QD) can improve the stability as per earlier reports (2,3). We, thus modelled and optimized the PSC device performance using Lead Sulphide QDs along with methyl ammonium lead iodide ($MAPbI_3$) as the absorber, taking the effect of various materials as HTL (NiO, P3HT, Spiro-MeOTAD and PEDOT: PSS) and ETL (C_{60}, PCBM, TiO_2 and ZnO) using SETFOS. In addition, the impact of layer thicknesses, doping concentrations of absorber layers along with optimized HTL/ETL as well as temperature, on the photovoltaic parameters, including PCE, are also thoroughly investigated. The optimized device obtained has a configuration of ITO/Spiro-MeOTAD/$MAPbI_3$/PbS/ZnO/Ag with an open circuit voltage of, 1.022914 V a short circuit current density of 27.39669 mA/cm^2, fill factor of 88.3114 %, a power conversion efficiency of 24.73963% and an external quantum efficiency of 90.504%. The results of this investigation shall gain increasing scientific interest in future and conjointly find applications in the design of more stable, low-cost, efficient Solar Cells based on QD's and perovskite materials.

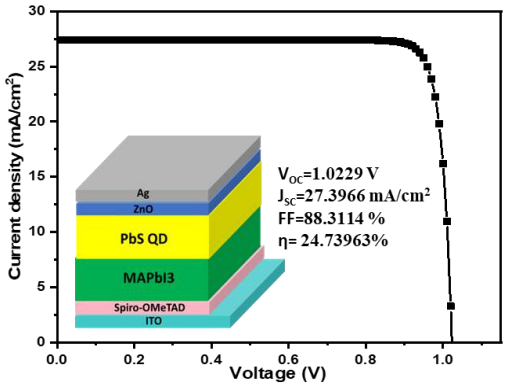

Fig.1. Current density-voltage graph of QD/perovskite solar cell.

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E 087

Metal-Organic Framework Based Triboelectric Nanogenerator for Smart Parking

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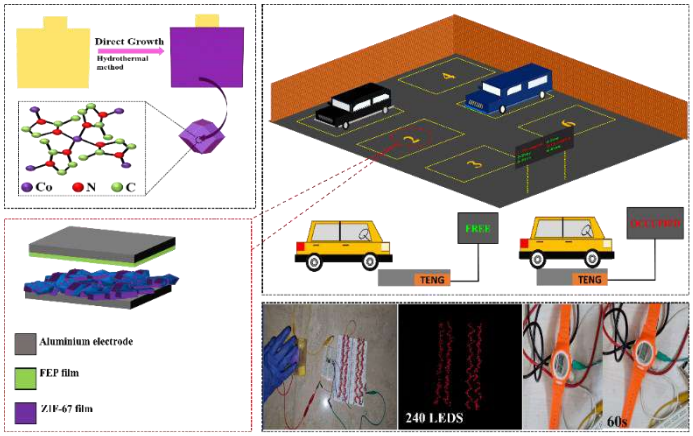
ABSTRACT

In recent years, Metal-organic framework materials (MOFs) has emerged as a promising candidate in the field of Triboelectric nanogenerators (TENGs) due to their numerous unique properties. Most of the existing literature has opted for a composite material approach, combining MOFs with polymer or binder materials to fabricate TENG device. While this method enables the integration of MOFs materials, it may not accurately reflect the intrinsic triboelectric properties of the MOFs. Hence, growing MOFs directly on conducting substrates is a major roadblock to realizing their potential in TENG devices. The novelty of this paper lies in the direct coating of ZIF-67 on conductive aluminium (Al) substrate by using a simple and cost-effective hydrothermal method. ZIF-67 film coated on Al substrate and fluorinated ethylene propylene (FEP) has been employed tribolayers. Under repeated hand tapping of 4Hz the proposed TENG produced an open circuit voltage, and short circuit current of 280V, 70µA respectively. The device exhibited highest power density of ~ 2.35W/m^2 at a matching load resistance of ~10MΩ and was used to light up 240 LEDs, and run various electronic devices. Finally, the fabricated device was demonstrated in smart parking system to deliver the real-time information about the parking slots and their locations. This work highlights the triboelectric properties of MOF material and integrating MOFs-based TENG in energy harvesting application.



E 088

Effect of $MASnI_3$ Buffer Layer on FTO/SnS_2/MEH-PPV/Cu_2O/Au Solar Cell Using Numerical Simulation

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ABSTRACT

Polymer-based solar cells are currently gaining interest due to their advantageous properties, such as a suitable band gap, high absorption coefficients, and excellent charge carrier mobility. Earlier reports have claimed that in the polymer such as poly[2-methoxy-5-(2ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV)-based solar cells, Power conversion efficiencies (PCE) can be increased to 13.38% from 9.65% using a thin layer of $MAPbI_3$ perovskite. The results in the said investigation suggests a new procedure to enhance the PCE of the Polymer based solar cell using a thin layer of Perovskite. Motivated by this, we in this investigation proposed a new thin film lead-free perovskite layer i.e., Methyl Ammonium Tin Iodide ($MASnI_3$) using which the efficiency can be enhanced from 7.33% to 22.71%. The work has been carried out using Setfos-5.3. We also calculated various parameters of the proposed solar cell, including fill factor (FF), open circuit voltage (V_{oc}), short circuit current density (J_{sc}) are found as 60.88%, 1.27 V and 29.18mA/cm^2 respectively. To the best of our knowledge the increase of PCE by 15.3% in a polymer based solar cell using a thin layer of perovskite is reported for the first time here in this investigation.

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E 089

Estimation of Band Bending and Hole Selectivity of MoO_3/n-Si Interface Subjected to Different Treatment Processes

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ABSTRACT

Dopant -Free Carrier Selective Solar Cells employing Transition Metal Oxides (TMO) have emerged as a potential alternative to conventionally doped amorphous Silicon a-Si(H) contacts, owing to their ease of deposition, low thermal budget and tunable electronic properties[1,2]. Thermally evaporated MoO_{3-x} thin films serve as hole-selective layers (HSL) in carrier-selective silicon solar cells resulting from their elevated work function and substantial band gap. The heightened work function induces upward band bending in n-type silicon creating a barrier for the electrons from Si and facilitates excellent hole transport to the HSL layer. Kelvin Probe Microscopy has been previously employed to investigate and quantify surface voltage, oxide thickness, oxide charge density, and recombination lifetimes[3,4]. Here, we adapt a novel approach using contact potential difference (CPD) from a gold tip to measure the extent of band bending at the MoO_{3-x}/n-Si interface, for a range of post- deposition processed MoO_{3-x} thin films over Si using contactless surface work-function measurements based on the principle of Kelvin Probe Force Microscopy (KFM). The surface work functions of 15nm MoO_{3-x} films on silicon are investigated in this study, considering their responses to UV exposure, vacuum anneal, air anneal, and forming gas anneal (FGA), through contactless electrostatic voltmeter measurements, with a simultaneous calculation of band bending with respect to the bare silicon surface. A series of test diode structures is fabricated using these MoO_{3-x} films as HSL, and their dark current characteristics (J-V) are systematically studied. The ideality factor η and reverse saturation current density(J_0) of the diodes are subsequently extracted and compared, shedding light on the variation in work function and thus the band bending, resulting from different treatments and exploring their impact on the hole selectivity of MoO_{3-x} films. This novel approach offers a versatile, contactless, vacuum-less method for rapid measurement of band bending at the interface between semiconductor thin films and silicon surface.

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E 090

Medical Waste Material-Inspired Triboelectric Nanogenerators for Sustainable Energy Harvesting and Self-Powered Sensors

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ABSTRACT

This work explores the environmental challenges associated with medical plastic waste in healthcare facilities and proposes an innovative solution using triboelectric nanogenerator (TENG) technology. In this study, we have used medical plastic waste, such as X-ray films and saline bottle sheets to fabricate a triboelectric nanogenerator (TENG) for the first time. The fabricated TENGs are operated in vertical contact separation mode (VCS) using Silicone rubber as the opposite triboelectric layer. The X-ray film based TENG (X-TENG) produced an open circuit voltage (V_{oc}), short circuitcurrent(I_{sc}), and instantaneous power density(P_d) of 201 V, 62.8 µA, and 1.39 W/m^2 while the saline bottle based TENG has a V_{oc}, I_{sc} of 508 V, 105 µA, and power density of of 8.78 W/m^2 which is one of the highest power density values reported for a waste material based TENG. This TENGs can directly power commercial red LEDs and turn on a calculator, digital watch, and hygrometer with a charged capacitor. Furthermore, this TENG can be utilized as a self-powered touch sensor for various security applications, human-machine interfaces, and IoTs. The suggested concept of employing medical waste for fabrication of TENG has the potential for broader application to encompass other non-hazardous plastic waste generated within the medical sector.

E 091

Investigating Liquid-Immersed Laser Ablation of Thin Film Stack Over C-Si for Laser Processed Solar Cells

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ABSTRACT

Pulsed laser ablation is becoming increasingly popular in micromachining due to the growing need for precise manufacturing and functional surfaces. Nevertheless, the effectiveness of laser processing in air is mainly hindered by particle redeposition, necessitating supplementary cleaning procedures to achieve optimal surface quality. During the laser assisted fabrication of c-Si IBC solar cells, where a stack of layers are required to be removed or patterned, the silicon substrate beneath these thin films will also get ablated and also result in the particle redeposition. This may have critical influence on the interface quality and the passivation of the silicon surface. A minimum damage to the silicon is beneficial for achieving less surface recombination velocity. A technique is being investigated in this work where this Femto second laser processing (800 nm,1kHz) is carried out in liquid medium rather than in air to control redepositions. Laser ablation in liquid enables a substantial decrease in particle redeposition, as particles quickly cool down without adhering to the substrate surface. Laser ablation in liquid is accompanied by complex interactions such as plasma formation, cavitation and persistent bubbles [1], which can induce chemical reactions on the surface. Here, we present the results of changes in surface morphology and surface chemistry and the comparative study of current voltage characteristics of the heterojunction diodes fabricated in air ambient and in liquid medium.

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E 092

Spinel-Based Thermoelectrics: Emerging Materials for Efficient Waste Heat Harvesting

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ABSTRACT

Thermoelectric materials and devices have garnered significant attention in recent years as a promising avenue for sustainable energy harvesting. This abstract provides a concise overview of the current state of thermoelectrics, emphasizing recent advancements and challenges in the field. The focus is on the utilization of waste heat as a valuable resource for power generation, with a particular emphasis on enhancing the efficiency and practicality of thermoelectric systems. Spinel compounds have recently emerged as a promising class of materials for thermoelectric applications due to their unique electronic and thermal transport properties. This abstract provides an overview of the current research landscape focused on spinel-based thermoelectrics, highlighting the distinctive characteristics of spinel structures and their potential for efficient waste heat harvesting. A significant portion of the abstract is dedicated to recent advancements in the synthesis and characterization of spinel-based thermoelectric materials. This includes discussions on innovative doping strategies, nanostructuring techniques, and the use of advanced characterization tools to tailor the thermoelectric properties of spinel compounds for optimal performance.

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E 093

Enhancing Charge Transfer and Electrocatalytic Properties of MoO_3 Counter Electrode for Pt-Free DSSC Applications

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ABSTRACT

Recent advancements in dye-sensitive solar cell (DSSC) research have been directed towards replacing expensive platinum (Pt) counter electrodes. This study explores the application of Co-doped MoO_3 as a counter electrode (CE) in DSSCs. Pure MoO_3 and MoO_3 doped with different concentrations of Co (5 wt% and 10 wt%) were synthesized using the hydrothermal method. X-ray diffraction (XRD) confirmed the mixed crystal structure (hexagonal and orthorhombic) in Co-MoO_3. Field emission scanning electron microscopy (FESEM) images revealed a decrease in rod size and the appearance of particles in Co-MoO_3. The bandgap reduction after Co-doping in MoO_3 further confirmed the presence of Cobalt in MoO_3. Additionally, Co-MoO_3 demonstrated a 94.5% improvement in charge transfer properties. Current-voltage (I-V) results indicated enhancements in J_{SC}, V_{OC}, and PCE in Co-MoO_3 CE-based DSSC devices. Specifically, devices with 5 wt% Co-doped MoO_3 exhibited a 34% higher PCE compared to pure MoO_3 (1.2%). Furthermore, a detailed analysis of electrocatalytic properties through cyclic voltammetry revealed that the incorporation of Co as an impurity in MoO_3 refined the morphology and electrical properties of MoO_3, leading to improved electrochemical performance in iodide-based electrolytes.

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E 094

Investigation of Ni-Doped MoO_3 as Counter Electrodes in Dye-Sensitized Solar Cell Application and Electrochemical Properties

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ABSTRACT

The substitution of costly platinum counter electrodes has been a central focus in the research of Dye-Sensitized Solar Cells (DSSC). Here, we present a hydrothermally synthesized nickel-doped molybdenum tri-oxide nanomaterial (Ni-MoO_3) used as a counter electrode (CE) in DSSC. The motivation for doping nickel in MoO_3 was to explore the synergic effect on electrocatalytic and charge transfer properties. The presence of nickel changes the valence band energy level of MoO_3 and appropriately aligns with electrolyte redox potential for facilitating hole transport. The XRD, FESEM and UV-DRS confirm Ni impurity presence in MoO_3. The electrochemical impedance spectroscopy (EIS) demonstrates the 5 wt% of Ni in MoO_3 (MN5), reduced the charge transfer resistance by 73.3% than pure MoO_3 (M). I-V results exhibited 1.8 % of PCE for MN5 CE-based devices, which is 30 % higher than M-CE (PCE-1.2 %). This work indicates that the Ni-MoO_3 with high electrocatalytic activity for the oxidation/reduction process can be simply obtained by the hydrothermal method and induction of nickel.

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E 095

Fabrication of CIGS Thin Films Using at Various Deposition Potential Via Electrochemical Route for photovoltaic application

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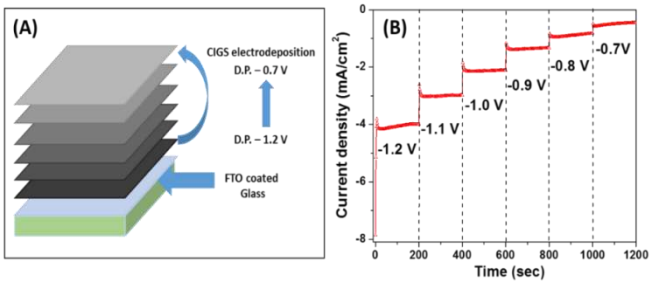
ABSTRACT

We have developed CIGS thin films by a simple electrochemical route. Cyclic voltammetry study is employed to obtain the optimum deposition potential. Chronoamperometric measurements are recorded to investigate the nucleation and growth mechanism of individual Copper Indium Gallium Selenide (CIGS) layers electrodeposited at various deposition potential ranging from -0.7 V to -1.2 V. The CIGS layers grown at lower deposition potential, shows progressive nucleation, while other deposition potential shows that the instantaneous deposition potential is dominant. The effects of deposition potential on various properties of CIGS layers have been thoroughly studied. Deposition potentials can easily tune the value of energy band gap, type of conductivity, elemental composition, etc. Raman spectra confirms that ordered defect compound (ODC) layer are deposited at lower deposition potential, while higher deposition potential layer reports the growth of In-rich CIGS layer. A systematic increase observed in the band gap from 1.04 to 1.20 eV upon increasing the deposition potential revealed the addition of more Ga in CIGS. The variation in the bulk elemental composition determined by Energy dispersive X-ray analysis (EDAX) goes similar with the structural analysis carried out from X-ray diffraction (XRD) and Raman analyses which confirm the formation of polycrystalline growth of CIGS layers. EDAX study confirms the growth of stoichiometric CIGS layers grown at -0.9 V. Photochemical analysis confirmed the growth of n-type and p-type CIGS layer electrodeposited lower and higher deposition potential, respectively. Field emission scanning tunneling microscopy (FESEM) confirms the growth of compact, void free CIGS layers. The prepared CIGS thin films grown at -0.9 V are suitable for photovoltaic application.



Keywords: *CIGS, Electrodeposition, Raman spectra, ordered defect compound, FESEM*

E 096

Unveiling CO_2 Radical Anion Mediated Pathways for Enhanced Ammonia Production from Nitrates via Photocatalysis

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ABSTRACT

Green ammonia production through photocatalysis emerges as a sustainable alternative to the energy-demanding Haber-Bosch process. This work utilizes nitrate, which is a common pollutant in wastewater, as a nitrogen source for ammonia production. Converting nitrates into ammonia presents a dual advantage: it helps diminish nitrate pollution and facilitates the creation of valuable ammonia as the product. In this work, we report an impressive ammonia production of 1.12 mmol/g_{cat}/h utilizing TiO_2-Cu_xO as the catalyst and formic acid as the sacrificial agent. We further explored the influence of different sacrificial agents in the reaction mechanism for ammonia production. When formic acid was used as a scavenger, we obtained highly selective ammonia production with negligible evolution of hydrogen as a byproduct. However, in the presence of methanol, the selectivity towards ammonia is lowered and hydrogen production is increased. Our ESR studies showcased how the $\cdot CO_2^-$ generated from formic acid oxidation contributes to the selective synthesis of ammonia. Apart from serving as hole scavengers, sacrificial agents can play a crucial role in generating highly reactive species like $\cdot CO_2^-$ that can activate and reduce nitrate ions. We attribute the exceptional activity of the TiO_2-Cu_xO catalyst in formic acid for ammonia production to the Cu_xO surface's special ability to rapidly break down formic acid and generate $\cdot CO_2^-$ radicals.

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E 097

Thermoelectric Performance of Bi-Sb Co-Doped Mg_2Si for Mid Temperature Applications

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ABSTRACT

Magnesium silicide is a promising thermoelectric material due to its low toxicity, abundance on Earth and thermal stability. In this work, Bi and Sb co-doped n-type magnesium silicide samples were prepared with the stoichiometric ratio of (x = 0.01, 0.02, 0.03, 0.04 and 0.05) by vacuum melting followed by hot-press method. XRD analysis confirms the phase purity of samples while HRTEM analysis confirms the existence of polycrystalline nature. The Bi-Sb co-doping effectively enhance the carrier concentration of -1.6×10^{18} resulting the improved electrical conductivity at 5817 Sm^{-1}. The obtained Seebeck co-efficient value of -173 $\mu V\ K^{-1}$ and improved electrical conductivity significantly boosting the power factor of 349.27 $\mu Wm^{-1}K^{-2}$ which is ~197.88% enhanced compared to pure sample. The contribution of dislocations drastically reduced the thermal conductivity of 2.536 $Wm^{-1}K^{-1}$ leads to improve the thermoelectric figure of merit of 0.08 at 753K.

Keywords: *Magnesium silicide, Phonon Scattering, weighted mobility, Effective mass.*

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E 098

Realization of Low Potential Barrier in MoS_2/rGO Heterojunction with Enhanced Electrical Conductivity for Thin Film Thermoelectric Applications

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ABSTRACT

Transition metal dichalcogenides of molybdenum disulfide (MoS_2) have significant properties of anharmonicity, large effective mass and tunable band gap of 1.2 eV to 1.9 eV. The reduced graphene oxide (rGO) is an effective material due to its high mobility and semi-metallic nature with high σ by forming the charge carrier network in a functional composite. MoS_2 and MoS_2/(rGO) thin films were grown on SiO_2/Si substrate through atmospheric chemical vapor deposition technique and to study the thermoelectric performance. Few layered MoS_2 was confirmed by the vibrational analysis and the composition elements are confirmed by the XPS technique. The reduced phonon lifetime in A_{1g} and low activation energy improved the electrical property of MoS_2/rGO. The reduced energy barrier at the interface, rGO sheets allow the flow of charge carriers between MoS_2 layers[1]. MoS_2/rGO attained a high σ of 22622 S/m at 315 K because of an electron-rich cloud around the electrons in S atoms near the adjacent layer of rGO[2].

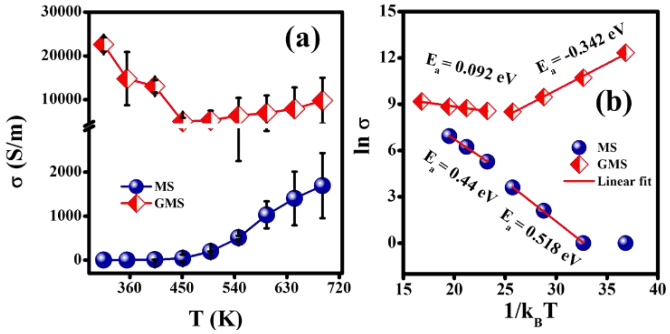

Fig. 1. (a) Temperature dependent electrical conductivity and (b) activation energy for MoS_2 and MoS_2/rGO

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E 099

Investigation of Interface Induced Thermoelectric Properties of Ag_2S Decorated MoS_2 On Carbon Fabric for Wearable Thermoelectric Application

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ABSTRACT

Wearable Thermoelectric Generators (WTEG), being flexible and safe are the only replacement for the conventional batteries for mobile applications. In the present work we have grown MoS_2 nanostructures on the conductive carbon fabric via in-situ binder-free hydrothermal technique and created a MoS_2/Ag_2S interface through dip coating technique and have studied the effect of interface formation on thermoelectric properties of MoS_2. From the structural and morphological analysis, it can be confirmed that the 2H-MoS_2 is uniformly grown on the entire fabric and on dip coating, few agglomerated particles can be spotted. Further the TE properties of pristine MoS_2/CF and MoS_2/Ag2S on CF is investigated from the temperature ranging from 303 to 373 K. The findings indicate that the interface effect of MoS_2/Ag_2S/CF constitutes a promising route for enhancing its thermoelectric performance for wearable TEG applications.

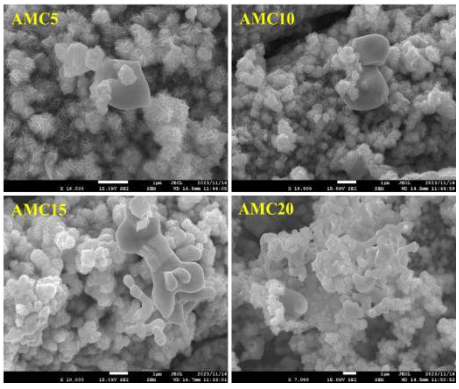

Fig. 1. FE-SEM image of MoS_2/Ag_2S on Carbon fabric

Keywords: *Wearable TEG, MoS_2, Ag_2S, Carbon fabric*

E 100

Seebeck-Coefficient of Si Ribbons Evaluated by Kelvin-Probe Force Microscopy

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ABSTRACT

The nanometer-scale materials have been expected to enhance the efficiency of thermoelectric devices because of an increase in Seebeck coefficient and a decrease in thermal conductivity [1]. However, it is difficult to evaluate the thermoelectric characteristics of nanomaterials due to their quite small dimensions. We are constructing a new technique for the Seebeck coefficient evaluation using Kelvin-probe force microscopy (KPFM) [2,3]. The potential gradient in Si ribbons with millimeter-scale width and length fabricated in a Si-on-insulator (SOI) wafer could be observed by KPFM under a temperature gradient. In this measurement, on the other hand, the temperature difference was measured by thermocouples set at the positions distant from the Si ribbon on the SOI wafer. Therefore, it is difficult to apply this method to micro/nanometer-scale Si ribbons.

In this report, we established a technique of local temperature measurement by KPFM and observed the thermoelectromotive force and the temperature difference, simultaneously. For this purpose, the n-type Si sample was designed to consist of a Si ribbon and two Si probes with micrometer-scale width and length. These Si probes are used for estimating the local temperature from the Fermi energy shift. The Seebeck coefficient was experimentally estimated to be -3.91 mV/K. Although this was 5 times larger than the expected value, the Seebeck coefficient could be evaluated by KPFM without thermocouples.

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E 101

$AgCrS_2$: A Layered Semiconductor with Low Thermal Conductivity

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ABSTRACT

The energy crisis and thermal management have been the two main issues of the twenty-first century. If the thermoelectric concept's figure of merit is high enough to rival that of conventional methods, it is thought to be the ideal solution for both problems. There has been a major push to improve the figure of merits (zT) of semiconductor materials for thermoelectric applications to make them commercially feasible. The layered semiconductors with low thermal conductivity are of great interest in recent times. With this motivation, the present work indulges in unveiling the thermal conductivity (kL) of AgCrS2. The results of this study show that the titled compound has a low kL of 1.48 W m-1 K-1 at 300 K. The major outcome of the work recommends the possible usage of chalcogenide in the thermoelectric industry.

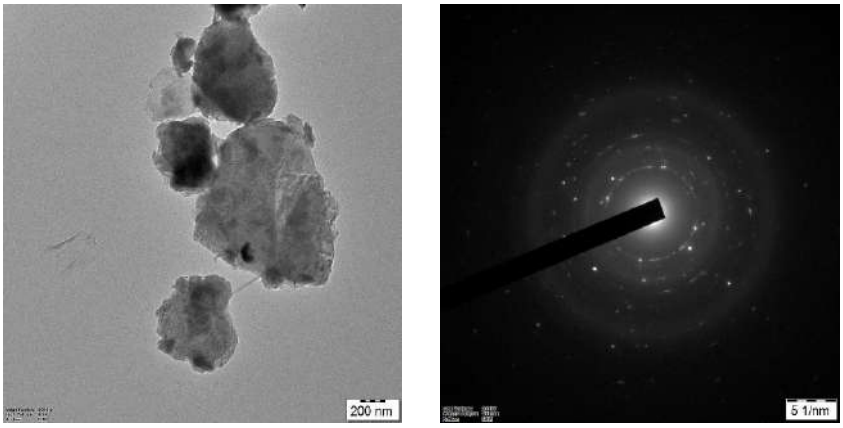

Figure 1 Transmission electron microscope image (left panel) and selective area electron diffraction (right panel) of $AgCrS_2$.

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WS_2/Conducting Polymer Nanocomposites-Based Flexible and Binder-Free Electrodes for High-Performance Supercapacitors

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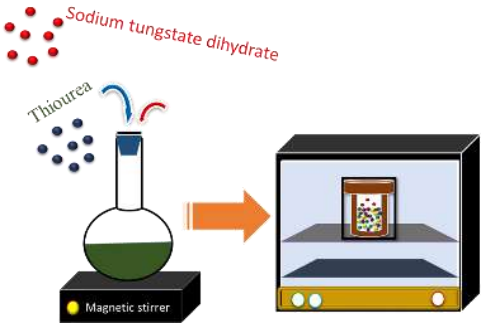
ABSTRACT

The 21st century is rapidly approaching a significant energy crisis. It is essential to promptly develop new environmentally sustainable activities in order to address the impending problem. Supercapacitors are very promising energy storage technologies due to their inherent performance benefits. 2D WS_2 transition metal dichalcogenides are regarded as favourable components in energy storage devices because of their expansive surface areas, elevated theoretical capacitance, and occurrence of effective redox processes at their surfaces. Here in this study WS_2 /conducting polymer-based nanocomposites are prepared and fabricated a symmetric supercapacitor based on these electrodes. Conducting polymers are generally attractive as they have a high charge density and low cost. It is possible to develop devices with low equivalent series resistance (ESR), high power, and high energy density. WS_2/Polyaniline and WS_2/polypyrrole based nanocomposites were synthesized via a facile hydrothermal deposition method, followed by one-step oxidative polymerization. Electrochemical characterizations conducted in a symmetric two-electrode configuration. The WS_2/PANI electrode supercapacitor demonstrates a specific capacitance of 500 F g^{-1}, and WS_2/PPy exhibited a specificcapacitance of 400 F g^{-1}. The devices exhibited excellent energy density and power density.



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E 103

Electrical Simulation of Ternary Layer-By-Layer Organic Solar Cell

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ABSTRACT

Recently, researchers have been interested in incorporating a third component into the active layer of organic solar cells (OSC). Introducing a third component aims to improve the efficiency of light absorption, charge separation, and transport within the solar cell. It is widely observed that varying active layer thicknesses result in different device competencies due to the behaviour of charge transportation and charge collection in such volume morphology of active layer. In this paper, a layer-by-layer (LbL) devices based on BTR-Cl as donor and IT-2Cl as acceptor was incorporated with Y6 acceptor as a third component in the active layer. These devices had been electrically characterised using organic and hybrid material nano (OghmaNano) simulation tool. A thickness ranging between 10 nm and 150 nm of each material in the active layer was evaluated in this simulation. This simulation shows the current-voltage (I-V) and current density-voltage (J-V) patterns for ternary LbL OSC devices at various thicknesses. The short circuit current density (Jsc), open circuit voltage (Voc), and fill factor (FF) for each device's active layer thickness were also provided. At a thickness ratio of 50:80:30 nm (BTR-Cl to Y6 to IT-2Cl) and a light intensity of 10 mW/cm^2, the maximum attainable efficiency, 9.94%, was found.

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E 104

Geometrical Approach for Size Optimization in Micro/Nano Textured Absorber Functional Layer to Improve Photon Absorption

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ABSTRACT

With the power conversion efficiencies of different solar cell technologies reaching their saturated limits, light management is now one of the strategical step in photovoltaics research to surpass the limits. It is widely accepted fact that light management with the geometrical modifications to the surface of the light absorber in the micro/nano size regime, aids the light conversion capability compared to plain absorber surface[1-3]. Different shapes and sizes are considered and evaluated for their conversion improvement with respect to their plain counterparts. Experimental evidence confirms that size dependency of different shapes is crucial in achieving maximum light absorption[4]. Mathematical estimations on the approximate absorption is calculated based on the available experimental data to explore the performance of different shapes over a wide size range. This work aims to arrive at a mathematical model to calculate the optimal dimension for substrate texturing. Optical ray tracing simulations will be done with the same geometrical dimensions to verify the applicability of the mathematical model.

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E 105

DFT Study of V-decorated Graphdiyne for Efficient Hydrogen Storage

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ABSTRACT

Hydrogen serves as a desirable substitute for fossil fuels because it is a very clean and sustainable fuel. Using Density Functional Theory, we investigated the hydrogen storage capacity of synthesized 2D carbon allotrope, 'Graphdiyne' (GDY)[1]. We discovered that since pristine GDY exclusively bonds the hydrogen molecules by van der Waals interactions, it is not ideal for storing hydrogen under ambient conditions. The adsorption energy can be increased by decorating GDY with metal atoms, especially Transition metals, where the Kubas interaction [2] helps in binding hydrogen to the adsorbent. We, therefore, explored the possibilities of enhancing the hydrogen storage capacity of GDY by adsorbing Vanadium on GDY. Without V, we noticed that the binding energy for hydrogen on GDY was -0.16eV, which improved when V was bound, satisfying the requirements of DoE. We have also examined the structural integrity of the system using ab initio Molecular Dynamics Simulations (AIMD)[3]. This can assist us in determining the feasibility of our system.

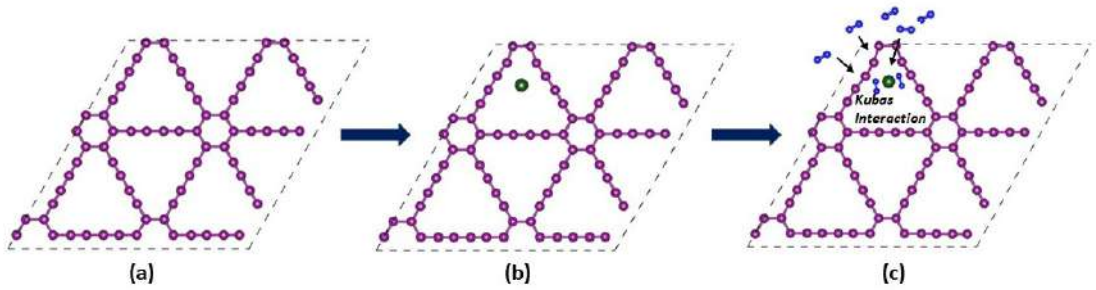

Fig.1. (a) Pristine Graphdiyne (GDY) (b) GDY+V (c) H_2 adsorption on GDY+V where Kubas interaction comes into play.

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E 106

Wearable Textile Based Thermoelectric Generator for Harvesting Low Grade Heat Energy

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ABSTRACT

The growing demand for power solutions in portable devices has driven the advancement of wearable energy-harvesting technology. Researchers have explored that oxide materials are capable for power generation which are economical, less toxic, stable at high temperatures, etc. In our study, we present the synthesis and characterization of Bi_2Te_3 and doped ZnO nanocomposites coated on fabrics. Structural and morphological analyses using FESEM, XRD, and EDAX confirmed the formation of Ni:ZnO and Bi_2Te_3 on the fabrics. The average Seebeck coefficient of Ni:ZnO coated cellulose fabric was found to be 310 µV/K, significantly higher than that of pristine ZnO coated fabrics. Subsequently, these p-type and n-type thermoelectric components were assembled to create an array of 2 thermocouples. The resulting thermoelectric generator, utilizing the coated fabrics, exhibited an output power of 80nW/cm2 with a 25 K temperature difference. Additionally, a wearable thermoelectric module comprising the p-type and n-type thermocouples displayed a device output voltage fluctuating between ~0.3mV and ~0.7mV as human body temperature varied from 308K to 309K when applied on the arm. This analysis underscores the suitability of the flexible device for energy harvesting from the human body, particularly in powering biomedical signal and sensing applications.

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E 107

Recent Advancement on $ZnIn_2S_4$ Based Material for Photocatalytic Water Splitting to Generate Hydrogen Energy

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ABSTRACT

In past years, the overdependence of fossil fuel, and ever-increasing demanding of sustainable, clean and environmental friendly for industrial and domestic's applications has been a major issues of concern. As a ternary metal sulfide (chalcogenides), $ZnIn_2S_4$ photocatalyst has attracted widespread of attentions in the field of photocatalysis due to its unique properties such as, easy synthesis, high stability, low cost, non-toxicity, high chemical durability, suitable band gap and superior absorption of visible light. However, despite all these novelty, $ZnIn_2S_4$ has some distinct drawback that hindered the photocatalytic H_2 generation via photocatalytic water splitting such as, high charge recombination, low utilization of solar energy as well as inferior redox capacity. Many review articles have been published on $ZnIn_2S_4$ for photocatalytic H_2 generation. However, most of them were focuses on application of $ZnIn_2S_4$ and heterojunction. Herein, recent advancement on $ZnIn_2S_4$ based material for photocatalytic water splitting to generate H_2 are discussed in details. Furthermore, the study widely identified and discussed the challenges related to $ZnIn_2S_4$ based photocatalyst, recent synthesis method, properties and morphology, modifications strategies such as heterojunction, elemental doping etc. Thus, this study would guide the future researchers to broaden the modifications $ZnIn_2S_4$ -based materials for photocatalytic water splitting.

Keyword: Zinc Indium Sulfide; Solar Fuel; Photocatalysis; Water-Splitting; Clean Energy.

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E 108

A Recent Trends in Photocatalytic Water Splitting using Titanium Dioxide Based Photocatalysts for Solar Fuel (Hydrogen) Production

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ABSTRACT

The hydrogen has been utilized in different applications like, production industries, transportations and so on, as a source of energy over the years. Its mode of productions mostly is through fossil fuel, particularly, natural gas. However, when the production is engineered via photocatalytic processes using renewable energy with net zero carbon emission, the resulting hydrogen is known as solar fuel (H_2). Also, photocatalytic H_2 generation through water splitting with titanium dioxide (TiO_2) based photocatalyst is one of the efficient method. The most widely explored material in photocatalysis with unique features is TiO_2. Despite it wide band gap of (3-3.2) eV with narrow light absorption, it turn to be the most suitable candidate of photocatalytic hydrogen production. Herein, the strategic modification of polymorph, morphology and crystal structures, metal doped and nonmetal doped of TiO_2 photocatalyst were discussed. Additionally, the processes of enhancing the photocatalytic hydrogen evolution such as; water splitting, photoreforming and oxidation of organic substrate, development of sensitive TiO_2-based photocatalysts, separation of photogenerated charges in TiO_2-based photocatalysts and many more modifications of such kinds were reviewed. Lastly, future research needs and challenges of TiO_2-based photocatalysts that must be overcome, to fully utilize it in photocatalytic hydrogen production through water splitting were discussed.

Keywords: *Hydrogen; Titanium dioxide; Photoreforming; Bandgap; Water splitting*.

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E 109

Investigation of Lead-Free Halide Perovskites for Thermoelectric Applications

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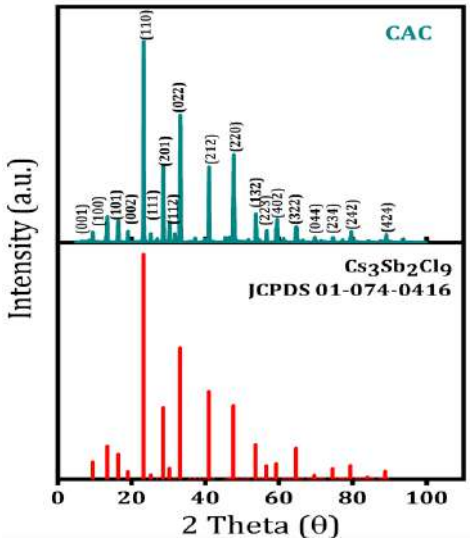
ABSTRACT

In recent years, metal halide perovskites have been the subject of extensive research with potential applications ranging from solar cells to chemical sensors. With respectable charge carrier tunability and ultralow lattice thermal conductivity (<1 $Wm^{-1}K^{-1}$) originating from soft elastic moduli and low acoustic cutoff frequency, halide perovskites were considered to be a potential contender for future thermoelectrics. In search of lead-free halide perovskites, we investigated the thermoelectric performance of **$Cs_3Sb_2Cl_9$** synthesised via reflux method and densified by Spark Plasma Sintering. Theoretical studies show the direct band gap of 2.86 eV making it suitable for efficient energy conversion in the mid-temperature region. XRD analysis reveals that $Cs_3Sb_2Cl_9$ has a trigonal crystal structure with a space group $P\bar{3}m1$. The substitution of antimony (Sb) in place of lead (Pb) leads to the formation of electron rich region which forms complex electronic structure and polar bonds with cesium (Cs) and chloride (Cl) resulting in enhanced carrier mobility. A considerable reduction in lattice thermal conductivity was achieved due to the variation in valence states of Cs^{+} and Sb^{+3}. The fundamental understanding of carrier and phonon dynamics will be crucial in developing eco-frinendly metal halide based thermoelectric materials for mid temperature applications.



Keywords: *metal halide perovskites, ultra-low lattice thermal conductivity, soft elastic moduli, low acoustic cutoff frequency*

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NiO/CdS-Bi_2MoO_6 Ternary Nanocomposite with n-type and p-type interfaces for the enhanced Photocatalytic Hydrogen Production under Solar light

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ABSTRACT

NiO/CdS-Bi_2MoO_6 ternary nanocomposite was synthesized and evaluated for the photocatalytic hydrogen production under direct solar light radiation. 1wt% of NiO and CdS loaded Bi_2MoO_6 produced the highest amount of H_2. The characterization results revealed the porous and orthogonal structure of Bi_2MoO_6. High-resolution transmission electron microscope (HRTEM) images showed heterogeneous connections at the interfaces of nanocrystals NiO (p-type) and CdS (n-type) with nanoparticles Bi_2MoO_6 (n-type), this resulted n-n and p-n type junctions at nanocrystal interfaces. These interfaces played an important role in improving interfacial charge transfer (IFCT) and prolonging the lifetime of photogenerated charge carriers. These phenomena were validated by photoelectrochemical and photoluminescence studies. Dopants acted as a donor (n-type) and acceptor (p-type) of Bi_2MoO_6 to improve the charge transfer process and significantly reduced the band gap, which shifted the light absorption edge position to longer wavelengths than pristine materials as shown in DRS UV-Vis spectra. Thus, NiO and CdS loading facilitated the desirable characteristics for Bi_2MoO_6 to enhance the H_2 production rate three times higher than the intact Bi_2MoO_6. This study provides deep insights into the development of solar-responsive Bi_2MoO_6 based photocatalysts for efficient H_2 production.

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E 111

Ultra-Low Thermal Conductivity of MoS_2/CuS Nanocomposites Via Interface Acoustic Phonon Scattering

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ABSTRACT

Dramatic enhancements in the figure of merit have been obtained in bulk thermoelectric materials by doping, band engineering, and nano structuring. Here, we investigated the electrical and thermal transport properties of *p*-type MoS_2/CuS. Over the temperature, non-degerate semiconductor (303 −700 K) with dominancy of acoustic interface phonon scattering (above 503 K) crossover is noticed. The high electrical conductivity (σ) of 927 Scm^{-1} in due to large density of states around Fermi energy (0.2) an increased Cu^{2+} and resulted in high power factor ($S^2\sigma$) of 44 $\mu Wm^{-1}K^{-2}$ at 653 K. MoS_2/CuS enhances the electrical conductivity through band engineering, improving carrier mobility and shifting the Fermi level to the conduction band. The obtained electrical conductivity is 1.2 times greater than pure MoS_2. The ultralow thermal conductivity (κ) of 0.2 $Wm^{-1}K^{-1}$ at 653 K for MC20 is achieved via acoustic interface phonon scattering and carrier mediated lattice softening. Moreover, the incorporation of CuS into MoS_2 composites can increase the power factor and thermoelectric figure of merit, which arises from the combination of following factors, i) The concentration of CuS increases the hole concentration, which resulting in an increase in electrical conductivity, ii) The MoS_2/CuS composites creates the acoustic interface boundary scattering and restricts the charge carriers with low energy effectively in turn increase the mean energy and Seebeck coefficient through the energy filtering effect, iii) The dominance of acoustic phonon scattering strongly scattered the phonons and suppress the lattice thermal conductivity. The phonons will be significantly scattered for heat transport when they pass through the MoS_2 and CuS interfaces due to the significant mismatch of the phonon DOS and softened chemical interaction. As a result, the phonon mean free path is suppressed, and the thermal conductivity is decreased effectively for the CuS composites samples.

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The synthesis of precursor for a Hydrogen fuel cell by sol-gel method

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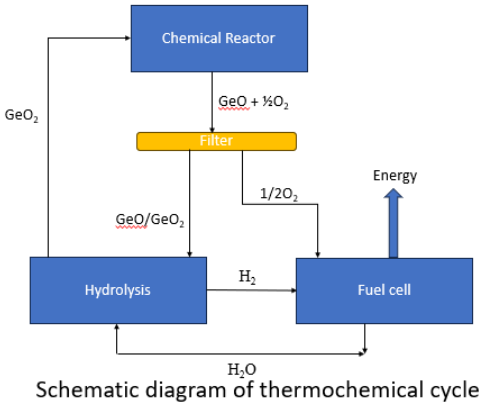
ABSTRACT

Over the years, humanity has heavily depended on finite natural resources like fossil fuels and natural gas to satisfy its essential energy requirements which resulted in carbon emissions. To overcome this, renewable energy source like hydrogen fuel cells are recognized as a cleaner alternative due to its non-emission during combustion is emerging as a promising contender. In this pursuit, hydrogen (H_2) production via water splitting(WS) using metal oxide (MO) redox reactions is explored. Transition temperatures (T_H) for ZnO/Zn and SnO_2/SnO WS cycles were 2070 K and 2055 K, respectively [1,2]. Recent studies on germanium oxide-based WS cycle showed a lower T_H of 1785 K, prompting further research to address high-temperature challenges. A novel method is implemented for synthesizing a precursor for H_2O splitting by reducing GeO_2 with $LiAlH_4$. GeO_2 in water forms complex compounds; NaOH converts them to $Ge(OH)_4$. $Ge(OH)_4$ reduction with $LiAlH_4$ yields GeO_x/Ge in this innovative procedure. By carefully controlling parameters like temperature, pH, and initial concentration of the starting materials, it becomes possible to achieve GeO_x/Ge in the GeO_2 matrix. This has been confirmed by XRD, Raman, and PL results. The noteworthy fact is that this reaction takes place at much lower temperatures (T_H) at 1023 K. Furthermore, GeO_x/Ge in the GeO_2 matrix may be used as a precursor of H_2O splitting for hydrogen gas production for future studies.



Schematic diagram of thermochemical cycle

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E 113

Unravelling effect of light-harvesting implemented by Au decorated on TiO_2/rGO plasmonic photoanode layer for dye-sensitized solar cell application

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ABSTRACT

Charge transport layer (i.e, photoanode) is a primary responsive component for the maximal light absorption to extract the photo-induced charge carriers which is considerably more important than other counterparts of dye sensitized solar cell (DSSC). Hereby, we tried to resolve the low electrical conductivity and poor light absorption behaviour of frequently used TiO_2 based photoanode. To aim this, we present an inclusive study on the effect of plasmonic Au nanoparticles (Au NPs) embedded (mesosphere TiO_2) Meso-TiO_2/rGO (TiO_2/rGO/Au) hybrid nanostructure. The plasmonic hybrid nanostructure (TiO_2/rGO/Au) were prepared by varying Au concentration (0, 0.3%, 0.5% and 0.7%) with Meso-TiO_2/rGO prepared via simple solvothermal and chemical reduction method. The as-prepared samples were named as Meso-TiO_2, TG (TiO_2/rGO), TGAu-3, TGAu-5 and TGAu-7. Then, the prepared sample were further analysed by XRD, TEM, BET and UV-DRS. The TGAu-7 sample has strong light absorption in the visible region and substantial surface area (152.61 m^2 g^{-1}) which impacts high dye impregnation. As a result, The DSSC device integrated with TGAu-7 photoanode achieved an excellent power conversion efficiency (PCE) of 10.58 % with an open circuit voltage (V_{OC}) of 0.72 eV and a short circuit current (*Jsc*) of 23.50 mA/cm^2. The obtained results ~94 % higher over the DSSC device constructed with Meso-TiO_2 (4.01 %).

Keywords: *Mesosphere, porous, visible, plasmonic and LSPR*

Hydrophobic Rose Petal Structure Designed using Soft Lithography for Triboelectric Rain Sensing and Fog Harvesting

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ABSTRACT

Apart from their beautiful attraction and nice smell, flowers can generate electricity, providing new opportunities for sustainable energy development. This research investigates the creative possibilities of using flower petals, significantly rose petals, as a new way to make electricity. The study uses soft lithography to transfer the complex designs on the surfaces of rose petals to polymer films. The surface roughness of the replicated petal pattern is evaluated using goniometric drop morphology and 3D optical profilometry, which carefully examine the contact angles, microscopic characteristics, surface morphology, and structural components. The study utilizes the single electrode mode, employing a spray bottle filled with tap water to examine electrical performance and fog conditions to evaluate fog harvesting capabilities. The practical efficacy of various applications is correctly assessed by practical trials that involve adapting umbrellas into warning lights on wet evenings.

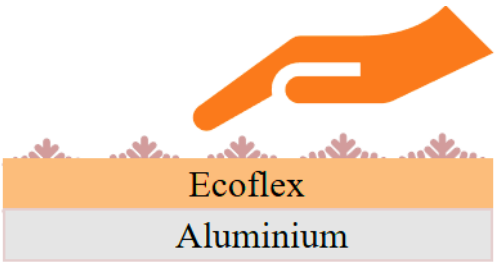

Fig. 1. Schematic structure of the device

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E 115

Hybrid Composites of $AgSbSe_2/MoS_2$ and $AgSbSe_2/CuO$ on Carbon Fabric for Wearable Thermoelectric Application

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ABSTRACT

Smart wearable devices are still powered by batteries requiring constant recharging, which is a key challenge faced in wearable technologies. Fabrication of flexible thermoelectric that can utilize body heat for wearable applications are an attractive alternative to batteries. Designing a low-cost, flexible, and high-performance thermoelectric material remains a considerable challenge due to the low thermoelectric efficiency of conducting polymers and the rigidity of inorganic materials. Here we have integrated $AgSbSe_2$ into conductive carbon fabric as a flexible thermoelectric material via a microwave-assisted hydrothermal method. Additionally, MoS2 and CuO were screen printed onto the $AgSbSe_2$ grown on carbon fabric to improve its thermoelectric performance. The XRD analysis was used to confirm the phase presence of $AgSbSe_2$, MoS_2 and CuO on carbon fabric (CF). The thermoelectric properties, like electric conductivity and seebeck coefficient of $AgSbSe_2$-CF , MoS_2/ $AgSbSe_2$-CF and CuO/ $AgSbSe_2$- CF were compared and analyzed. The analysis shown that $AgSbSe_2$-CF screen printed with MoS2 and CuO offers promising thermoelectric properties.

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Enhanced Growth of ZnO on Ag Fabric for Wearable Thermoelectric Applications

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ABSTRACT

The present need for batteries as a source of power for smart wearable devices is one of the most significant challenges associated with wearable technology. It is possible that the creation of wearable thermoelectric devices that are capable of generating electricity via the utilization of body heat might be a potential alternative for batteries. Due to low thermoelectric efficiency of conducting polymers and rigidity of inorganic materials, creating a low-cost, flexible, and high-performance thermoelectric material is still a challenging task. Therefore, in this work, we focus on the fabrication and characterization of low-cost and large-area flexible thermoelectric materials with nanocrystalline ZnO applicable for wearable power generator. Fig.1 shows the ZnO nanostructures were coated on Ag fabric (SF) by dip coating process. It was demonstrated that the polarity of Seebeck coefficient in ZnO-covered SF can be controlled by tuning the dipping process. On the other hand, as the thickness of the material increases in SF, there was enhancement in the thermoelectric properties. The analysis shows that the ZnO-coated SF material offers promising thermoelectric properties.

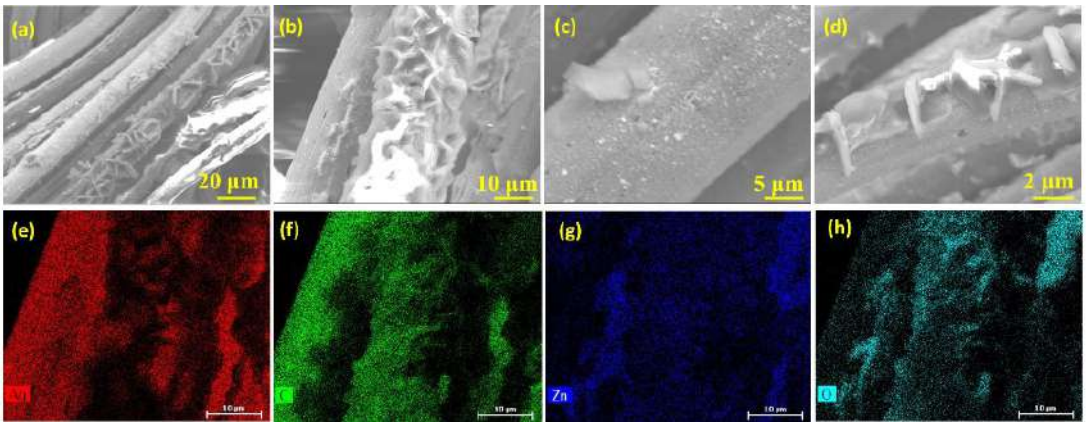

Fig. 1: FE-SEM Image and elemental mapping of ZnO nanostructures

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E 117

Seebeck Coefficient Characterization under Oscillated Temperature Difference

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ABSTRACT

The inability of conventional methods to measure the thermoelectric properties simultaneously, results longer measurement time and higher measurement cost. In this study, with the aim of characterizing the Seebeck coefficient and the thermal diffusivity of thermoelectric material, simultaneously, a Seebeck coefficient characterization system based on AC Calorimetry technique with the addition of voltage measurement system has been constructed. In this method, a periodic heating was performed by using a diode laser irradiation and the corresponding periodic temperature were measured by using an infrared camera. A copper bar was used as a reference material and the experiment was carried out near room temperature. The Seebeck coefficient of copper was evaluated from the temperature difference and thermoelectromotive force which were analysed by the measured voltage and oscillated temperatures on the surface of copper bar. The Seebeck coefficient was found to depend on the heating frequency and become close to reported value with decreasing the frequency. The Seebeck coefficient value was evaluated to be 1.52 ± 0.29 μV/K, which is close to the reported value of copper, 1.83 μV/K at frequency of 20 mHz. From the simulated results using finite element method, this dependency is likely governed by the heat flux at the heat sink. Consequently, the developed system was considered able to measure the Seebeck coefficient with an acceptable accuracy and able to realize the simultaneous measurement with the thermal diffusivity.

E 118

Phase modulation – An Effective Strategy to Optimize the Thermoelectric performance of GeSe.

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ABSTRACT

GeSe is an IV–VI chalcogenide compound with an orthorhombic structure similar to SnSe, which is an excellent thermoelectric material. Theoretically, orthorhombic GeSe is predicted to have a high thermoelectric performance, but experimentally doping did not serve the purpose [1]. Phase modulation is one of the ways to tune the thermoelectric performance of orthorhombic GeSe. Alloying GeSe with alloys like Ag (Sb/Bi) (Te/Se)2 (incipient metals) leads to phase change from room temperature orthorhombic to room temperature rhombohedral or cubic phase, resulting in a substantial increase in the thermoelectric performance of GeSe [2-4]. In this work, we study the structural and thermoelectric properties of $GeSe_{1-x}Te_x$ ($0.00 \leq x \leq 0.50$) without any additional dopant on the Ge site; here, we see that with the increase in tellurium content, the phase changes from room temperature orthorhombic(x=0) to hexagonal ($0.2 \leq x \leq 0.3$) to rhombohedral ($0.4 \leq x \leq 0.5$) phase. Also, increasing the annealing temperature from 300°C to 500°C leads to the of the hexagonal phase into the orthorhombic and rhombohedral phases, confirmed by the X-ray diffraction. This new rhombohedral phase with higher symmetry leads to a multivalley Fermi surface and a drastic increase in carrier concentration, as seen from both the Seebeck coefficient as well as electrical resistivity measurement. Also, the lattice thermal conductivity of the rhombohedral phase is the least due to anharmonicity developed by metavalent bonding in that phase. The zT of the rhombohedral $GeSe_{0.6}Te_{0.4}$ sample reaches ~ 0.63 at 573 K, which is around 16 times higher than that of pristine covalent bonded orthorhombic GeSe. This study will be helpful in finding the actual origin of high thermoelectric performance in Ge (Se, Te) based thermoelectric material systems.

Keywords: *Metavalent, Seebeck coefficient, Electrical resistivity, Thermal conductivity*

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E 119

Computational Analysis and Numerical Simulation to Improve the Efficiency of $CuInGa(S,Se)_2/In_2S_3$/Al- ZnO Thin Film Based Solar Cells

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ABSTRACT

Developing operative approaches to address the energy crisis reveals a gap in recent solar cell technologies. This research investigates the fundamental optoelectrical characteristics of thin films. The study explores the single buffer layer (In_2S_3) based solar cells, various replacements for conventional based various composition of copper–indium–gallium–diselenide and disulfide (CIGS) absorber layers have been studied by solar cell capacitance simulator (SCAPS) in terms of layer thickness, absorber layer band gap and operating temperature to find out the optimum choice. An efficiency of 23.28% (with V_{oc} of 0.7372 V, J_{sc} of 37.68 mA/cm^2 and fill factor of 83.77) has been achieved with $CIGSe_2$ and 19.47% (with V_{oc} of 1.2909 V, J_{sc} of 16.8326 mA/cm^2 and fill factor of 89.51) for $CIGS_2$ based absorber layers as the reference case. It is also found that the high efficiency $CIG(S/Se)_2$ cells have the absorber thickness between 2 µm and 5 µm. It is also revealed that the optimum thickness of buffer layer is within the range of 500 nm. In light of these findings, it is indicated that $CIGSe_2$ holds potential as a viable thin-film material for photovoltaic solar cell applications.

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E 120

Tribological properties of Laser Surface Textured Tools during Dry Machining of Aluminium Alloy AA2024

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ABSTRACT

Premature tool failure, variations in cutting forces, and a decline in the quality of the machined surface are all brought on by friction at the tool-chip interface and tool-chip adhesion during machining. While machining ductile materials chips get fused with rake face of the cutting tool, and leads to the formation of Built-up edge. Built up edge protects the rake face of the tool from wear but make the machined surface rough. Surface texturing of tools is a potential way to modify the tribological properties of mating surfaces in order to increase the tribological qualities and decrease the tool-chip adhesion. The performance of surface textured tools depends upon orientation, dimple depth, width and pattern. Under lubrication regime, microholes in surface textured tools acts both as lubrication reservoir and traps wear debris to reduce abrasive wear. Surface texturing is a technique used to modify the topography and properties of tool surfaces, with the goal of enhancing cutting performance, reducing friction and wear, improving chip evacuation, and optimizing tool life. In terms of surface roughness of machined work pieces and tool-wear, the machining efficiency of laser surface textured tools is analysed.

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E 121

Controlled carrier-phonon dynamics in MoS_2/WO_3 nanohybrid for high performance thermoelectric applications

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ABSTRACT

Molybdenum disulphide (MoS_2) has paid great attention owing to its fascinating characteristics such as anisotropy, anharmonicity, direct narrow bandgap, low thermal conductivity with size effect, large effective mass, low cost. Here, we report MoS_2/WO_3 hybrid prepared by hydrothermal method. The material formation is confirmed by presence of Mo^{4+}, S^{2-}, W^{6+} and O^{2-} oxidation state from X-ray Photoelectron Spectroscopy (XPS) and X-ray diffraction (XRD). The mobility reveals the evidence of weaker electron-phonon coupling, suppression of optical phonon scattering on electrons and large polaron under carrier optical phonon scattering. Meanwhile $n \rightarrow p$ transition is noticed with increasing the WO_3 in MoS_2. This is due to the transition metals electronic configurations of Mo $(4d^5\ 5s^1)$ W $(4f^{14}\ 5d^4\ 6s^2)$, where the *d-d* states of Mo have 5 electrons and W has 4 electrons. The five electrons from Mo 4d $(4d^5\ 5s^1)$ can share electrons with W 5d $(4f^{14}\ 5d^4\ 6s^2)$, resulting in *p*-type conduction. The results revealed that utilizing an appropriate amount of WO_3 in MoS_2 is an effective way to improve thermoelectric performance.

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F 001

Silver Doped Zinc Stannate (Ag-$ZnSnO_3$) Nanocomposite for Efficient Photocatalytic Degradation of Crystal Violet Dye

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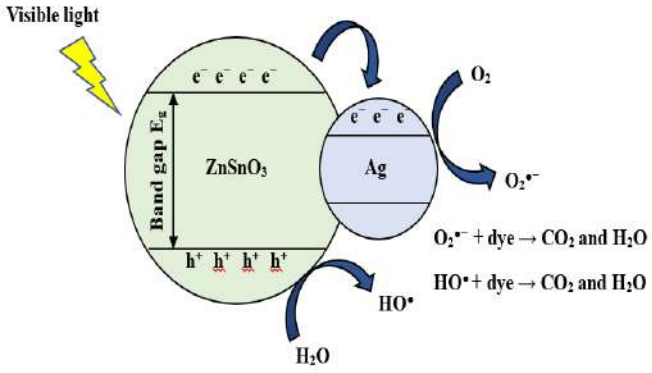
ABSTRACT

All living things are adversely affected by untreated dye effluents from textile factories, which are one of the main causes of water pollution. More effectively than the currently used conventional approaches, photocatalytic activity using semiconductor nanoparticles facilitates the degradation of organic contaminants. Among many semiconductors, zinc stannate ($ZnSnO_3$) is considered to be an important ternary semiconductor due to its high electrical conductivity, high electron mobility, low visible adsorption, and high optoelectronic properties. $ZnSnO_3$ absorbs only UV light due to its large bandgap which leads to low degradation yield. Therefore, in this work silver (Ag) loaded on the surface of $ZnSnO_3$ enables visible light absorption due to the Schottky barrier effect. Pure and Ag-doped $ZnSnO_3$ nanocomposites were prepared using chitosan biopolymer without changing the pH value. The structural analysis confirms the orthorhombic perovskite structure of $ZnSnO_3$. From the optical analysis, there is a redshift of absorbance edge for Ag-doped $ZnSnO_3$ over the pure $ZnSnO_3$. The morphological analysis shows that the samples are spherical in shape and also confirms the crystallinity of the samples. The presence of Zn-O and Sn-O functional groups was established by FTIR analysis. Raman analysis shows the various energy modes of synthesized pure and Ag-doped $ZnSnO_3$. For the photocatalytic activity, crystal violet dye (CV) was taken as a model pollutant for both the pure and Ag-doped $ZnSnO_3$ nanocomposite as a photocatalyst under visible light irradiation. The modification of $ZnSnO_3$ nanocomposite using Ag-doping can further enhance the photocatalytic activity of the photocatalyst, due to its low bandgap and larger surface area. Overall, Ag-doped $ZnSnO_3$ nanocomposite can serve as a highly efficient photocatalyst to treat wastewater for environmental remediation.



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F 002

Efficient $SrFe_2O_4$ Nanoparticles for Photodegradation of Congo Red Dye Under Visible Light Irradiation

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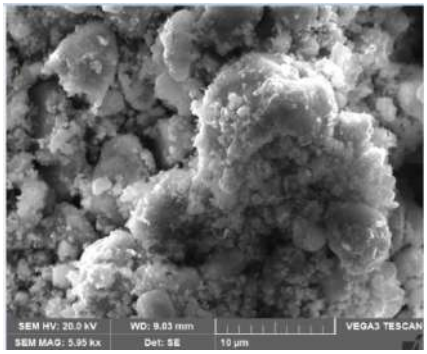
ABSTRACT:

Strontium ferrite nanoparticles ($SrFe_2O_4$) is a permanent magnetic material, which have received a great deal of attention due to their unique chemical, thermal, and magnetic properties in different field of applications. Photocatalytic activity has emerged as the easiest and eco-friendly technique for removing dye contaminants in wastewater treatment. In this work, the $SrFe_2O_4$NPs were synthesized by using *Erythrina variegata* leaf extract as a capping and reducing agent for photodegradation under visible light irradiation. The spinel cubic crystal structure of prepared green assisted $SrFe_2O_4$NPs was confirmed by powder X-ray diffraction studies (PXRD) and average crystalline size found as 25 nm using Scherer formula. FTIR shows the tetrahedral and octahedral sites of the prepared nanoparticles. The optical properties were analyzed using UV–Vis-diffuse reflectance spectrophotometer with bandgap was calculated using Tauc's plot and is found to be 1.7 eV. The irregular shapes of $SrFe_2O_4$NPs were examined using a scanning electron microscope (SEM) and compositional analysis studied by EDX. Towards application, the photocatalytic activity of the synthesized $SrFe_2O_4$NPs was studied under visible light and the maximum efficiency was obtained as 70 % degradation of congo red (CR) dye.



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F 003

Optical Properties of Gadolinium Doped EuF_3 Nanoparticles Surface Modified with Tryptophan

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ABSTRACT

Gadolinium doped EuF_3 nanoparticles were synthesized via chemical precipitation method at room temperature in presence of tryptophan (Trp). The product was investigated by XRD, SEM, TEM, FT-IR, FT-Raman, UV-Vis and Photoluminescence spectra. The average size was calculated using XRD spectra and found to be 73.54 nm at FWHM for most intense peak. SEM studies shows flake like morphology having size of the order of 56 nm – 71 nm with nanoparticles has average size of 13 nm which is in agreement with TEM studies which has globular aggregates formed due to small granules of size 24 nm. The binding of organic ligand on the surface of host nanoparticles were confirmed by FT-IR & FT-Raman studies which indicated the absorption band due to surface modifier. Luminescent properties of EuF_3: Ho surface modified with tryptophan are investigated. The comparative studies of pure and doped sample shows increase in the luminescent intensity at the wavelength of 654 nm corresponding to transition $^5D_0 \rightarrow {}^7F_3$ under the excitation wavelength of 341 nm. The UV-Vis spectra shows absorption at three different wavelengths 236 nm, 336 nm & 364 nm having band gap of 5.26eV, 3.87 eV & 3.41 eV. The absorption in the lower wavelength region confirms the quantum dot nature of synthesized nanoparticles.

Keywords: *Gadolinium, surface modification, tryptophan, quantum dot*

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F 004

Synthesis and Electrochemical Application of Mixed-Spinel Magnesioferrite

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ABSTRACT

This work presents an efficient non-enzymatic electrochemical sensor based on catalytic oxidation by the $MgFe_2O_4$ magnetic spinel for the sensitive determination of ascorbic acid. $MgFe_2O_4$ spinel ferrite is synthesized via the simple and cost-effective solid-state reaction route. X-ray photoelectron spectroscopy and X-ray diffraction studies reveal a mixed spinel structure of the synthesized material with the formula $(Mg_{0.65}Fe_{0.35})A[Fe_{1.65}Mg_{0.35}]BO_4$ with Fe^{3+} and Mg^{2+} occupying both the tetrahedral and octahedral sublattices. The Raman and Fourier-transform infrared spectroscopic analyses confirm the spinel structure formation. The Furthermore, the magnesioferrite spinel integrated glassy carbon electrode displays an enhanced catalytic activity toward ascorbic acid compared to the bare electrode in the phosphate buffer solution of pH 7.4 owing to the mixed-valence cationic states in the spinel ferrite. The electrochemical performance of the modified electrode under the influence of various parameters such as scan rate, analyte concentration, and interference are studied in detail. The sensor provides a linear increase in the oxidation peak current as a function of increasing concentration with a limit of detection and quantification of 24.09 µM and 80.30 µM, respectively. The synthesized ferrite shows good selectivity toward interfering agents, such as potassium chloride, sulfuric acid, hydrogen peroxide, sodium hydroxide, glucose, and choline chloride.

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F 005

Improved Polaron Hopping in Ag Substituted Fe_2O_3 for Efficient Photo-Catalysis: Experimental Studies and First-Principle Calculations

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ABSTRACT

Unveiling the polaron hopping mechanism and the subsequent transport properties in Fe_2O_3 is crucial for achieving cost-effective applications. Thus, in this work the electron-phonon coupling strength in Fe_2O_3 was favorably tuned with Ag dopants, thereby improving the polaron conduction for efficient phtoto-catalysis. Initially, solid state sintering technique was employed to prepare Fe_2O_3 and Ag doped Fe_2O_3, and then the structural confirmations were done with XRD, HR-TEM and XPS analysis. Following that, the carrier-phonon interactions in pure and Ag doped Fe_2O_3 were quantified via Fano resonance approach. The results confirm that the self-trapped carrier in Fe_2O_3 undergoes easy hopping with the Ag dopants. Consequently, an improved carrier lifetime in Ag doped Fe_2O_3 has been observed from time resolved photoluminescence measurements. Importantly, the photo-catalytic measurements were carried out towards aqueous methylene-blue solution and the improved degradation was obtained with the Ag doped Fe_2O_3 due to the improved polaron hopping as evidenced from the Fano-resonance approach.

Keywords: *Fe_2O_3, Polaron, Fano-resonance, Carrier lifetime, Electron-Phonon interactions.*

F 006

Solvothermal Synthesis of Oxide Nanoparticles and their Applications for IR-Light Induced Functional Materials

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ABSTRACT

Solvothermal synthesis process is a powerful tool for the synthesis of functional materials with improved physical and chemical properties applicable to both industrial and nanomaterials research areas. Water molecules play an important role in the crystal growth of nanomaterials during the solvothermal synthesis process. Compared with organic solvents, the water molecule as reaction media generally results in large particle size and hard agglomeration, because of its large dielectric constant and large solubility. In the present talk, a novel water molecular controlled release solvothermal process (WCRSP) for synthesizing multiscale homogeneous and morphology-controllable inorganic materials will be introduced. It is found that the WCRSP process results in very homogeneous particles with unique morphologies and superstructures of the surface and results in novel properties of oxide materials. The WCRSP process is an effective method for synthesizing various inorganic functional nanomaterials, such as TiO_2, Cs_xWO_3, $W_{18}O_{49}$, and their composites. Some novel applications, such as infrared light shielding smart window, photo-thermal transformation, cancer cell IR thermal therapy, and multifunctional photocatalytic activity of these materials, will also be introduced in details.

F 007

Functionalized Nanomaterials in Pancreatic Cancer Theranostics and Molecular Imaging - An Understanding

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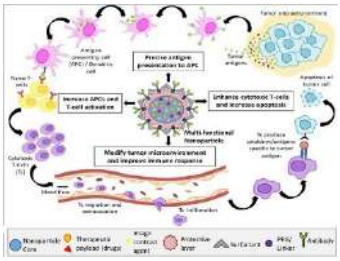
ABSTRACT

Pancreatic cancer (PC) is one of the most fatal and aggressive malignancies in the world. As of 2022, pancreatic cancer contributes to about 3% of all cancers globally. Over the years, research has characterised germline predisposition, the origin cell, precursor lesions, genetic alterations, structural alterations, transcriptional changes, tumour heterogeneity, metastatic progression, and the tumour microenvironment, which has improved the understanding of PDAC carcinogenesis. By using molecular based target therapies, these fundamental advancements support primary prevention, screening, early detection, and treatment. The main focus of this work is the use of targeted nanoparticles as an alternative to conventional pancreatic cancer treatment due to the various side effects of the latter. The principles of nanoparticle based cancer therapy is efficient targeting of tumour cells via enhanced permeability and retention (EPR) effects and decrease the chemotherapy side effects due to their non-specificity. To increase the efficiency of existing therapies and modify target nanoparticles, several molecular markers of pancreatic cancer cells have been identified. Thus, pancreatic cancer cells can be detected using appropriately functionalized nanoparticles with specific signalling molecules. Once cancer has been identified, these nanoparticles can kill the tumour by inducing hyperthermia, medication delivery, immunotherapy or gene therapy. As potent co-delivery methods for adjuvants and tumor-associated antigens, nanoparticles (NPs) have demonstrated significant promise as delivery vehicles in cancer therapy. This ensures the precise internalization of the functionalized nanoparticle and thus also activates the immune system effectively against tumor cells. This review also discusses the immunological factors behind the uptake of functionalized nanoparticles in cancer therapies. Theranostics, which combine imaging and therapeutic chemicals in a single nanocarrier, are the next generation of medicines. Pancreatic cancer treatment may be revolutionised by the development of a tailored nanocarrier with diagnostic, therapeutic, and imaging capabilities.



Keywords: *Targeted therapy; immunotherapy; nanomedicine; theranostics; functionalized nanoparticles; pancreatic cancer*

F 008

Green Synthesis of Iron Oxide Nanoparticles using Justicia Adhatoda Leaf Extract and their Photocatalytic Activities

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ABSTRACT

Eco-friendly, plant derived materials have been fascinated as a substitute for synthesising nanoparticles in recent trend and also green synthesis is an economic and clean technology. In this study, iron oxide nanoparticles were synthesised with the implementation of simple bio-reduction method taking aqueous leaf extract of justicia adhatoda as a reducing agent. The phase structure, composition and morphology were confirmed by the characterization techniques such as XRD, FTIR and FE-SEM with EDS. Vibrating sample magnetometer was used to reveal the magnetic properties of the nanoparticles. The photo catalytic activity of the synthesised iron oxide nanoparticles were monitored using UV-Visible Spectroscopy. Thus, it could be concluded that aqueous leaf extract of justicia adhatoda can be used efficiently in the production of iron oxide NPs for commercial applications in environmental fields.

Keywords: *Green synthesis, Bio-reduction method, Justicia Adhatoda, Iron oxide nanoparticles, Photocatalytic Activity.*

F 009

Impact of Excess Sulphurization of MoS_2 towards Piezo-Catalytic H_2 Production

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ABSTRACT

In this work, we study the impact of excess sulphur on MoS_2 on structural and piezo catalytic activity towards H_2 production under ultrasonic vibration conditions. The piezo response force microscopy indicates a considerably higher piezo potential in MoS_2 with excess sulphur (MOS-EX). Benefiting from the increased piezoelectricity, higher concentration of carriers, higher Hall mobility and lower resistivity, the MOS-EX exhibits an improved activity of piezocatalytic H_2 production, and the corresponding H_2 evolution rate reaches up to 561 $\mu molh^{-1}g^{-1}$, which is 1.2 times higher than the hydrogen production rate of MoS_2 is only 439.06 $\mu mol \cdot h^{-1} \cdot g^{-1}$. This work not only provides a new strategy for modulating the piezoelectricity of transition metal dichalcogenides but also breaks new ground for developing high-efficiency piezo catalysts.

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F 010

One Dimensional α-MnO_2, ZnO and α-MnO_2/ZnO Nanocomposite Electrodes for Enhanced Supercapacitor Applications

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ABSTRACT

Supercapacitors are spotlight of energy storage devices due to long cycle stability, fast charge-discharge performance and high-power density [1,2]. Manganese dioxide (MnO_2) is an ideal electrode material for supercapacitors due to its low cost and large theoretical specific capacity (~1370 Fg^{-1}). However, electrochemical performance of α-MnO_2 is limited by its poor electrical conductivity [3,4]. Therefore, ZnO is used as a composite due to its low-cost, long-life cycle, non-toxic and electrical conductivity which will enhance the electrochemical performance of α-MnO_2 [5,6]. We report in this paper, one dimensional α-MnO_2/ZnO nanocomposites and pure α-MnO_2, pure ZnO were synthesized through a one-step hydrothermal method. The Crystalline structure and elemental composition were analysed using X-ray diffraction and Fourier transmission infrared spectra. The morphological study was explored using HR-SEM analysis which showed that the α-MnO_2 and ZnO reflected the nanowires and nanorods morphology respectively. Electrochemical characterizations like CV, GCD, and EIS were utilized to analyse the super capacitive properties of the synthesized electrode material [7]. Hence, the synthesized α-MnO_2/ZnO nanocomposite is a highly potential material for energy storage application.

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F 011

Cerium Metal-Organic Frameworks: Catalysts for Electrochemical and Photocatalytic Transformations

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ABSTRACT

In the realm of advanced materials science, the exceptional capabilities of cerium-based metal–organic frameworks (Ce-MOFs) in both electrochemical and photocatalytic applications are of paramount importance. These unique attributes not only enhance the versatility of Ce-MOFs but also provide effective solutions to complex challenges in diverse industries, from environmental remediation to cutting-edge sensing technologies. Our study delves into the synthesis, characterization, and applications of Ce-MOF and a composite material comprising cerium benzene tricarboxylic acid (Ce-BTC) and graphitic carbon nitride (gC_3N_4), known as Ce-BTC/gC_3N_4. Through an eco-friendly stirring route, we successfully synthesized Ce-BTC MOFs and the composites, demonstrating their remarkable features such as expansive surface area, multiple oxidation states, high homogeneity, stability, and efficient electron charge transfer behavior. Our investigation includes an in-depth analysis of the redox behavior exhibited by the Ce-BTC/gC_3N_4/GC electrode using cyclic voltammetry, showcasing its potential for sensitive dopamine detection. Furthermore, we explore the catalytic prowess of Ce-BTC/gC_3N_4 in the complete degradation of MB dye under visible light, achieving an impressive efficiency of approximately 98%. These results highlight the versatility of Ce-MOFs and their potential in addressing critical environmental and analytical challenges. As we further explore the synthesis, characterization, and applications of Ce-BTC/gC_3N_4, it becomes evident that this material's dual capacity for electrochemical and photocatalytic performance represents a significant advancement in materials science. This dual functionality opens new avenues for innovative solutions across various industries, ushering in a future where metal–organic frameworks play a central role in the development of practical and sustainable technologies.

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F 012

Synthesis, Structural, Optical Characterization of Olivine Structured Co_2SiO_4

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ABSTRACT

Olivine structured compounds of general formula M_2SiO_4 are of great interest for geologists and mineralogists due to their good optical and magnetic properties. Herein, we have synthesized the olivine structured cobalt orthosilicate Co_2SiO_4 via high temperature solid state reaction route. The crystallization in orthorhombic structure with non-centrosymmetric space group Pbnm have been confirmed by Rietveld refinement of X-ray diffraction data. The bond lengths between the atoms computed using Bond_Str program in Fullprof Suite are supporting the results obtained from Rietveld refinement. The morphological and elemental distributions in the compound were assessed by scanning electron microscopy. The FTIR spectrum confirms the formation of Co-O and Si-O bonds as well as absence of organic functional groups indicating the phase pure synthesis of Co_2SiO_4. The optical band gap determined from the UV-Vis-NIR spectroscopic data by utilizing the Kubelka-Munk function was found around ~3.5eV suggesting its semiconducting nature.

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F 013

The Optimization of $Sm_{1-x}Sr_xMnO_3$ (x = 0.1, 0.2, 0.3, and 0.4) Perovskite (SSM) with A-Site Deficiencies as a Promising Approach for Designing Efficient Electrocatalyst for Oxygen Reduction Reaction (ORR)

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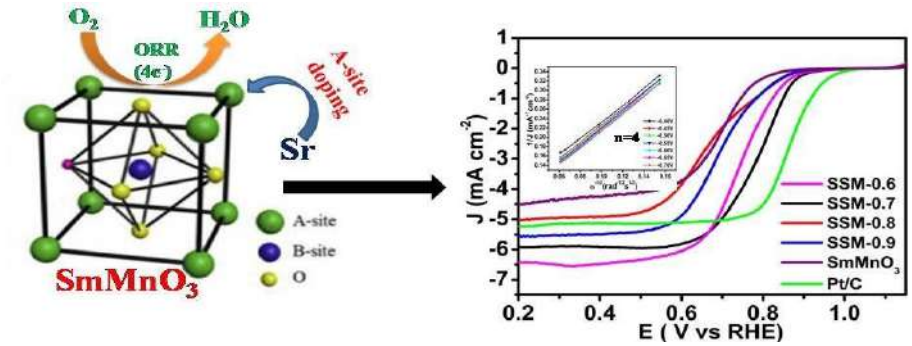
ABSTRACT

A non-precious metal catalyst that is highly selective, stable and efficient is crucial for alkaline fuel cell applications. Recently, rare earth-based perovskite-type oxides showed improved oxygen reduction reaction (ORR) performance which is comparable to commercial Pt/C. Here, the strontium doped $SmMnO_3$ ($Sm_{1-x}Sr_xMnO_3$ (x = 0.1, 0.2, 0.3, and 0.4)) with A-site deficiencies are prepared via a sol-gel method with post calcinations. The structure, morphology, valence state and oxygen adsorption behaviors of these samples were characterized, and their catalytic activities toward ORR were studied by the rotating ring-disk electrode (RRDE). The results showed that with appropriate doping of Sr and introducing A-site deficiencies effectively tailor the Mn valence and increase the oxygen adsorption capacity of the prepared catalysts. With high electron transfer number and outstanding stability, the prepared catalysts with A-site deficiencies can be used as a promising electrocatalyst in fuel cell. Chronoamperometric measurements showed that SSM-0.7 had superior durability and methanol tolerance than Pt/C. The findings provide a new insight into the design of A-site Sr doped rare earth manganite perovskites nanoparticles as highly efficient catalysts for ORR in alkaline media.



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F 014

Multifunctionality Exploration of Dy substituted $NiFe_2O_4$: An Efficient Bifunctional Electrocatalyst toward ORR/OER

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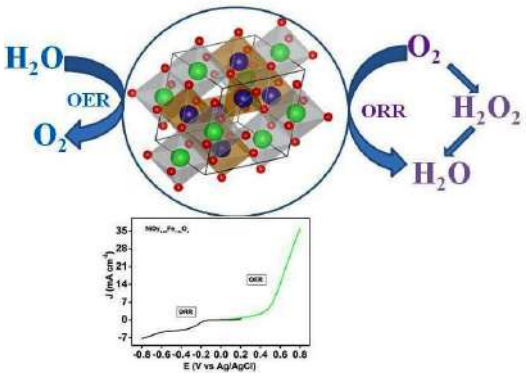
ABSTRACT

Oxygen reduction reaction (ORR) and Oxygen evolution reaction (OER) and are important reactions of energy storage and conversion devices. Therefore, it is highly desirable to design efficient, long -lasting and dual electro catalysts for replacing the traditional noble-metal-based catalysts. We devise a relatively low- temperature Co-precipitation strategy for producing a spinel based oxide catalyst composed of Dysprosium substituted $NiFe_2O_4$ as $NiDy_xFe_{2-x}O_4$(x=0.025,0.05,0.075,0.1) the catalyst performs admirably, with improved kinetics and activity for ORR and OER. The NDFO 0.05 shows bifunctional behavior having an onset potential of -0.12V vs (Ag/Agcl) and a current density of 7.25mA/cm^2. For OER, NDFO 0.05 exhibited an onset potential of 0.56V vs (Ag/Agcl) and a current density of 36mA/cm^2. A high electron transfer number "n" nearly 4, performed by RRDE and long-term stability better than that of Pt/C is observed. As a result, the resultant NDFO- 0.05 has greater potential to be applied as a efficient ORR and OER electro catalyst.



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F 015

$SrSnO_3$ Perovskite Oxide in Situ Grown on N-Doped Reduced Graphene Oxide as High Performance for ORR

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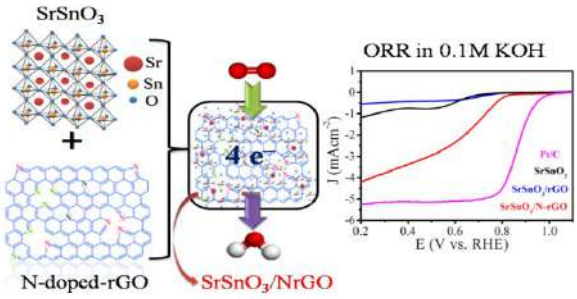
ABSTRACT

Development of new materials that can efficiently transfer energy in a variety of energy conversion and storage systems is the need of the hour. There is growing need for energy and the environmental challenges posed by rapid population growth and economic development. The sluggish kinetics of oxygen electrode reaction involving the oxygen reduction reaction (ORR) is the major drawbacks in the energy devices. Perovskites, a unique class of multi-metal oxides, are rapidly emerging as promising high-performance catalytic materials. One example is $SrSnO_3$, a stannate-based perovskite with high electrical conductivity and thermal stability. In the past decade, N-doped graphene have been extensively studied as catalysts for the ORR. Therefore, it is logical to investigate the ORR performance of $SrSnO_3$/N-rGO catalysts, which could benefit from the synergistic coupling effect of the two materials. In this study, $SrSnO_3$/NrGO catalysts were made using a hybrid and economical technique. Synthesized $SrSnO_3$/NrGO composite catalyst has shown ORR in $4e^-$ pathway.



Keywords: Perovskite, $SrSnO_3$, $SrSnO_3$/NrGO, ORR

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F 016

Electrical Properties of Polymer Blend Electrolyte on Dye-Sensitized Solar Cells (DSSC) Application

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ABSTRACT

Polymer blend electrolyte (PBE) based on poly-methyl methacrylate (PMMA) and polyvinylidene fluoride (PVdF) polymers have been prepared using a solution casting technique [1]. Prepared PBE has been investigated using various ratios of PMMA and PVdF polymers. The Electrical Impedance Spectroscopy (EIS) shows the optimum conductivity value is PMMA:PVdF (70:30) with 3.82×10^{-5} Scm^{-1}. The temperature dependence conductivity has been performed in the 300–373 K range, which is observed to obey the Arrhenius behaviour [2]. The dielectric constant (ε') and loss (ε") increases with temperature at lower frequencies and approach negligible values at higher frequencies. This behaviour can be explained based on electrode polarization effects [3]. The plot of the real, M_r and imaginary part, M_i versus frequency, indicates that the systems are predominantly ionic conductors. DSSC's performance's efficiency value is impressive by using PBE, standing at 0.06%. The interaction between these two polymers influences the performance of DSSC.

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F 017

Impact of Different Ag Nanostructure on the Photo-Catalytic Properties of ZnS

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ABSTRACT

ZnS is a versatile semiconductor with tunable optoelectronic properties, making it suitable for wide range of applications. However, its wide bandgap limits the light harvesting efficiency, which, in turn, affects its photo-catalytic activity. To overcome this drawback, we provide a novel strategy through incorporating noble metal nanostructures on the ZnS surface. Initially, we prepared Ag nanospheres and Ag nanoprisms of different edge lengths, and loaded onto the ZnS structure. The localized surface phenomena of Ag will improve the light harvesting ability of ZnS and consequently improve its photo-catalytic efficiency. Importantly, the role of different morphologies of Ag nanostructures on the catalytic activity of ZnS is evaluated. To start with, the structural confirmations of Ag:ZnS were performed with XRD and HR-TEM and XPS analysis. Then, the optical properties are studied with absorption and FTIR spectra. Finally, the photo-catalytic studies were carried out under visible-light irradiation and the results shows that, there is a strong correlation between the Ag morphology and the catalytic performance of ZnS.

Key Words: Photo-catalysis, ZnS, Ag, LSPR, nanoprism.

F 018

A Comparative Study of In Vitro Antimicrobial Activity of PEG and Gallic Acid Capped Silver Nano Particles

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ABSTRACT

In this work, the physic-chemical properties and anti-microbial potential of the silver nanoparticles synthesised using two different reducing agents (Chemical reducing agent and green reducing agent) are compared. In both approaches, silver nitrate is used as precursor of Ag^{2+} ions, whereas Poly Ethylene Glycol and Gallic acid are used as the reducing agents. The appearance of yellow coloured colloid after the synthesis indicate the formation of silver nano particles which is attributed to the excitation of surface plasmon oscillations. The XRD spectrum confirms the crystalline nature of silver silver nanoparticles. FTIR spectrum confirms the presence of PEG and Gallic acid on the surface of silver nanoparticles. The PEG capped samples show good anti-microbial potential on different microbes and it is observed that the growth of microbe colony is very much reduced and even a halo (a region without microbes) appearing around the filter paper. But an entirely different result is observed in the Gallic acid coated silver nanoparticles as they do not show any anti-microbial potential. This may be due to the fact that the natural anti-oxidant activity enables the Gallic acid to protect these microbial cells from the oxidative damage caused by reactive species.

F 019

Photocatalytic Degradation of Pharmaceutical Contaminants using Novel Nanocomposites

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ABSTRACT

Due to the global generation of waste and effluents, evolutionary concepts of waste remediation have emerged, leading to concepts of pollutant reduction in the environment Pharmaceuticals have been found in industrial zones, hospitals, and are most common in developed countries. However, antibiotics are now overused, with unambiguous amounts produced. According to research, pharmaceuticals and their metabolites are dumped into the aquatic environment all over the world. Effluents from industries and common effluent treatment plants have frequently detected pharma contaminants ranging from 1ng/L to a few mg/L. It is also clear that ciprofloxacin traces in wastewater near industries exceed 1000 times the permissible limits, leading to antimicrobial resistance. Currently, the removal efficiencies achieved at wastewater treatment plants are insufficient. Advanced oxidation techniques are a new technology for advanced waste water treatment. It has been discovered that photocatalysis can be used as a polishing step to degrade ciprofloxacin and many other recalcitrant chemical compounds. This work primarily focuses on developing a unique coupled nano photocatalyst to degrade the antibiotic, ciprofloxacin. This research explores the efficiency and mechanisms of this innovative approach, shedding light on its potential for sustainable water purification.

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F 020

Facet-Dependent in Boosting Electron Mobility of Cu-Doped Rutile TiO_2 Film-Based Methylene Blue Degradation

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ABSTRACT

Titanium dioxide (TiO_2) is widely used as an active photocatalyst to degrade wastewater[1]. In general, the photocatalytic activity of the anatase phase is superior to that of the rutile phase[2]. However, the rutile phase also possesses certain advantages, such as high chemical stability and strong absorption of UV rays. In a typical rutile TiO_2 nanorod, the {111} and {110} facets play the role of oxidative and reductive sites, respectively, for capturing photoinduced holes and electrons to inhibit recombination. Hence, doping rutile-phase TiO_2 with copper oxide (CuO) can alternate the facet and enhance the photocatalyst's crystal structure and optical properties of the rutile phase. CuO has been incorporated into the TiO_2 lattice, as confirmed by XRD analysis and Raman spectroscopy in the rutile phase. The synthesized TiO_2 in the rutile phase had a flowerlike structure. HR-TEM analysis confirmed an alternate facet upon CuO doping, indicating a change in the facet structure. The (110) facet alternates with the co-exposed (111) and (220) facets upon doping with CuO. Doping rutile-phase TiO_2 with 5% CuO results in a reduction of the bandgap to 2.89 eV. Adding 5% CuO dopant to the TiO_2 film resulted in the degradation of 98.47% of methylene blue through photodegradation. The co-exposed facet (111) and (220) helps separate the charge carriers generated by light and extends their lifespan, enhancing their ability to perform their intended role[3].

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F 021

Upconversion and Photoacoustic Measurements of Ho^{3+}/Yb^{3+} doped Gd_2O_3 Phosphor through 980 nm Excitation

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ABSTRACT

The Ho^{3+}/Yb^{3+} doped Gd_2O_3 phosphor samples were synthesized by the combustion method and then upconversion (UC) and photoacoustic (PA) spectroscopic studies were done. Prepared phosphor samples were annealed at 800-1300°C for 3 hours and all samples were found in cubic phase confirmed by X-ray diffraction (XRD) analysis. From Field Emission Scanning Electron Microscope (FE-SEM) images it is found that particle size increases with increase in annealing temperature. The frequency UC emission spectra of samples were recorded by exciting the sample with 980 nm diode laser and maximum intensity is obtained for the sample annealed at 1000°C for 3 hours. A PA cell was designed for comparative study of UC (happen due to radiative transition of photon) and PA (happen due to non-radiative transition of phonon) through 980 nm laser. Then PA absorption spectra of the optimized sample recorded through 500 Watt. Xenon lamp excitation. The result show that this phosphor is appropriate for generating strong UC emission along with strong PA signal. Therefore, the present phosphor have dual functionality properties that are useful in upconversion imaging and photothermal therapy. Also, the present sample has shown its potential for detection of fingerprint and security ink.

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F 022

Flexible, Lightweight, and Ultrathin Graphene-Polymer Composite Film for Ku-Band Electromagnetic Interference Shielding

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ABSTRACT

With the quick development of electronic gadgets, many electromagnetic waves are disturbed in the living environment, potentially affecting human health. Designing and producing highly efficient materials for electromagnetic interference (EMI) has become a crucial challenge that requires immediate concern. Consequently, we have successfully developed an ultrathin and flexible composite thin film using a simple solution casting technique. This composite, is composed of poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP)/reduced graphene oxide (rGO) at a remarkably low rGO loading of 6.75 wt.%. Uniform distribution of rGO sheets throughout the polymer matrix, confirmed through high-resolution transmission and field-emission scanning electron microscopy. Further, we conducted an array of investigations, including X-ray diffraction, Raman, Fourier transform infrared spectroscopy, and contact angle analysis to interpret the interfacial interaction between the matrix and filler. Remarkably, PVDF-HFP/rGO composite film exhibits a tensile strength of ~64.8 MPa and Young's modulus of 4.2 GPa. Impressively, the ultrathin PVDF-HFP/rGO composite film, with a thickness of ~80 µm, demonstrated a substantial EMI shielding effectiveness (SE) of ~18.3 dB in the Ku-band region, despite containing only a meagre 6.75 wt.% of rGO. This impressive EMI SE is attributed to the well-established network of interconnected rGO sheets within the matrix. This work not only demonstrates a scalable and effective method for producing ultrathin, light, and flexible composite films but also reveals the enormous possibilities for EMI shielding applications in the fields of miniature electronic devices and aerospace technology.

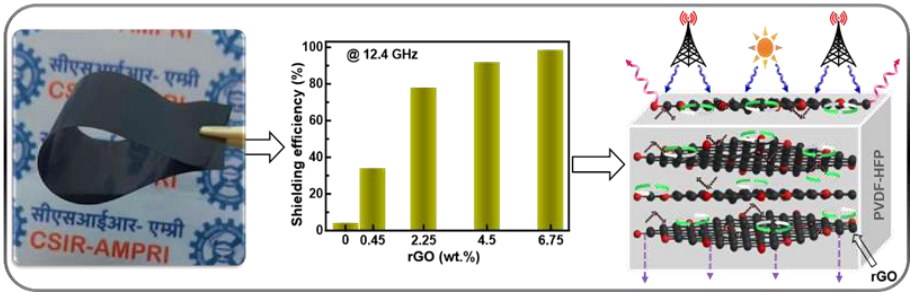

Figure. Optical image of PVDF-HFP/rGO composite thin film and its EMI shielding efficiency & mechanism.

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F 023

Synthesis of Rare Earth Doped Fe_3O_4/Tio_2 Core-Shell Photocatalysts for Degradation of Nitrobenzene and Rhodamine B

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ABSTRACT

During the degradation of contaminants through advanced oxidation processes using TiO_2 nanoparticles (TiO_2 NPs), the recovery of NPs is a challenge. The incorporation of a magnetic core in the TiO_2 nanoparticles allows them to be easily recovered by using a magnet. [1,2] Furthermore, in recent years, doping TiO_2 with rare earth metals has proven to be an effective method to improve its photocatalytic properties. [3] Rare earth-doped Fe_3O_4/TiO_2 photocatalysts were synthesized via a two-step process. Initially, Fe_3O_4 nanoparticles were prepared using the co-precipitation method proposed by Wang [4]. An aqueous medium was prepared by dissolving $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$, and then a solution of NaOH was added. In the second phase, the TiO_2 shell deposition was carried out using the sonication process to simulate Rather's methodology [1]. Briefly, the synthesized Fe_3O_4 NPs were dispersed into isopropanol and subsequently mixed with titanium isopropoxide. During this step the rare earth element was also added. The synthesized nanomaterials were analyzed by physicochemical techniques including XRD, BET, SEM, UV reflectance and DLS. Finally, to evaluate the photocatalytic activity of the doped and undoped Fe_3O_4/TiO_2 NPs some experiments of photodegradation of nitrobenzene and rhodamine-B [5] were carried out in a Rayonet photochemical reactor using ultraviolet light at a wavelength of 254 nm, the remaining concentration of the contaminants was determined by UV-Vis spectrophotometry to estimate the % of degradation.

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F 024

Sulphur and Nitrogen Co-doped Carbon Nanoparticles Via Hydrothermal Route

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ABSTRACT

Quantum dots fabricated from carbon precursors are poised to reach the pinnacle of fresh preferences in the field of carbon materials. Carbon Quantum Dots (CQDs) are zero-dimensional carbon-based materials with sizes less than 10nm that are comprised of sp^2/sp^3 hybridised carbon atoms and unique surface functional groups. Many factors dictate the physical characteristics of carbon dots, embarking on the choice of the carbon source (precursor) and the synthesis procedure. The synthesis of carbon nanoparticles hires readily available and inexpensive carbon precursors and is relatively effortless to carry out while reducing the production of toxic byproducts. In the current study, carbon nanoparticles were synthesised by implementing an expeditious hydrothermal synthesis process and through the use of citric acid and thiourea. In this experiment, we have employed TGA as a surface modification agent with the aim of enhancing the long-term stability of carbon nanoparticles. The average size of the particles was computed from the XRD depict. Along with this, functional group analysis and optical property analyses were executed.

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F 025

Formation of Calcium-Alginate Microbeads Encapsulated Gold Nanorods and its Potential for Long-Term Fungal Treatment

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ABSTRACT

Anisotropic gold nanoparticles (GNPs) colloids have stability issues maintaining their size and shape for a long time. In fungal treatment, controlled release is crucial to ensure optimal functionality and overcome lifetime limitations. Hence, encapsulation of GNPs was proposed to stabilize and protect the particles from unwanted chemical interaction and simultaneously extend the use time with controlled release. In this study, gold nanorods (GNRs) were encapsulated with varied sodium alginate (SA) ratios and calcium chloride. The GNRs were synthesized using seed-mediated growth methods (SMGM), which comprised the preparation of seed solution for 2 hours and a 20-hour ageing growth period. The formation of encapsulated gold nanorods (EGNRs) was done using an extrusion method, in which the mix of centrifuged GNRs and SA was dropped into CaCl2 solution at a flow rate of 1 mL/min. The optical response of GNRs shows two plasmon peaks after the centrifuge process at 528 nm and 699 nm, whereas the structural results exhibit two XRD peaks on the (111) and (200) planes, confirming the formation of GNRs. The synthesized GNRs have an average surface density of 74.81% and an aspect ratio of 4.23 ± 0.36. The encapsulation process suggests increased SA concentration causes larger Ca-Alg microbeads EGNRs. The characterization of EGNRs resulting in the 3:1 ratio of SA to CaCl2 is the most optimal for encapsulation and potential for controlled release application. The optimum sample shows an excellent hydrophilic surface with an angle of 39.30° and a good response to the control release test. Therefore, the EGNRs were proposed for long-term fungal treatment due to their exceptional ability to control the release of the anisotropic GNPs colloids.

F 026

Electrochemically Driven Water Splitting in Tb (DAB), a Lanthanide Based Coordination Polymer

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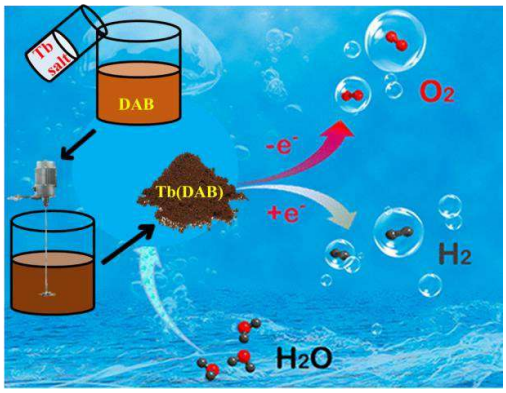
ABSTRACT

The pursuit of sustainable energy sources has led to extensive research in the field of electrochemical water splitting, a promising technology for renewable hydrogen production. Coordination polymers, a novel upcoming class of materials have gained significant attention as potential catalysts for this crucial process. The rational design and synthesis of coordination polymers offer numerous advantages, including precise control over the active sites, enhanced catalytic activity, and stability under harsh electrochemical conditions. These versatile materials exhibit tailored architectures and well-defined coordination environments, offering precise control over their electrocatalytic activity and stability. In the present work, we report a facile method for synthesis of a unique lanthanide metal coordination polymer, Tb(DAB) comprising 3,3'-Diaminobenzidine (DAB) as the ligand. The multi-stacked hierarchial layers of the polymer are analysed for their composition and morphology using XRD, XPS, FT-IR, Raman, FESEM and HRTEM. The synthesized coordination polymer is seen to give remarkable results for hydrogen evolution reaction with an overpotential of 228 mV measured at current density 10 mA cm^{-2}.



Keywords: Coordination polymer; Tb, diaminobenzidine, electrochemical water splitting, hydrogen evolution reaction.

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F 027

Fabrication of Graphene Quantum Dot Engrained in MOF-Derived Carbon@$NiCo_2S_4$ High-Performance Counter Electrode in Dye-Sensitized Solar Cells and Degradation of Tetracycline from Aqueous Solution

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ABSTRACT

Photocatalytic water purification is an effective environmental protection technique for removing toxic and harmful compounds from water, and solar energy conversion is a trustworthy and sustainable option for the future due to rising energy demands and the depletion of fossil fuels [1,2]. Herein, we report the construction of Graphene Quantum Dot (GQD) embedded MOF-derived carbon@$NiCo_2S_4$ by a facile solvothermal reaction, which in turn is utilized for specific applications such as counter electrodes (CEs) for dye-sensitized solar cells (DSSC) and visible-light-driven photocatalysts for the degradation of tetracycline. The developed GQD entrenched MOF-derived carbon@$NiCo_2S_4$ exhibits outstanding electrochemical performance when employed as CE in DSSC because of their favourable structural and morphological features. In particular, MOF-C@NCS/GQD delivered impressive power conversion efficiency compared to other electrodes and demonstrated superior electrocatalytic activity for the reduction of I_3^- to I^-. In addition, the formation of ternary composites has excellent photocatalytic decomposition of tetracycline under white light irradiation. Furthermore, the cycling test confirms the stability of MOF-C@NCS/GQD heterostructure. In order to improve photocatalytic activity and electron conductivity, the development of heterostructure and synergistic effects contributes to an increase in light absorption capacity, effective charge separation and a decrease in electron transfer resistance. Hence, this nanostructured MOF-C@NCS/GQD might be an excellent candidate for the counter electrode and photocatalyst in energy conversion and environmental applications.

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F 028

Biotic Synthesis of Silver Nickel Oxide Nanocomposites intending Bio-Medical Applications

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ABSTRACT

A single pot biotic synthesis has been carried out in order to achieve organic AgNiO Nanocomposites aiming Bio-Medical Applications. This work presents fabrication of Silver Nickel-Oxide Nanocomposites through bio-mediated reduction of Silver and Nickel salts using Catharanthus roseus (L.) G.Don (Vinca Rosea) plant crude extract. Crystalline nature of the green Nanocomposites is confirmed from sharp spectral peaks in XRD pattern at (111), (200), (220) and (311) planes. Crystallite size is calculated to be around 5nm using Debye Scherrer formula. EDX Analysis confirms presence of Silver, Nickel and Oxygen along with other elements. SEM and TEM images authenticate presence of spherical nanoparticles that would be helpful in diagnostic and therapeutic applications. FTIR Peaks identify phytochemical functional groups of the bio-source responsible for the reduction process. UV-Visible Absorption Spectra with peak at 207nm enables investigation on optical and electronic properties. Zeta potential of the Nanocomposites gives information on its charge and electrostatic compatibility in bio-medical applications. This simple synthesis of AgNiO Nanocomposites might be a promising tool in various bio medical and technological applications in pharmaceutical industries.

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F 029

Insitu Synthesis and Characterization of Bimetallic Nanoparticles

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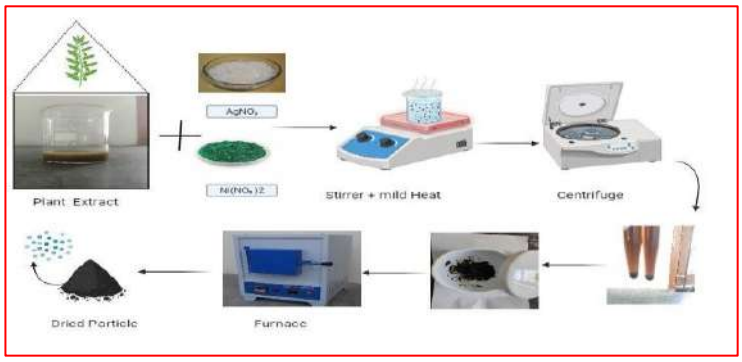
ABSTRACT

The green synthesis of metal nanoparticles (MNPs) is an emerging branch of nanotechnology with significant advantages over chemical and physical techniques for the environment and far-sighted. Bimetallic nanoparticles (BMNPs) are gaining attention in technology and science due to their superior physicochemical properties and diverse shapes, sizes, and structures when compared to monometallic nanoparticles. The production of BMNPs by natural extracts is straightforward, low-cost, and eco-friendly. For decades Phyllanthus niruri has been the focus of extensive investigation into the active components and their pharmacological efficacy**.** Several bioactive molecules, such as lignans, phyllanthin, hypophyllanthin, flavonoids, glycosides, and tannins, are present in the aqueous extracts of P. niruri. In this synthesis, the bio-reduction of metal ions was carried out in the presence of gallic acid as a surface modification agent, while using Phyllanthus niruri as a green source. The nanoparticles were examined using characterization studies such as UV, XRD, FTIR, SEM-EDX, and ZETA-POTENTIAL.



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F 030

Synthesis of WO_3/g-C_3N_4 Nanocomposite with Enhanced Photocatalytic Activity for Wastewater Treatment

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ABSTRACT

A simple and cost-effective hydrothermal method was used to synthesize graphitic carbon nitride (g-C_3N_4) nanosheets loaded with WO_3 nanoparticles. The morphological, structural, optoelectronic, and vibrational properties of the photocatalysts were investigated with the goal of gaining a better understanding of their photocatalytic activity. The surface morphology of synthesized WO_3 and g-C_3N_4 are shown in Figure 1. The crystal violet (CV) dye degradation and elimination of organic pollutants in water and the photocatalytic kinetics were analyzed to determine the corresponding pseudo-first-order reaction constants (k). The photocatalytic degradation efficiency of CV was 92.46% with WO_3/g-C_3N_4 under Visible light irradiation. Trapping experiments were able to show that the main active species for photocatalytic reduction of CV dye corresponding photocatalytic degradation comes via both holes and superoxide radicals. The greater catalytic efficiency of WO_3/g-C_3N_4 may be owing to a synergistic interaction between the WO_3 and g-C_3N_4 tighter interface and better optical absorption in the visible range. Additionally, a bigger specific area and increased visible light absorption contribute to the breakdown of organic dye. The mechanism of the photocatalytic process, as well as its reutilization capabilities, were also studied.

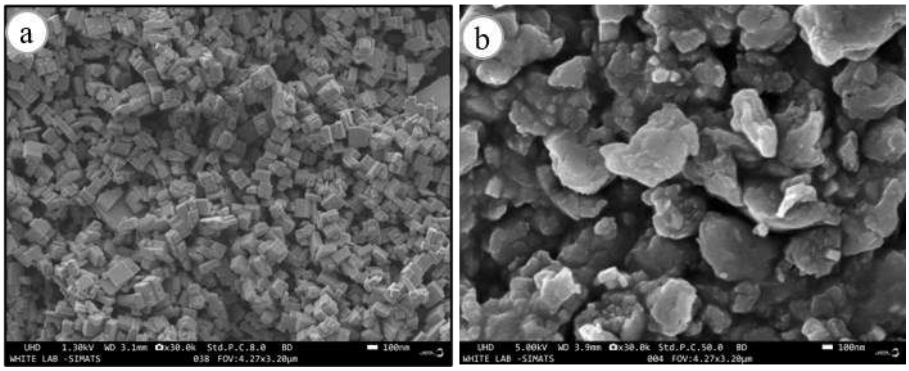

Fig.1a &b.SEM images of pure WO_3 and WO_3/g-C_3N_4 composites Heterojunction

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F 031

Impact of Ion Irradiation on the Optical and Structural Properties of ZnO Films: Insights from PL and UV-Vis Analyses

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ABSTRACT

This study investigates structural and optical transformations in ZnO films deposited on glass substrate using PLD. The films underwent irradiation with 100 keV Xe^+ beam at varying fluencies. Surface morphology, analyzed using SEM, reveals a transition from random particle distribution in pristine film to a more uniform arrangement in irradiated films, with increased roughness at higher ion fluencies. UV-Vis absorption measurements were conducted to assess the band gap energy. Interestingly, the band gap energy of irradiated films showed only minimal deviations from pristine films, implying that the ZnO crystal structure remains largely intact. This lack of impact on the electronic gap suggests that the small band gap changes are due to the morphological modifications, confirmed by SEM. Photoluminescence measurements done at room temperature with an excitation line of 310 nm from Xe lamp revealed a near band edge emission at 392 nm and additional visible emissions attributed to crystal defects. Emission intensity decreased in irradiated films, indicating a reduced concentration of specific recombination centers, aligning with previous researches that suggest ion irradiation induces defect center formation. Additionally, a blue shift in band edge emission occurred at low and medium fluencies, while a red shift was observed at the highest fluence, exhibit interesting PL emission properties. Thus, this study elucidates the effects of Xe^+ beam irradiation on ZnO films, offering insights into morphology and optical property transformations. These findings highlight, potential of ion beam irradiation for engineering the structural and optical characteristics of ZnO films, with implications for applications in optoelectronics and material sciences.

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F 032

Development of $ZrPo_4$ Based Magnetically Retrievable Photocatalyst for Removal of Azo Dyes from Industrial Wastewater.

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ABSTRACT

Now a days, synthetic dye production exceeds 7×10^5 tons annually, causing pollution in natural streams and water bodies. Photocatlysis, a cost-effective method combining material science, chemistry, and environmental engineering, is being investigated to remove these dyes from industrial and municipal water effluents. The study presents synthesis of a magnetically retrievable visible light driven amorphous zirconium phosphate supported on iron oxide doped graphitic carbonnitride$ZrPO_4/g\text{-}C_3N_4$ /Fe_3O_4(CFZ)nanocomposites, which shows superior photocatalytic efficiency for the degradation of anionic azo dyes congored(CR),reactive blue 1(RB-1). The composite's common structure, which provides multichannel photocatalytic sites while inhibiting photogenerated electrons and holes recombination, enables it to be utilized multiple times without affecting its photocatalytic activity significantly. The reusability of composite and low cost makes it a promising alternative for azo dye degradation in water. Under visible light irradiation (110w, IP67 klx) at room temperature and PH 7, 10 mg of the photocatalyst could destroy about 100% of 10 mL of 10 mg/L of an aqueous dye solution in 25 minutes. Various analytical techniques were used to characterise the prepared $ZrPO_4/g\text{-}C_3N_4/Fe_3O_4$ composite. FTIR, XRD, VSM, XPS, SEM, and TEM investigation revealed that $ZrPO_4/g\text{-}C_3N_4/Fe_3O_4$ nanocomposites with average particle sizes of (8 ± 1.2) nm were successfully prepared. To summaries, the synthesized nanocomposite CFZ has potential to efficiently degrade the azo dye with environmentallyfriendly strategy to deal with the ongoing problem of dye contaminated wastewater.

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F 033

Comparison study of Polymer Nanocomposites and Biosorbents using Adsorption Technology in Heavy Metal Removal

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ABSTRACT

The global water contamination threat has been greatly exacerbated by the swift pace of industrialization. Nanostructured materials, with their notably high specific surface area-to-volume ratio, display distinctive features, such as catalytic potential and enhanced reactivity. Standard techniques employed for the extraction of heavy metals include reverse osmosis, electrodialysis, ion exchange, and activated carbon. Nevertheless, these approaches have notable drawbacks, including inefficacy in dealing with minute levels of contaminants, high operational and maintenance expenses, and the generation of tainted sludge. This research provides an overview of contemporary nanocomposite technologies utilizing polymers, and biosorbents for the purpose of eliminating heavy metals. However, in light of current environmental issues and the pollution linked to highly efficient polymer nanocomposite, there is a concern about the considerable toxicity they can leave in the environment. In contrast, biosorbents, which utilize waste agricultural materials for pollutant removal. Consequently, both nanocomposites show considerable promise for future applications. This study emphasizes the advantages of employing biosorbents as environmentally friendly nanocomposite materials for addressing environmental pollution when compared to polymer nanocomposites.

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F 034

Investigation on the Physico-Chemical Attributes and the Photocatalytic Ability of Novel BiOI/ZrO_2 Nanocomposite Prepared through Solvothermal Method

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ABSTRACT

Organic pollutants are a serious threat to the water resources and cause numerous health issues to humans. Photocatalytic degradation of these pollutants is one of the most efficient methods, which can be used to treat the water resources [1,2]. So, in this work, BiOI/ZrO_2 a novel binary nanocomposite is synthesized through a simple solvothermal method and this nanocomposite was characterized using X-ray diffraction (XRD) analysis, FTIR, UV-VIS analysis, Photoluminescence analysis, High Resolution Scanning Electron Microscopy (HR-SEM) to study about the crystal structure, functional groups present in the sample, optical properties and morphology of the prepared nanocomposite. Through XRD, the average crystallite size of BiOI/ZrO_2 nanocomposite was found to be 31.7 nm. Through the addition of BiOI a narrow band gap semiconductor (2.15 eV), to the wide band gap semiconductor ZrO_2 (5 eV), it's bandgap is adjusted and the resulting nanocomposite exhibited a band gap of 3.06 eV [3-5]. Hence the photogenerated electron hole pairs are efficiently separated in the resulting nanocomposite and it exhibits excellent photocatalytic ability against the degradation of organic pollutants (Eosin Yellow Dye).

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F 035

Visible-Light driven High Photocatalytic Activity of Mg Doped Tio_2 Nanoparticles Synthesized Via Wet Chemical Method

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ABSTRACT

The utilization of semiconductor photocatalysts for the removal of organic pollutants from wastewater has garnered significant attention due to their environmental compatibility and efficiency. In this study, we present the synthesis and characterization of Alkaline earth metal Magnesium (Mg)-doped titanium dioxide (TiO_2) nanoparticles as a promising photocatalyst for the degradation of Methylene Blue (MB) dye under UV, visible, and dark conditions. The doping of TiO_2 with alkaline earth metal is a well-established strategy to extend its photo response into the visible range and enhance photocatalytic activity. Mg-doped TiO_2 nanoparticles were synthesized through a wet chemical method, and their physicochemical properties were systematically characterized using various analytical techniques, including X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FT-IR), UV-Visible and Photoluminescence (PL) spectra. The XRD analysis revealed the formation of an anatase phase, with a noticeable shift in diffraction peaks corresponding to Mg doping. The optical properties of the nanoparticles were investigated through UV-Visible spectroscopy and PL spectra revealing shifts in absorption edges and bandgap due to Mg doping. while EDS revealed the successful incorporation of Mg ions into the TiO_2 lattice and Fourier transform infrared spectroscopy (FT-IR) for confirming the bonding nature. The photocatalytic performance of Mg-doped TiO_2 nanoparticles was evaluated by monitoring the degradation of MB dye under different illumination conditions, including UV, visible light, and in the absence of light (dark). The unique aspect of this study lies in the observation that Mg-doped TiO_2 nanoparticles exhibited appreciable photocatalytic activity even in the visible range, highlighting their potential for use in wastewater treatment scenarios. This intriguing photocatalytic activity can be attributed to the presence of Mg dopants, which create oxygen vacancies and trap charge carriers, allowing for enhanced electron-hole separation, reduced bandgap and prolonged radical species lifetimes. This research provides valuable insights into the versatile and enhanced photocatalytic properties of Mg-doped TiO_2 nanoparticles, which can potentially be utilized for the efficient removal of organic pollutants like methylene blue from water under different lighting conditions, contributing to the development of sustainable and environmentally friendly water treatment technologies.

Keywords: Mg doped TiO_2 nanoparticles, Wet chemical method, Methylene Blue Photocatalytic activity.

F 036

Synthesising Nanostructured Zinc Substituted Ni-Co ferrites by Combustion method: Investigation on their Structural, Magnetic and its Electrochemical Properties

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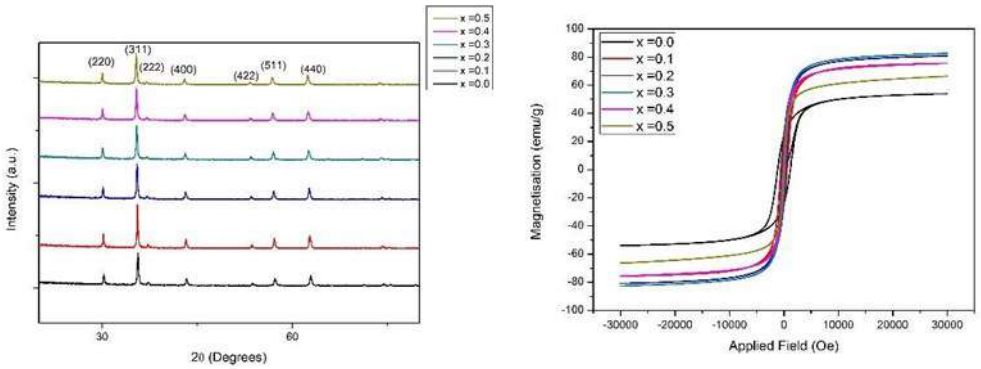
ABSTRACT

Nanoparticles of $Ni_{0.5-x}Zn_xCo_{0.5}Fe_2O_4$ (x=0.0-0.5) are prepared by combustion method using succinic acid as fuel. The structural, dielectric and magnetic properties were studied for the synthesised 'as prepared' zinc substituted Ni-Co ferrites. The XRD pattern of the 'as prepared' ferrites showed formation of monophasic cubic spinel structure (Fig.1a). There is a increase in the lattice parameter with an increase in zinc concentration [1]. The IR spectra depict two characteristic absorption peaks of spinel at around 600 cm-1 and 400 cm-1 [2]. The variation of dielectric properties as a function of frequency shows high values at lower frequencies and



remains constant at high frequencies [4]. The Curie temperature determined from A.C. susceptibility measurements found to decrease with increase in zinc content [1]. The VSM plots of all the ferrites indicate ferromagnetic nature (Fig.1b) and shows a random trend in saturation magnetisation (Ms) with increase in the zinc content in Ni-Co ferrites may be due to variation in particle size of the end products [3]. The corresponding Ni-Co ferrites shows a good amount of electrochemical properties which can be used as a supercapacitor.

Figure 1. a) X-Ray diffraction pattern of 'as prepared' $Ni_{0.5-x}Zn_xCo_{0.5}Fe_2O_4$ (x=0.0- 0.5) and b) The VSM plots of magnetic moment against magnetic field at room temperature of 'as prepared' $Ni_{0.5}xZn_xCo_{0.5}Fe_2O_4$ (x=0.0- 0.5).

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F 037

Anticancer Activity of Green Synthesized Manganese-Doped Cerium Oxide Nanoparticles using Acacia Concinna Fruit Extract

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ABSTRACT

In this study, pure Cerium Oxide (CeO_2) and Manganese-doped Cerium Oxide nanoparticles ($Ce_{1-x}Mn_xO_2$) were synthesized via sol-gel method using Acacia Concinna fruit extract as a capping and reducing agent. The synthesized nanoparticles were subjected to various characterization techniques, including X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Energy-Dispersive X-ray spectroscopy (EDX), Raman spectroscopy, UV-Visible Spectroscopy, and Fourier Transform Infrared Spectroscopy (FTIR). The XRD pattern demonstrated single phase of CeO_2, with cubic fluorite type structure. The morphology of the nanoparticles were analyzed by FESEM. Raman spectroscopy validate the phase purity of the synthesized samples and provide information about structural defects caused by the dopants. This study indicated the promising role of manganese-doped cerium oxide nanoparticles as a potential nanotherapeutic agent for cancer treatment. The as-synthesized samples signified remarkable anticancer effect against breast cancer (MCF-7) and colon cancer (HCT-116) cell lines. The green synthesis approach, coupled with significant anticancer efficacy, opens new ways for further research in the development of innovative cancer treatments and therapies.

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F 038

Green Synthesis, Characterization and Anticancer effects of Gd-doped CeO_2 NPs in Human Colon Cancer (HCT-116) and Breast Cancer (MCF-7)

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ABSTRACT

Nanoparticles have emerged as promising agents in the field of cancer therapy due to their unique physicochemical properties. This study investigates the green synthesis, characterization, and anticancer potential of pure Gadolinium-doped Ceria (Gd-doped CeO_2) nanoparticles in human colon cancer (HCT-116) and breast cancer (MCF-7) cell lines. Pure ceria and Gd-doped ceria nanoparticles were synthesized by sol-gel method using Acacia Concinna fruit extract as surfactant. Their structural, morphological, and physico-chemical properties were characterized using various analytical techniques, like X-ray diffraction (XRD), Raman spectroscopy, UV-Visible Spectroscopy, Field emission scanning electron microscopy (FESEM), Energy-Dispersive X-ray spectroscopy (EDX), and Fourier Transform Infrared Spectroscopy (FTIR). The XRD and Raman patterns have witnessed the cubic flourite-type structure of CeO_2 nanoparticles. FESEM images indicated the formation of monodisperse nanoparticles having spherical morphology. In vitro cytotoxicity studies were conducted to assess the anticancer activity of these nanoparticles. Both pure ceria and Gd-doped ceria nanoparticles demonstrated dose-dependent cytotoxicity against HCT-116 and MCF-7 cancer cell lines, while exhibiting minimal toxicity towards normal human cells. These nanoparticles exhibited promise as novel therapeutic agents, opening avenues for further exploration in the field of cancer nanomedicine.

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F 039

Highly Fluorescent Nanocarbon Materials Synthesised from Dicot Plant Using Microwave-Assisted Hydrothermal for Multifunctional Applications

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ABSTRACT

Nanotechnology and nanomaterial are a promising and rapidly growing technology in the field of research which works in the nanoscale regime. Carbon nanoparticles which are unique category of particles due to its excellent electrical and heat conductivity, mechanical properties, UV stability, heat and scratch resistance, which makes it suitable for wide range of applications. In our work carbon nanoparticle sample is extracted and synthesized from a dicotyledonous plant and its optical properties has been studied. It was observed that, the sample exhibited strong absorbance in UV region and excellent fluorescence emission in the visible region. When the sample is excited at 365 nm a bathochromic shift was obtained, due to these characteristic properties of the prepared nanocarbon material it could be used as down conversion material in energy harvesting devices to enhance the performance. Intrinsic property of these carbon-based nanoparticles could be utilized in applications of solar cells; devices which convert solar radiation into electricity by the phenomenon of photovoltaic effect. This Fluorescent behaviour of nanocarbon materials could be used for multifunctional applications like, LED manufacturing, biomedical applications, biomedical sensors, anti- counterfeit applications and many more due to their outstanding chemical and optical properties.

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F 040

Multifunctional Carbon Nanomaterials Derived from Edible Tubers Via Microwave-assisted Hydrothermal Method

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ABSTRACT

Nanocarbon is an emerging material because of its unique optical, electrical, and mechanical properties applicable to a wide range of applications. A number of eco-friendly techniques for producing nanocarbons are beginning to realize their full potential for industrial-scale manufacturing and usage in the creation of long-lasting applications. In this work, we synthesized nanocarbon materials from Edible Tubers and exhibited fluorescence characteristics suitable for multi-dimensional applications. These nanocarbon materials have been proven to be effective in LED (light-emitting diode), anti-counterfeit applications, and down-conversion in solar cell applications. It can be used for LED applications because of its optical phenomena like photoluminescence, and UV absorption due to its electron band structure where the electrons in the valence band excite to the conduction band when UV light of suitable energy falls on the material. The prepared nanocarbon materials have excellent fluorescence quantum yield and are nontoxic making them ideal for anti-counterfeit applications. Moreover, the carbon nanomaterial shows emission at the visible range with an excitation of 365 nm and acts as down conversion materials for solar cell applications. Hence, the synthesized carbon nanomaterials from biomass provide multifunctional applications.

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F 041

Fluorescent Carbon Nanomaterial Synthesized from Agrarian Waste for Multifunctional Applications

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ABSTRACT

Carbon nanomaterials have exceptional mechanical strength, large surface area, high thermal conductivity, high electrical conductivity, lightweight, chemical stability, and are versatile in terms of tailoring for various applications. The scientific community has been smitten by their exemplary properties and it drives one to unravel the unexplored domains. In this work, we have synthesized a fluorescent carbon nanomaterial from a nutritious agrarian waste, which gives an added advantage of developing an environmentally friendly material from biomass. Owing to their fluorescence, this material can be used for multifunctional applications including LEDs, anti-counterfeiting, UV absorption, and solar cells. The white emission obtained from the sample substantiates the use of this material in the above-mentioned applications. Integrating carbon nanoparticles into LEDs escalates their properties, like luminescence, stability, and durability. Further, due to their unique properties and optical features, carbon nanomaterials can be used for anti-counterfeiting. Exposing the sample to long UV rays (365 nm) shows an absorption affirming the use of this material in UV-absorption devices, like sensors, HPLC, and spectrometers. The emission in the visible region helps us use this material for down conversion in solar cell applications. Hence, the synthesized carbon nanomaterial is a boon to the material science and nanomaterial industry.

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F 042

Nickel-Cobalt Oxide Nanomaterials as Efficient Bifunctional Catalysts for Water Electrolysis

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ABSTRACT:

Water electrolysis, a vital technology for sustainable hydrogen and oxygen production, relies on efficient catalysts to facilitate the splitting of water into hydrogen and oxygen. In this study, we present nickel-cobalt oxide (NiCoO) nanomaterials as promising catalysts for this electrochemical process. The synthesis of NiCoO is achieved through a hydrothermal method, which offers a simple and cost-effective approach. One of the standout features of these NiCoO nanomaterials is their interconnected spherical morphology. This unique structure enhances their performance as bifunctional catalysts for water electrolysis. The interconnected spheres provide a high surface area, which allows for more active sites where the electrochemical reactions can occur. This improved surface area, in turn, results in better catalytic activity, making the NiCoO nanomaterials highly effective in promoting both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). Here synthesized material shows 391 mV and 137 mV overpotential at current density of 10 mA/cm2. This study demonstrates the potential of NiCoO nanomaterials to contribute to the development of sustainable hydrogen production technologies, bringing us one step closer to a greener and more environmentally friendly future.

Keywords: Nickel-Cobalt Oxide; Hydrothermal; Nanomaterials; Bifunctional Catalysts; Water Electrolysis

F 043

Synthesis and Characterization of MoS_2 Nanoflower and Nanosheets for Supercapacitor and Photocatalytic Applications

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ABSTRACT

In this article, we synthesize MoS_2 nanosheet and nanoflower to enhanced energy storage and photocatalytic activity. Herein, sample synthesis is performed using a facile hydrothermal method, followed by a detailed analysis of their physicochemical properties using various characterization technique. X-ray spectra confirmed the presence of a 1T/2H mixed phase of MoS_2. X -ray photoelectron spectroscopy (XPS) analysis of synthesized samples revealed their corresponding energy states. The MoS_2 Nanoflower exhibited a higher specific capacitance than the MoS_2 nanosheets. But MoS_2 nanosheets shows higher degradation efficiency compared to MoS_2 Nanoflower using Methyl orange as an organic dye under visible light irradiation. The findings of this study demonstrate that MoS_2 nanostructures are excellent materials for both supercapacitor and photocatalytic applications.

F 044

Synergetic Performance of Novel SnO_2/g-C_3N_5 Heterojunction with Enhanced Photocatalytic Performance for Degradation of Organic Pollutant

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ABSTRACT

The proper design of photocatalysts is essential to improving the photocatalytic decomposition of wastewater as well as degradation of organic pollutants still remains a challenging task. This work has been used as a nitrogen-rich carbon nitride(C_3N_5) that has received as more attractive and great concern available in the nitrogen-containing precursor of 3 amino 1,2,4 triazole [1]. Herein a novel SnO_2/g-C_3N_5 hybrid material has been prepared via simple solid state mixing method. The physicochemical properties were investigated by various spectroscopy techniques [2]. To examine the morphologies and microstructures showed that g-C_3N_5 was wrapped tightly on the surface of SnO_2 nanomaterial with large intimate interface contact areas between the sheet of g-C_3N_5 and SnO_2 nanomaterial [3]. The XPS results and PL spectra demonstrated that the intimate interface contacts could facilitate the transfer and separation of the photogenerated charge carriers at their interface, thus the recombination of the photogenerated electron-hole pairs was impeded [4]. The effective photocatalytic activity of the nanocomposite was owed to the combined effect of three core processes: effectual charge separation, charge transfers, and higher visible-light absorbance. The synergistic effect of g-C_3N_5 and SnO_2 components in the composite leads to efficient separation of photogenerated charge carriers via heterojunction pathway and results in remarkable photocatalytic activity compared to individuals.

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F 045

Antibacterial study of Green Synthesized Calcium Oxide Nanoparticles (CaO NPs) Using Leaves Extract of Murraya Koenigii

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ABSTRACT

In this study we have synthesized Calcium Oxide Nanoparticles (CaO-NPs) via thermal treatment of $Ca(OH)_2$ as precursors which were synthesized by adding NaOH solution to $CaCl_2 \cdot 2H_2O$ solution without the use of any surfactant and organic medium which were later act as a precursors , called Green synthesis method .Aqueous extract from Murraya keongii (Curry) plants leaves were used as capping agent for the synthesis of CaO NPs .Antibacterial study has done by Agar well diffusion method. In this study , Staphylococcus aureus and Escherichia coli were used as the microorganisms. The synthesized CaO NPs were characterized by using X-ray powder diffraction analysis , Raman spectroscopy. The crystalline size of the most intense peak located at 37.35° is about 33.25 nm & crystalline size of the lowest peak located at 42.81° is 0.96 nm . The average crystalline size is 32.08 nm. Raman spectrum features shows number of peaks corresponding to specific molecular bond vibration i.e., single-single bond (N-O, C=C), Group of bonds (benzene ring), Polymer chain vibration, Lattice modes. The spectra suggest that the peak at 315 ,612 and 1073 cm^{-1} bands are of function of calcium oxide content.

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F 046

$NaYF_4:Ho^{3+}/Yb^{3+}@NaYF_4$ Core-Shell Nanoparticles for Optical Temperature Sensing and Anti-Counterfeiting Applications

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ABSTRACT

This work presents a synthesis and upconversion emission study of $NaYF_4:Ho^{3+}/Yb^{3+}@NaYF_4$ Core-shell nanoparticles. The upconversion phosphor has been synthesized via a thermal decomposition reaction route. The information about crystallinity, phase formation, and morphology has been obtained by X-ray diffraction, SEM, and TEM imaging which revealed the formation of pure hexagonal phase of the nanoparticles. The absorption-related study is performed using UV-Vis-NIR and FTIR spectroscopy. The upconversion fluorescence spectroscopy experiment is performed with a laser having a wavelength of 980 nm coupled with an optical fiber and CCD. The synthesized phosphor shows strong emissions in the green and red regions due to various transitions of Ho^{3+} ions. The formation of the shell enhanced the emission around 2 times due to preventing the migration of energy to quenchers. The variation in emission intensity with temperature revealed the good thermal sensing capability of the synthesized phosphor. Moreover, the application of the synthesized phosphor for fingerprint detection and anti-counterfeiting has been demonstrated.

Keywords: Upconversion; core-shell; fluoride nanoparticles; lanthanides; optical thermometry; anti-counterfeiting

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F 047

Zirconium-Doped Zinc Oxide for Solar-Powered Environmental Remediation: Characterization and Photocatalytic Performance

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ABSTRACT

Environmental pollution is increasing due to the continuous usage of pesticides, dyes, heavy metals, and pharmaceuticals that contaminate the water. As a unique and significant photocatalyst, zinc oxide (ZnO) has great promise for environmental cleanup and renewable energy production. The problem can be resolved when these pollutants are degraded by photocatalytic active nano structural metal oxides such as TiO_2, ZnO, etc. This abstract emphasizes how ZnO-based photocatalysis can use solar energy for environmental remediation. Due to its unique characteristics, which include a broad bandgap, high electron mobility, cost-effectiveness, and eco-friendliness, ZnO is an excellent material for degrading organic pollutants and generating renewable energy. To reduce the amount of sunlight and fast charge recombination in the photocatalysis process, we are doping transition metals and noble metals into the photocatalyst in order to raise the photodegradation performance. This investigation employed co-precipitation to create undoped and doped ZnO with zirconium (Zr) at various concentrations (2, 5, and 10%). We carefully examined the structural, optical, morphological, and chemical properties of both doped and undoped ZnO samples using X-ray diffraction (XRD), photoluminescence (PL), Field emission scanning electron microscopy (FESEM), and Fourier-transform infrared spectroscopy (FTIR). XRD analysis showed a slight shift at higher angles as the doping concentration increased. The band gap obtained from PL analysis for undoped and doped varied from 3.20 to 3.22 eV. A hexagonal shape was obtained from SEM analysis of 10% doped Zr doped ZnO. FTIR analysis exhibited a peak corresponding to Zn-O stretching. Photocatalytic degradation of sulphanilamide was performed under sunlight and concluded that as the doping concentration increases, the time taken for reduction decreases from 180 to 150 min.

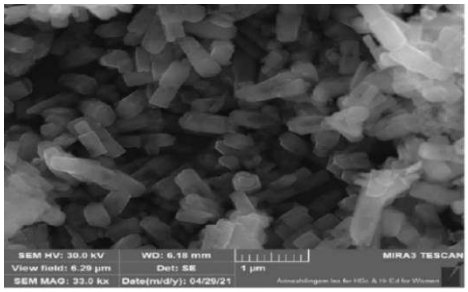

Figure: FESEM of 10% Zr-doped ZnO

F 048

Carbon Quantum Dots in Zinc Oxide Eugenol Cement for Enhanced Detection and Removal of Dental Implant Cement Residues

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ABSTRACT

Marginal retention of dental cement during implant cementation procedure causes peri-implantitis. The removal of these cement residues before setting time is challenging. We aim to detect and remove cement residues by embedding Carbon Quantum Dots (CQD) in dental cement. A 2 nm CQD is synthesized via thermal decomposition using citric acid and diethylene glycol as precursors. Physicochemical characterization reveals that CQD incorporated zinc oxide eugenol (ZOE-CQD) consisted of cuboid, hexagonal prism, thin rods, near-spheroid, and irregularly shaped particles. Zinc oxide particles are crystalline, and the hexagonal wurtzite phase of zinc oxide was observed in ZOE-CQD. The Infrared (IR) band at 3375 cm^{-1} is observed due to the extensive O-H stretching of eugenol and CQD. The absorption peak at 376 nm was accredited to the n-π* transition of the C=O band and π-π* transition of the conjugated C=C band of the CQD. Four different concentrations of CQD were tested with ZOE, namely 12, 16, 20, and 30 mg/ml. ZOE with 20 mg/ml CQD concentration exhibited greater luminescence. A quenching effect was observed in the CQD concentration above 20 mg/ml due to the chemical interaction between Zn^{2+} metal ion and CQD. The overlapping of the absorption and emission spectra of zinc oxide, eugenol, and CQD leads to the inner filter effect. Therefore, a CQD concentration of 20 mg/ml can be used for detecting cement residues. In conclusion, this research demonstrates that incorporating fluorescent CQD into ZOE cement can significantly aid in the detection of cement residues when compared to conventional zinc oxide cement.

Keywords: Carbon quantum dots, dental cement, peri-implant disease, fluorescent agent, nanoparticles, cement residues

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F 049

Semi Organic Nonlinear Single Crystals for Efficient Terahertz Generation

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ABSTRACT

Single crystals having significant nonlinear properties are the pillars of the terahertz photonics. The large nonlinear susceptibility and laser damage threshold value of the crystal is responsible for the generation of THz waves. The great sensitivity of the terahertz waves makes it an ideal candidate for imaging applications. The conventional slow evaporation solution growth technique is used to grow the single crystal. The structural parameters of the crystal have been determined by the single crystal X ray diffraction analysis. The UV-Visible spectroscopy analysis is performed to identify the linear optical parameters of the crystal. The Fourier transform spectrum was taken to confirm the functional groups present in the sample. The grown crystal was subjected to TG-DTA analysis for identifying the thermal stability of the material. The Kurtz-Perry technique is utilized for determining the SHG efficiency of the synthesized crystal. The Z scan analysis has been employed to determine the nonlinear refractive index (n_2), absorption coefficient (β), and third order susceptibility of the synthesized single crystal.

Keywords:. Semi organic crystal, Single Crystal XRD, TG/DTA, SHG, Z -Scan

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F 050

Hierarchical $Cr_2CT_x/NiFe_2O_4$ hybrid MXene Composite as a Bifunctional Electrocatalyst for Overall Water Splitting

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ABSTRACT

The electrocatalytic water splitting offers great potential as an environmentally friendly and sustainable method to produce hydrogen and oxygen, serving as a renewable energy alternative to traditional fossil fuels. MXene, a novel two-dimensional (2D) layered class of materials, has gained enormous attention as an electrocatalyst for water splitting. This versatile material can be tailored to enhance its electroactive surface sites and stability toward electrocatalytic performance. Herein, we designed a 2D hybrid material, $Cr_2CT_x/NiFe_2O_4$, via an in-situ hydrothermal approach. $NiFe_2O_4$ spheres decorated on layered-Cr_2CT_x are subjected to analysis using XRD, FTIR, XPS, FESEM, HRTEM, and Raman. The synthesized hybrid MXene material shows outstanding activity for overall water splitting compared to Cr_2CT_x and $NiFe_2O_4$. $Cr_2CT_x/NiFe_2O_4$ exhibits an overpotential of 144 mV and 159 mV at a current density of 10 mA cm^{-2} for hydrogen evolution and oxygen evolution reactions, respectively, and achieves overall water splitting of 1.69 V. This study reveals valuable insights on bi-functional 2D hybrid MXene materials for electrocatalytic water splitting.

Keywords: Cr_2CT_x MXene; $NiFe_2O_4$ Spinel; 2D/3D hybrid; electrochemical water splitting; hydrogen evolution reaction; oxygen evolution reaction

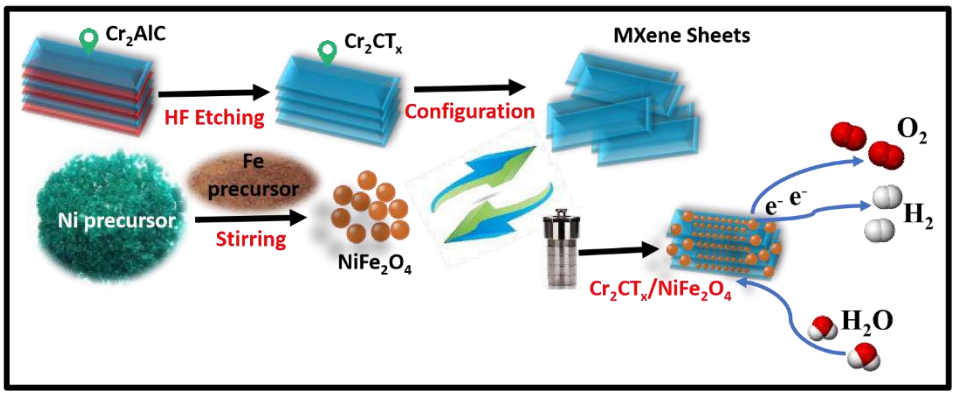

Fig. 1. Synthesis and water splitting application of $Cr_2CT_x/NiFe_2O_4$ hybrid MXene composite

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F 051

Chemoselective Oxidation of Vanillyl Alcohol using Cu/Co/SBA-15 Mesoporous Catalyst

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ABSTRACT

Heterogeneous catalysts possess the advantages of ease of recovery and recycling and, hence, are readily amenable to continuous processing. These advantages of heterogeneous catalysts have received much attention. The replacement of heterogeneous catalysts in the industrial segment instead of homogeneous catalysts has been increasing gradually. The use of mesoporous solid catalysts such as SBA-15 and related molecular sieves has additional benefits in organic synthesis, because of their large pores and high surface area. In this study, SBA-15 based catalysts were synthesized and characterized for a few reactions of commercial importance. The scope of the present investigation involves the synthesis of Cu- and Co-immobilized SBA-15 using hydrothermal and wet incipient impregnation technique. SBA-15 as catalysts for the chemo selective oxidation of vanillyl alcohol with tert-butyl hydroperoxide (TBHP). GC analysis proved 84% conversion of alcohol to vanillin.

Keywords: *SBA-15, Heterogeneous catalyst, vanillyl alcohol, vanillin, oxidation*

F 052

Synthesis and Characterization of Nickel Oxide (NiO) Nano Powder

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ABSTRACT

Recently Nickel Oxide (NiO) has been a material of attraction due to its wide band gap, hall selective behaviour and its application as a transparent conducting oxide (TCO). In this work, NiO is synthesized through the Chemical synthesis method (Sol- Gel Synthesis) and its optical and structural properties are studied. Sol-gel synthesis of NiO nanopowder has been carried out by using nickel nitrate hexahydrate as the precursor and sodium hydroxide as precipitator, and DI water as the solvent. The synthesized NiO is characterized by UV-Vis spectroscopy, X-ray diffraction (XRD), and Scanning Electron Microscopy (SEM). NiO nano powder exhibited a maximum absorption peak at 348 nm with a band gap of 3.19 eV. X-ray diffraction pattern confirms the formation of face-centered Cubic (FCC) crystalline structured NiO with average crystallite size of 37, 36, 27, 24 and 23 nm. The sol- gel synthesized NiO is further optimized by spin coating it on the glass substrate and annealing it at different temperatures and their Absorption spectra and I-V characteristics are studied.

F 053

Study of Field Emission Properties as a Function of Length of Silicon Nanowire Prepared by MACE Method

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ABSTRACT

Scientific community always have a great interest to analyze interplay between the bulk silicon (Si) and its nanostructures (NSs) like nanoparticles, nanowires (NWs) etc [1,2]. Si NSs / NWs facilitate a wide range of amazing optoelectronic properties to develop new generation nanoscale devices due to quantum confinement (QC) effect [3]. Many researchers reported remarkable electron field emission (FE) properties of Si NWs which makes it promising candidate for electron FE based devices [4]. The electron FE properties of Si NWs have been studied using current–voltage (I–V) measurements followed by a theoretical analysis through the Fowler Nordheim (F-N) equation as a function of the aspect ratio of Si NWs. In order to reveal a detailed understanding of FE properties of Si NWs, a simple and cost effective metal assisted chemical etching (MACE) technique have been used to fabricate Si NWs with different Si wafer resistivity at constant etching time. The surface morphology of fabricated SiNWs samples have been carried out through scanning electron microscope (SEM). Resistivity of Si wafer affects the length and alignment of NWs during MACE process. It has been observed that the electron FE characteristics are directly influenced by the length of the Si NWs due to QC effects. This study reveals that as the size of Si NWs increases, FE characteristics like the field enhancement factor increases which suggests that the turn-on voltage and enhancement factor could be tailored by tailoring the sizes of Si NWs. Such work provides optimized wafer resistivity to make proper understanding of FE properties for various potential applications of Si NWs like high energy accelerators, microwave amplifiers and X-ray sources, etc [5].

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F 054

Development of a UV-Excited Optical Luminescence (UVEOL) Imaging Agent using Chromium-doped Bismuth Oxide Nanoparticles.

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ABSTRACT

Developing advanced imaging agents is essential for achieving targeted imaging and tracking for cancer detection. Bismuth-based nanoparticles have excellent X-ray attenuation characteristics, making them an effective contrast agent for computed tomography (CT). However, it is difficult to distinguish between normal and malignancies from soft tissues. Optical imaging shows disease progression and tumor response quantitatively. To improve the optical properties of the bismuth nanoparticles, we developed a bismuth-doped chromium (Cr^{3+}: Bi_2O_3 NPs) hybrid imaging agent as a cancer imaging agent for X-ray and optical images. The polyol process was used for synthesizing the Cr^{3+}: Bi_2O_3 NPs with different doping concentrations (0.5%, 1%, 5%) of the chromium. Various analytical techniques were employed to characterize the samples. As the dopant concentration increases, the polydisperse values and size of the hybrid nanoparticles also increase, indicating the interstitial doping of the chromium. The peak-shifting behavior of the doped Cr^{3+}: Bi_2O_3 NPs from the UV-visible spectra is evidence of an increase in wavelength emission. The high energy band gap of the synthesized Cr^{3+}: Bi_2O_3 NPs shows emission from green to red region when excited with UV-A and UV-B wavelengths. Thus, our developed hybrid imaging agent can provide both X-ray attenuation and UV-excited optical luminous properties for hybrid imaging modalities.

Keywords: *Nanoparticles, Metal oxide, Luminous, UVEOL, Bioimaging.*

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F 055

Synthesis and Characterization of Copper Indium Sulfide Nanostructures via Solvothermal Method

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ABSTRACT

Copper indium sulfide (CIS) is a promising semiconductor material with applications in photovoltaics and optoelectronic devices. This study reports a solvothermal synthesis method for the fabrication of CIS nanoparticles. The solvothermal process offers advantages such as simple equipment, less chemical innovation, low cost, mild preparation conditions, scalability, and precise control over size. It uses a solution medium in a spherical closed reaction vessel to create a high-pressure and high-temperature reaction environment. In this research, the CIS nanoparticles have been synthesized at various precursor concentrations at different temperatures and pressures to produce high-quality CIS nanoparticles. The structural, compositional, morphological, and optical properties of synthesized CIS nanoparticles have been investigated via X-ray diffractometer, scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray Spectroscopy, UV-vis spectroscopy, and photoluminescence spectroscopy. The results obtained in this study are very close to that reported by earlier workers.

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F 056

Real-Time Detection of Doxorubicin by Nitrogen-Doped Carbon Dots

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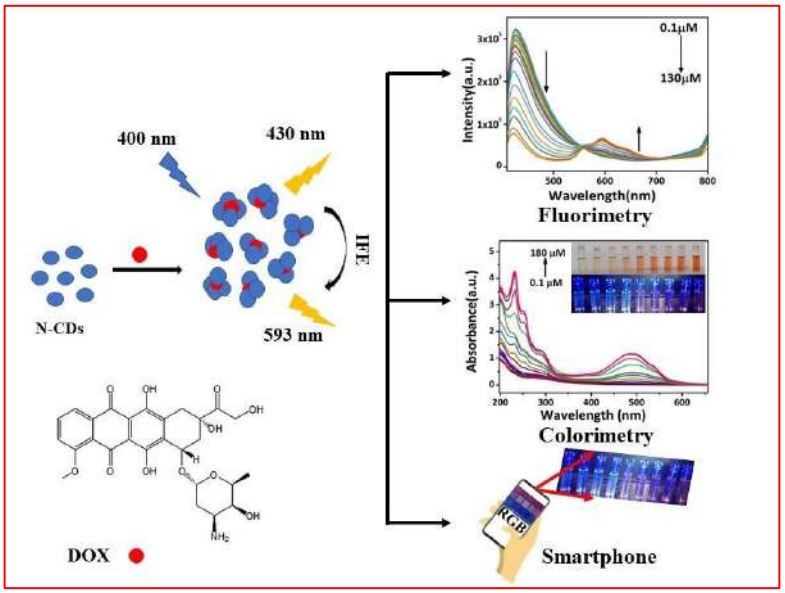
ABSTRACT

Therapeutic drug monitoring (TDM), essentially determines the drug concentration in blood and optimises the dosing range accordingly. TDM is essential for drugs like doxorubicin (DOX), a chemotherapeutic agent whose efficacy is compromised by the side effects of dosing. So, for egulation and usage control in biological systems, real-time DOX detection is crucial. Herein, a ratiometric fluorescence/ colorimetry/smartphone were employed for the detection of DOX using nitrogen-doped carbon dots (N-CDs). The N-CDs with a high quantum yield of 18% were synthesised by hydrothermal carbonisation of ascorbic5 acid and urea. The urea was chosen as the precursor because doping of nitrogen atoms in carbon dots increases the quantum yield. The full range of the XPS spectrum confirmed the presence of C, N and O elements in the synthesised N-CDs. The size and morphology were verified from the TEM image and the size of N-CDs varied from 2-5 nm. The N-CDs were nearly spherical in shape and evenly distributed. The as-prepared N-CDs help to detect the DOX within minute (0.5 mins) with high sensitivity, selectivity, and facilitate its visual detection by the naked eye. The limit of detection (LOD) for the fluorimetric and colorimetric methods were 0.058 μM and 0.70 μM respectively. The N-CDs can also detect the DOX in human blood serum in fluorimetry and colourimetry, with recovery percentages of 97.39-105.36% and 96.21104.99% respectively. The recovery percentage in smartphone method was 87.47-115.44 % [1].



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F 057

Low-temperature preparation of Graphitic Carbon Nitride from *Moringa Oleifera* leaves-Screening of Fluorescence and anti-oxidant property

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ABSTRACT

Two-dimensional metal-free graphitic carbon nitride (GCN) is receiving a lot of attention in the recent research world. The present study involves the preparation of graphitic carbon nitride through a one-step low-temperature thermal carbonization method from Urea and *Moringa Oleifera* leaves. The microstructure of the GCN was confirmed by the Powder X-ray Diffraction (PXRD) pattern and Micro-Raman spectra. The surface morphology and composition were well explored by X-ray Photoelectron Spectroscopic (XPS) analysis and High-Resolution Transmission Electron Microscopic (HR-TEM) images. The active surface principles of the GCN were extrapolated in terms of fluorescence and free-radical scavenging activity (DPPH quenching study). Ultimately the study provided a simple approach for the synthesis and application of GCNs.

Keywords: *Graphitic Carbon Nitride, Moringa Oleifera leaves, Urea, Low Temperature, Fluorescence, DPPH and Sensing.*

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F 058

Influence of Li-Nb co-doping on the Optoelectronic Characteristics of Spray-Pyrolyzed SnO_2 Films

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ABSTRACT

In order to tune SnO_2 thin films as an effective transparent conducting oxide electrode, the co-doping effects of niobium and lithium elements are examined for their structural, electrical transport, and optical characteristics. Cationic Li and Sb co-doping strategy into SnO_2 lattice has been reported to enhance the optoelectronic properties [1]. The coating of Li (0 - 4 wt.%) and Nb (2 wt.%) co-doped SnO_2 thin films on glass substrates is carried out using spray pyrolysis technique. Co-doping strategy reduces the value of contact angle on the film's surface by altering the surface morphology corroborating with literature reports [2]. Photoluminescence emission and visible light transmission measurements were conducted to understand the optical characteristics of the samples. Linear four-probe and Hall effect revealed sheet resistance and electrical transport properties with a minimum sheet resistance of 56 Ω/□ for 1 wt. % Li and 2 wt.% Nb doped SnO_2 thin film. These observed transparent conducting electrode characteristics will be discussed in detail.

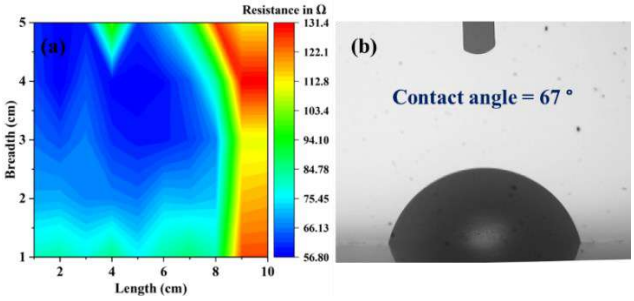

Fig. 1. (a) Sheet resistance mapping by linear four probe technique and (b) Contact angle measurement of the 1 wt.% 'Li'- 2 wt.% 'Nb' co-doped SnO_2 thin film.

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F 059

Growth and Characterization of n-type SnO_2 Nanostructures via p-type SnO formation during the Thermal Oxidation of Thin Sn films

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ABSTRACT

Tin oxide thin films are gaining much attention due to their excellent electrical, structural, optical, and chemical properties and show a wide range of applications in the field of optoelectronics, photovoltaics, gas sensing, and catalysts [1]. In general, tin oxide shows two major oxidation phases of stannous (SnO) and stannic (SnO_2) oxides with Sn^{+2} and Sn^{+4} oxidation states, respectively. Intrinsic SnO is a p-type semiconductor having an indirect energy band gap in the infrared regime, whereas SnO_2 appears as an n-type semiconductor with a direct energy band gap in the UV region. As a consequence, depletion layers of SnO-SnO_2 junction may naturally form during the oxidation process of thin Sn films [2]. Due to this unique possibility along with its gas sensing ability, tin oxide has become the most widely used oxide material for gas/vapour sensors. Depending on the growth conditions, SnO_2 appears in two different crystal phases such as tetragonal rutile structure at normal ambient whereas orthorhombic structure at extreme conditions of high temperature and pressure. In this work, we will present a controlled oxidation mechanism of thin Sn films with various oxide phases that leads to the formation of the most stable SnO_2 layers with faceted nanostructures. High purity metallic Sn films are deposited on chemically cleaned quartz substrates at room or elevated temperature, using a vacuum assisted thermal evaporation technique (~10^{-5} mbar). Thermal oxidation of as-deposited Sn films is performed using a muffle furnace in air ambient within a temperature range of 100ºC-1200ºC. Various surface characterization techniques such as XRD, FESEM, XPS, Raman, UV-Vis spectroscopy and I-V measurement have been performed to characterize the films. Initial oxidation of metallic Sn layers starts at about 250ºC. The P-type SnO phase is stable at lower oxidation temperature (250ºC-400ºC) while n-type SnO_2 starts to appear above 500ºC. Minor orthorhombic phase of SnO_2 is also observed during oxidation at higher temperatures (>800ºC). SnO_2 thin films appear with a granular surface morphology, uniformly distributed throughout the surface. However, a faceted morphology of these SnO_2 nanostructures are also observed at higher oxidation temperature. A sudden increase in electrical resistivity for oxide films oxidized at 500ºC is clearly observed, which indicates a transition of the p-type SnO layer into the n-type SnO_2 layer and hence the formation of depletion regions. These findings are very much complementary with Raman and UV-Vis spectroscopy. Due to this versatility of Sn oxides, it would be a potential candidate for the selective gas/vapor sensing at relatively lower operating temperature with a better sensitivity.

Keywords: Tin oxides, Thermal oxidation, Growth mechanism, Nanostructures

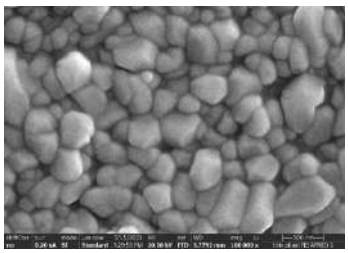

Fig. 1. Faceted nanostructures of SnO_2 grow at 1200ºC.

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F 060

Blue Emission from Ce^{3+}(x=0.1, 0.3 & 0.5 mol) Doped $SrLa_{1-x}AlO_4$ Phosphors

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ABSTRACT

In this present work, a host $SrLaAlO_4$ and $SrLa_{1-x}AlO_4$: xCe^{3+} (x=0,0.1,0.3.and0.5mol) phosphors have been successfully synthesized by a conventional solid-state reaction method at 1000 ^{0}C for 4hrs, and their structural and photoluminescence analysis has been studied. The XRD data confirms that all the prepared samples possess, a tetragonal structure possessing space group 14/mmm (139) with lattice parameters a=3.7564, b=12.6357, and c=3.3638. The crystal size of $SrLa_{1-x}AlO_4$: xCe^{3+} (x=0,0.1,0.3, and 0.5mole) varies from 19.266 nm, 20.250 nm, 19.934 nm, and 17.1931 nm. Photoluminescence studies were carried out by excitation of wavelength at 394nm, and the emission resulted peak 490nm($^5D_0 \rightarrow {}^2F_{7/2}$), corresponding electronic transition. The concentration quenching through dipole-dipole interaction. The Commission International de I′Eclairage (CIE) color coordinates were also determined from emission spectra and the value (0,3,0.33) was closer to white light. Efferent blue light-emitting diodes were prepared using Ce^{3+} doped phosphors under an excited UV light.

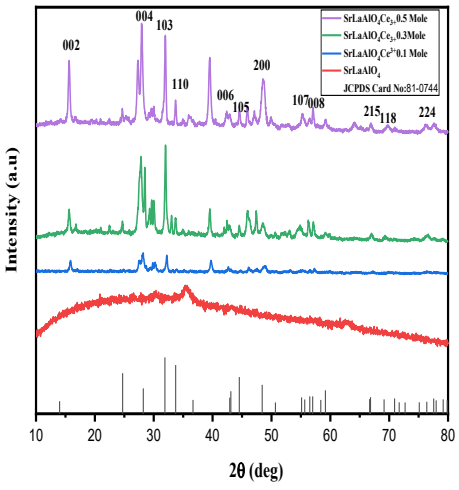

Fig. XRD of $SrLa_{1-x}AlO_4$: xCe^{3+} (x=0,0.1,0. 3 and 0.5mol) phosphor

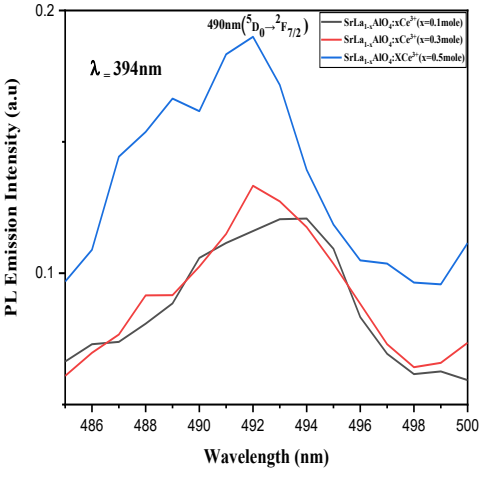

Fig. Emission of $SrLa_{1-x}AlO_4$: xCe^{3+} (x=0,0.1,0. 3 and 0.5mol) phosphor

F 061

Control of the Coating Structure on a Cathode Particle for Li-ion Battery

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ABSTRACT

Coating of Li ion conductors on cathode particles is indispensable not only for all-solid-state Li-ion batteries but also for those employing liquid electrolytes [1]. However, there are various reports discussing the optimal structure of the coating layer for these demands. In this presentation, we introduce a nanocoating process for Li-ion conductors on cathode particles using chemical reactions and deposition phenomena. In our previous study, our research group demonstrated that the coating structure can be controlled by manipulating key process parameters, including electrostatic interactions [2]. Consequently, this presentation serves an example for material development in the realm of Li-ion batteries based on this technology. As an example, Figure 1 elucidates TEM+EDS results, portraying the uniform oxide-based Li-ion conductor coating on the cathode particle's surface. Furthermore, this presentation delves into the impacts on cell properties when employing nano-coated cathode particles, showcasing an array of structures prepared using this technique, all within the context of a Li-ion battery system.

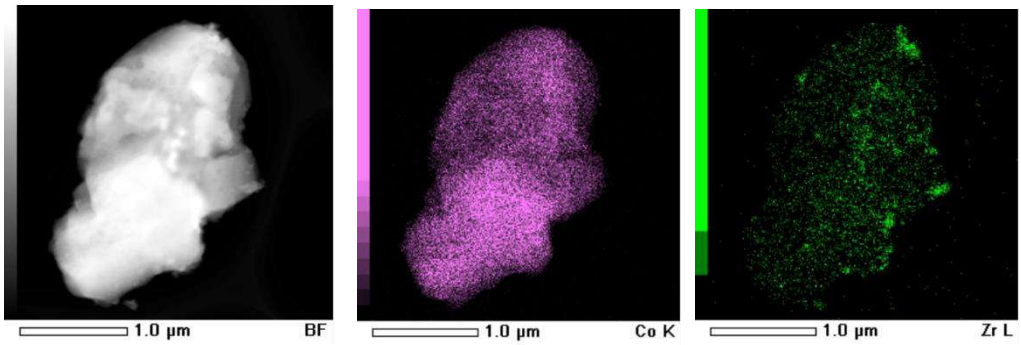

Fig.1 TEM+EDS analysis for $Li_7La_3(Zr_{1.75}Ta_{0.25})O_{12}$ coated $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ particle. Co: core part, Zr: Shell part

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F 062

Enhanced Cold Cathode Emission Properties of Titanium Dioxide Nanorod Decorated SiNW Hierarchical Structures

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ABSTRACT

Silicon nanowires functionalized by Titanium Diode (TiO_2) nanorods have been fabricated by time-varied hydrothermal synthesis of TiO_2 nanorods on chemically etched vertically aligned silicon nanowire (SiNWs) backbone. The electron field emission properties of these SiNW-TiO2 nano heterostructures have been are explored in this study. The effect of morphological variation, surface edges, surface roughness of the as-synthesized nano heterostructure in field emission properties have been studied in detail and enhancement factors have been calculated from the Fowler-Nordheim equation. The TiO_2 decorated SiNWs demonstrated enhanced cold emission properties compared to bare SiNW that is mainly contributed by the morphological structures. The hydrothermal synthesis time has been varied from 2 to 6 h and the nanorods show the optimum field emission properties in 4 h synthesis time. Electric field distribution simulations have also been carried out via finite element method around an isolated SiNW-TiO_2 emitter in a manner parallel to the experimental setup. The simulated field distribution results display good corroboration with the experimental findings. The obtained field emission properties strongly indicate SiNW-TiO2 hierarchical structures as probable candidate of cold cathode emitter used for electron emission-based applications such as field emission displays and vacuum nano-electronic devices.

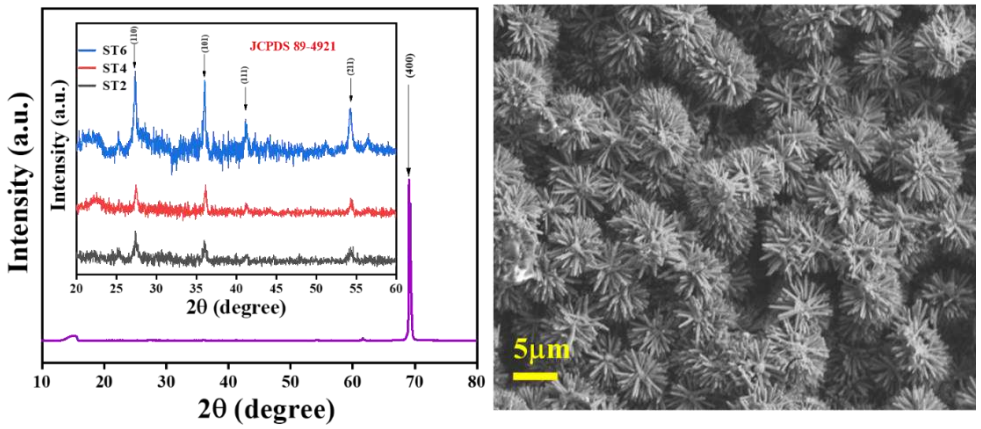

Fig 1. (a)XRD spectra of SiNW and SiNW-TiO_2 nanoheterostructures (b)FESEM image of SiNW nanoheterostructures.

F 063

Exploration of Novel Semiconducting Polymer Nanocomposites for Lithium- Ion Batteries *via* SET - LRP: Synthesis, Properties and Application

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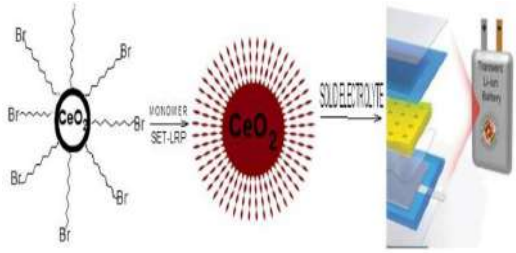
ABSTRACT

In the recent decade, lithium-ion batteries have flourished in the mobile market to a greater extent due to its wide physical and chemical properties, lifecycle, durability and cost effective. Despite its versatile commercial applications in various fields, it faces critical issues that restrict by safety concerns including leakage, combusting, or even explosions due to low boiling point of organic reagents as liquid electrolyte support. In order to mitigate these difficulties, solid electrolytes can be a potential choice and especially polymeric materials had wide challenging advantages among them. In current day, researchers focused more on Nano-Polymer based solid Li-ion batteries to accomplish high performance and to enhance the overall performance. In our work we reported the incorporation of the semiconducting nanoparticles into the polymer matrix which have been investigated to a greater extent. Cerium oxide (CeO_2) nanoparticles have been chosen to prepare polymeric nanocomposites due to its excellent physiochemical properties and electronic application. The surface functionalization of the nanoparticle was achieved by silylation followed by bromine termination result in the nano initiator which was further utilized for the polymerization of monomers specifically for battery applications. The controlled formation of semiconducting polymeric nanocomposites was achieved by SET-LRP, a controlled living radical polymerization method with a lower polydispersity index, which was further characterized by various spectroscopic techniques including XRD, TGA, GPC and electron microscope analysis. The polymerization proceeded in a "living" polymerization manner as indicated by linearity kinetic plot of the polymerization with minimal no of dead chains especially less than 5%. Plot of the molecular weight versus conversion showed a linear dependence, indicating a constant number of propagating species throughout the polymerization. The synthesized material was evaluated for its efficiency by analysing it with lithium-ion batteries as a solid polymer electrolyte and ion conductivity of the material was examined for its conductivity behavior for successful implementation in comparison with literature reports. Pictorial representation for the formation of solid polymeric nanocomposites electrolyte



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F 064

Photocatalytic Performance of g-C_3N_4/WO_3 Nanocatalyst for the Organic Dye Degradation for Waste Water Treatment

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ABSTRACT

Photocatalysis holds great promise as an efficient and sustainable oxidation technology for application in wastewater treatment. Rapid progress in developing novel materials has propelled photocatalysis to the forefront of sustainable wastewater treatments. In this work, g-C_3N_4 /WO_3 nanocomposite as photocatalyst was constructed by physical grinding of g-C_3N_4 and WO_3. The as-synthesized photocatalysts were characterized by X-ray powder diffraction, Fourier transform infrared spectroscopy, UV–vis diffuse reflectance spectroscopy, SEM, and photoluminescence. The photocatalytic activity of the photocatalyst was evaluated by degradation of Methylene Blue (MB) dye under a 300 W visible lamp. Compared to WO_3 and g-C_3N_4, the g-C_3N_4 /WO_3 composite exhibits an enhanced photocatalytic activity. The enhanced performance of g-C_3N_4 /WO_3 composite photocatalyst was mainly ascribed to the effect between WO_3 and g-C_3N_4, which improved the photogenerated carrier separation.

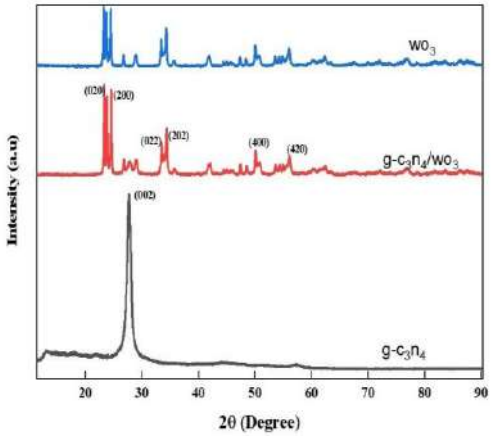

Figure 1: Comparison between the measured XRD pattern of g-C3N4, WO3, and g-C3N4/WO3 composite synthesized via physical grinding for 2 h and heated at 500°C.

Keywords: *Photocatalysis, Methylene Blue (MB), photogenerated carrier separation.*

F 065

Green Synthesised Carbon Dots - Chitosan Composite Electrospun Nanofiber Strips for Coconut Water Adulteration Test

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ABSTRACT

Cocos Nectifera L.water is the endospermic liquid inside coconut fruit, which has organoleptic characteristics according to the harvesting maturity. The Tender Kernel water is an energy drink and a detoxicant due to its plenty of minerals and antioxidants. The packaged drink available in the market may be added with adulterants like sugars, isovaleric acid, acetic acid and water for dilution. Also, preservatives such as rosemary extract, hops, salt, sugar, vinegar, alcohol, diatomaceous earth and castor oil can also be added. The loss of these minerals will not serve the purpose of drinking coconut water. In this study, we synthesised green luminescent C-Dots from coconut husk via hydrothermal synthesis and incorporated these carbon dots into the chitosan nanofiber sheets using electrospinning technique. These nanofiber sheets were used as indicator strips for the quality checking of tender coconut water. In the first step, the sheets were prepared with carbon dots and have been characterised using FTIR, UV-visible analysis, FESEM imaging with EDX, XRD and Raman spectroscopy to understand the quality of the material. The coconut water was then prepared with different concentrations of glucose and added flavours. The indicator strips show luminescent properties according to the adulteration and the pattern has been studied thoroughly for the accuracy of indicator strips.

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F 066

Highly Efficient Ultrasound-Driven Cu-MOF/$ZnWO_4$ Heterostructure: An Efficient Visible-Light Catalyst with Robust Stability for Complete Degradation of Tetracycline

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ABSTRACT

Metal-organic frameworks (MOFs) are a significant class of porous, crystalline materials composed of metal ions (clusters) and organic ligands. The potential use of copper MOF (Cu-BTC) for the sonophotocatalytic degradation of Tetracycline (TC) antibiotic was investigated in this study. To enhance its catalytic efficiency, S-scheme heterojunction was created by combining Cu-BTC with Zinc tungstate ($ZnWO_4$), employing an ultrasound-assisted hydrothermal method. The results demonstrated that the Cu-BTC/$ZnWO_4$ heterojunction exhibited complete removal of TC within 60 min under simultaneous irradiation of visible light and ultrasound. Interestingly, the sonophotocatalytic degradation of TC using the Cu-BTC/$ZnWO_4$ heterojunction showed superior efficiency compared to individual sonocatalytic and photocatalytic degradation processes using the same heterojunction. This enhancement in sonophotocatalytic activity can be attributed to the formation of an S-scheme heterojunction between Cu-BTC and $ZnWO_4$. Within this heterojunction, electrons migrated from Cu-BTC to $ZnWO_4$, facilitated by the interface between the two materials. Under visible light irradiation, the built-in electric field, band edge bending, and coulomb interaction synergistically inhibited the recombination of electron-hole pairs. Consequently, the accumulated electrons in Cu-BTC and holes in $ZnWO_4$ actively participated in the redox reactions, generating free radicals that effectively attacked the TC molecules. This study offers valuable perspectives on the application of a newly developed S-scheme heterojunction photocatalyst, demonstrating its effectiveness in efficiently eliminating diverse recalcitrant pollutants via sonophotocatalytic degradation.

Keywords: Copper-BTC, Zinc tungstate, S-scheme heterojunction, Sonophotocatalytic degradation, Tetracycline antibiotic

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F 067

Enhancing Photocatalytic and Optical Properties of ZnS Nanostructures through Cu@ZnS Nanocomposite Formation

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ABSTRACT

Zinc sulfide (ZnS) photocatalysts are widely used for harnessing light energy to catalyze chemical reactions. In this study, we tailored the band gap of ZnS by manipulating the concentration of the zinc precursor during the synthesis process, while also introducing copper metal ions into the ZnS matrix. By controlling the concentration of Cu in the nanocomposite, we can tailor the band gap to absorb specific wavelengths of light. Here, we employed a wet chemical method to prepare Zinc Sulfide samples (ZnS1, ZnS2 and ZnS3), with varying concentrations of the Zinc precursor, Zn $(NO_3)_2$. The prepared ZnS nanoparticles were incorporated with Cu nanoparticles obtained through a reduction method to create a Cu@ZnS nanocomposite. These samples were analyzed for their structural and optical properties. The band gap value of pure ZnS nanoparticles is measured at 3.45 eV, while in the case of the Cu@ZnS nanocomposite, it is reduced to 3.35 eV. To examine the surface properties of the prepared samples, they were subjected FESEM analysis. The catalytic efficiency of the Cu-ZnS nanocomposite was assessed by studying its ability to degrade Congo red dye solution. It is observed that the formation of the metal/semiconductor Cu@ZnS nanocomposite resulted in substantial alterations in the optical and catalytic properties of the ZnS nanostructures, primarily owing to the presence of Cu metal nanoparticles in close proximity.

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F 068

Probing the Oxidation Mechanism and Properties of Nickel Oxide

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ABSTRACT

Nickel Oxide (NiO) is a versatile *p*-type transition metal oxide semiconductor with a direct band gap of 3.6 eV - 4.2 eV, having a cubic rock-salt crystal structure is wide used in various field of applications such as electronic devices, volatile memory, gas sensor, catalysis, energy storage and many more [1-2]. However, the performance of NiO thin films is highly sensitive to its growth process. Therefore, a detailed understanding of the oxidation mechanism of thin Ni layer towards the oxide formation is found to be crucial for various applications of NiO based nanostructures in materials science and nanotechnology. In this study, we present a controlled thermal oxidation od thin Ni films deposited using an electron beam evaporation technique. A comprehensive analysis of these NiO films are performed using various surface characterization techniques such as XRD, FESEM, Raman spectroscopy, I-V measurements, UV-Vis spectroscopy, and XPS. XRD analysis reveals that the initial oxidation of Ni layer starts at 400°C and appears with (111), (200) and (220) diffraction peaks (Fig. 1(a)). FESEM images indicates the formation of homogeneous Ni film after room temperature deposition. With increase in oxidation temperature, NiO grain size increases due higher thermal diffusion and island coalescence (Fig. 1(b)). XPS peak of Ni-$2p_{(3/2)}$ at 853.6 eV confirms the Ni^{+2} oxidation state. All these findings reveal the structural, morphological, electronic, optical, and chemical properties of NiO films which can be explain in terms of thermal diffusion and chemical reactivity and are crucial for tailoring the nickel oxide based nanomaterials for various technological applications.

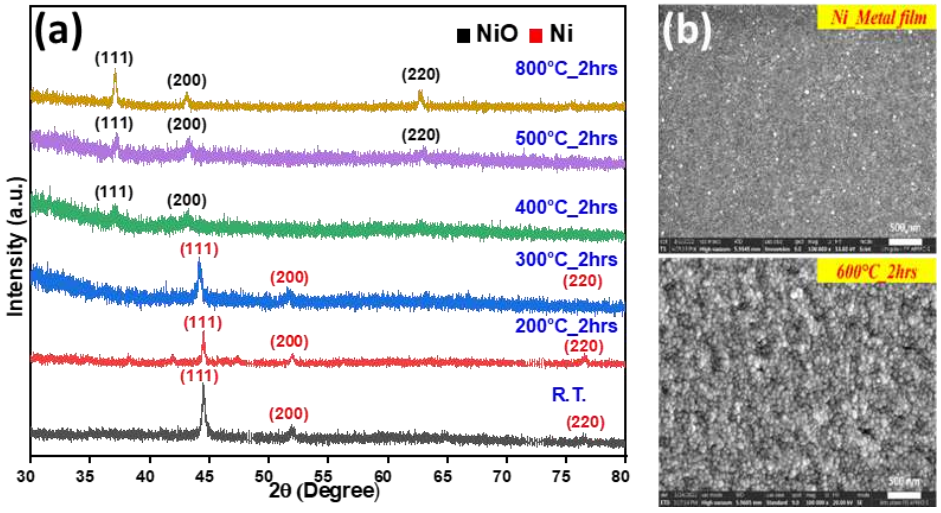

Figure 1. (a) XRD of Ni films oxidized at different temperature and (b) FESEM images of Ni and Oxide films.

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F 069

Barium Manganese Titanate (Ba_2MnTiO_6) Double Perovskite Based Phosphor

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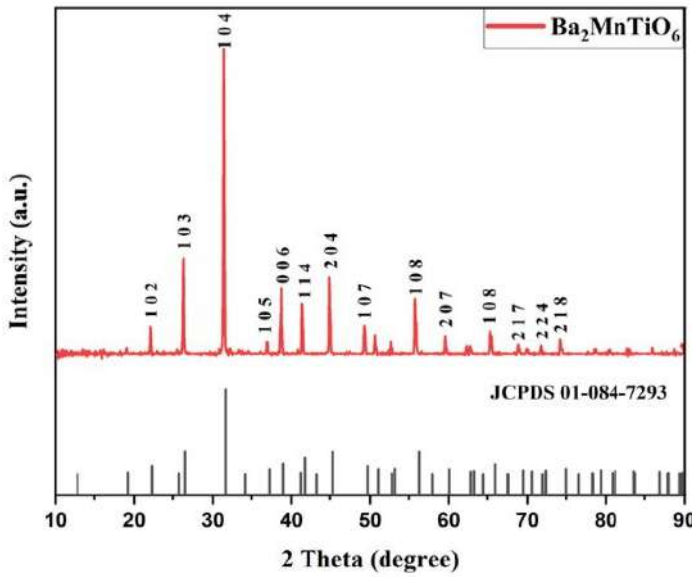
ABSTRACT

Next generation phosphor converted white-LEDs (pc-WLEDs) demand an efficient red emitter having a broad absorption in the UV/NUV region with a strong and narrow emission in the red region [1 - 2]. Recently, more research studies are focused on Eu^{3+} /Sm^{3+}/Mn^{4+} ion doped inorganic compounds with good optical performance [3-4]. Among them, double perovskites doped with Eu^{3+} have attracted researchers as attractive red phosphor materials because of their structural and thermal stability. Considering this, we prepared Eu doped Ba_2MnTiO_6 (BMT) double perovskite by high temperature solid state reaction method and their potential for red phosphor is studied at different Eu^{3+} concentration. Pure BMT was synthesized by mixing stoichiometric amounts of barium carbonate, manganese dioxide and titanium dioxide in an agate mortar for 1 hour with ethanol, followed by heat treatment at 600 °C for four hours and subsequently sintered at 1300 °C for 5 hours. The prepared compound was subjected to XRD study. XRD pattern (Figure) shows that Ba_2MnTiO_6 belongs to hexagonal structure with the space group P63/mmc. Lattice constants are calculated to be a = b = 5.6 Å, c = 13.8 Å, and β = 90°, according to the JCPDS card (JCPDS Card No. 01-084-7293). Optical properties of Eu Doped samples show characteristic absorption and emission bands of Eu^{3+} ions.



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F 070

Highly Efficient Electrochemical Lysing Platform for Pathogenic Bacteria with Optimized Electrode Design and Pt-rGO Modified Electrode

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ABSTRACT

Microorganisms are detected in resource-constrained settings by examining the genetic material (DNA/RNA) using nucleic acid amplification tests (NAATs) [1]. Cell lysis is required to retrieve the DNA present inside the cell. Electrochemical cell lysis (ECL) is a rapid, cost-effective, and reagent-less method, among other lysis techniques [2]. A small DC potential is applied between the electrodes, which causes electrolysis of water-producing H^+ and OH^- ions, which break the phospholipid bonds on the cell membrane, leading to the lysis of the cell [3]. Hence, the electrochemical method is an efficient cell lysing and DNA retrieval method that can easily be translated to a handheld point-of-care device. Optimally designed electrodes with electrocatalyst-modified surfaces can improve the efficiency of the electrochemical lysing to maximize the OH^- ions generation. This work optimizes design parameters, including size, shape, and distance between the electrodes, using COMSOL Multiphysics software. Tertiary current distribution Nerst-Planck module simulated the water electrolysis reaction and observed the generation and flux of H^+ and OH^- ions with time. Platinum nanoparticles decorated reduced graphene oxide (Pt-rGO) electrocatalyst has a low overpotential for water electrolysis (-0.77 V) and a low cathodic slope (0.073 V/dec), which directly results in lower energy required to drive the reaction. To fabricate a disposable electrode, Pt-rGO is synthesized by wet chemical method, mixed with printable carbon ink, and printed onto a PET sheet. The lysing efficiency of the new electrode material was improved by 33.33% compared to an unmodified carbon electrode and achieved complete lysis of pathogenic bacteria *E.coli* and *S.aureus* at 3 V under 2 minutes.

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F 071

Vertically Aligned ZnO Nanorods coated with AgBr for Dark-Light Dual Mode Disinfection

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ABSTRACT

Thin film coatings with antimicrobial properties find applications in various fields, including medical devices and food packaging, to combat microbial growth. Photocatalytic antimicrobial coatings offer a high actual-to-apparent surface ratio, holding immense potential for this purpose. However, achieving antimicrobial effectiveness not only in light but also in dark conditions poses a challenge. To address this, we introduce a novel approach using AgBr-coated vertically aligned ZnO nanorods (NRs) thin films. This method utilizes surfactants to achieve a uniform deposition of AgBr onto ZnO NRs. The resulting ZnO NRs/AgBr structures have undergone comprehensive characterization to assess their morphology, elemental composition, and wettability. Our studies confirm the ability to adjust the AgBr content by varying the concentration of the surfactant-based precursor solution. These ZnO NRs/AgBr structures exhibit a dual functionality, acting as both photosensitizers and antimicrobial agents. This dual role significantly enhances the visible-light photodisinfection efficiency of ZnO NRs, as demonstrated in our dark-light dual-mode antibacterial studies. Electron paramagnetic resonance measurements reveal that hydroxyl radicals play a pivotal role in the visible-light photodisinfection process.

Keywords: Antibacterial, AgBr, photocatalysis, reactive oxygen species, ZnO.

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F 072

One-Step Synthesis of Versatile $PbMoO_4$@$CdMoO_4$ Microspheres Hybrid for the Enhanced Photocatalytic Dye Degradation

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ABSTRACT

In this work, we have demonstrated the productive synthesis of novel and versatile $CdMoO_4$@$PbMoO_4$ microspheres hybrid photocatalysts by a facile in-situ hydrothermal method. Fabricated $CdMoO_4$@$PbMoO_4$ hybrid microsphere photocatalyst characteristics were analyzed using various techniques such as UV-visible spectroscopy, photoluminescence spectroscopy, powder X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray analysis, transmission electron microscopy and nitrogen isotherms. The photocatalytic degradation properties of $CdMoO_4$@$PbMoO_4$ hybrid microspheres were evaluated against methylene blue (MB) and congo red dyes (CR) under UV light. The hierarchical structure of $CdMoO_4$@$PbMoO_4$ along with the modulated bandgap, interfacial valence state electrons shift, and quick conversion of the Cd^{2+}/Pb^{2+} cycle led to display the 94.3% and 91.4% degradations of CR and MB under UV light irradiation, respectively which is superior to the corresponding pure structures degradation efficiency, signifying their boosted catalytic properties. Furthermore, degradation mechanism endorsed the excellent dye photodegradation under UV illumination by the novel $CdMoO_4$@$PbMoO_4$ microspheres hybrid catalyst. The observations resulted the more insight to progress the advancement of $CdMoO_4$@$PbMoO_4$ microspheres hybrid to effectively detoxify perilous and toxic water effluents for industrial purposes.

Keywords: Photocatalyst; Microspheres; Congo red; Methylene blue; Dye degradation

F 073

Development of $CaWO_4/C_3N_4/WO_3$ Ternary Nanocomposites for Effective Photodegradation of Organics and Antibiotics

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ABSTRACT

Environmental pollution is a major concern which imparts huge constraints on industrial and economic development. Environment pollution possesses serious threat to human and animal life. So, the quest for novel technology to produce clean energy and pollution free environment is continuous. There are several technologies in use to clean the pollutants. Each of the existing technology exhibits has its own limitation. Photocatalysis is one such environmental remediation technology having capability to mineralize the pollutant completely. Photocatalysis by heterostructured semiconductor material combines advantages of two or more dissimilar materials with unique properties. In the present work, ternary $CaWO_4/C_3N_4/WO_3$ nanocomposite were prepared and employed to test the photocatalytic performance against the organics. Heterostructured $CaWO_4/C_3N_4/WO_3$ ternary nanocomposites were constructed via multistep synthesis combining hydrothermal method, thermal polymerization and ultrasonication. The nanocomposites were characterized using XRD, UV, FTIR, FESEM, TEM and XPS. Photocatalytic studies were performed against RhB, ARS and tetracycline. The results reveals that the composition of nanocomposites has strong impact on the photocatalytic performance of the photocatalyst. Key reactive species responsible for photodegradation of organic compounds was found by radical trapping experiments. Kinetic experiments revealed that the photodegradation of organics follows pseudo-first order kinetics.

F 074

Enhancing Antibacterial Efficacy: A Novel, Magnetically-Recoverable AgBr-Loaded Iron Oxide/Alumina Nanocomposite Synthesized via Polymerizable Sol-Gel Method with Dark-Visible Light Activation

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ABSTRACT

Efficiently creating versatile nanocomposites is increasingly vital for a range of applications. This study details the synthesis of polymerizable sol-gel for magnetic iron oxide nanocomposites on alumina nanopowder. A calculated amount of iron (III) methacrylate and ethylene glycol dimethacrylate (EDMA) crosslinker are deposited on alumina nano powder to initiate the synthesis. Free radical polymerization is then thermally induced and allowed to run for 30 minutes at 125 °C. The resulting powder was calcined at 400 °C for 150 minutes and was characterized by field-emission scanning electron microscopy (FE-SEM), vibrating sample magnetometer (VSM), attenuated total reflectance – Fourier Transform infrared (ATR-FTIR) spectroscopy and ultraviolet-diffuse reflectance spectroscopy (UV-DRS). Saturation magnetization (Ms) values of 12–14 emu/g have been observed in the nanocomposites with 15 and 20 wt.% iron oxide. 5 wt.% of AgBr was added to the nanocomposite containing 20 wt.% iron oxide by completely mixing the surfactant-based precursor, silver-tetraoctyl ammonium bromide (Ag-TOAB), and then thermolyzing it. The antibacterial efficacy of the nanocomposites was assessed under both dark and visible light conditions against Escherichia coli. Remarkably, a 3 mg/mL loading of the AgBr-loaded nanocomposite achieved complete bacterial clearance within 90 minutes in the absence of light, while comparable activity was observed within 60 minutes in illuminated conditions. This underscores the multifunctional and highly promising nature of the AgBr-loaded iron oxide/alumina nanocomposite, serving as a dual-mode antibacterial agent and a magnetically recoverable photocatalyst material.

Keywords: iron oxide; photocatalysis; sol–gel; silver bromide; antimicrobial

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F 075

Efficient and Reusable Free-Standing CdS/ZnS/PVDF Nanocomposite Films for Visible-Light-Activated Malachite Green Dye Degradation

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ABSTRACT

In the present study, we develop a novel composite material comprising of Cadmium sulfide (CdS), Zinc sulfide (ZnS) and polyvinylidene fluoride (PVDF) as an efficient and reusable visible light active photocatalyst for the degradation of Malachite green dye. The polymer-based nanocomposite with different weight percentage of CdS/ZnS (5%, 10%, 15%, 20%) were prepared by co precipitation and solution casting technique. The structural, morphological and optical properties of the synthesized nanocomposite were characterized using X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM), Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis absorbance, transmittance, reflectance and photoluminescence spectroscopy. The photodegradation study demonstrated that CdS/ZnS/PVDF displayed significantly enhanced photocatalytic performance compared to both the individual CdS/ZnS and PVDF materials. It achieved a remarkable 99% degradation of the dye within 3 hours of visible light exposure. This may be attributed to the synergistic effect of the nanofillers and the PVDF matrix. The utilization of PVDF polymer serves a dual role, acting not only as a supportive matrix but also enhancing the photodegradation performance of the nanofiller. PVDF's excellent piezoelectric properties contribute to the generation of a spatial electric field, facilitating the separation of photogenerated charge carriers, a fundamental requirement for the photodegradation process. Furthermore, polymer-based nanocomposite materials offer the advantage of easy recovery and reusability, making them highly practical. In our study, the examined nanocomposite material demonstrated remarkable reusability, maintaining its activity even after undergoing five consecutive experimental cycles. Additionally, we conducted a scavenging study to investigate the major reactive species in the photodegradation process.

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F 076

Creating Self-Cleaning and Dual-Mode Antimicrobial Nanocomposites: CuO/AgX (X = Cl, Br, or I) Heterojunctions from Metal-Organic Frameworks

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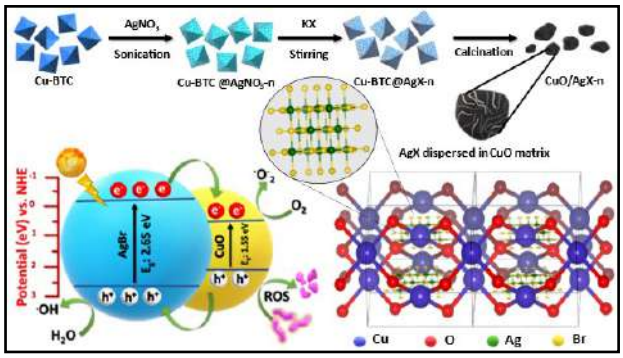
ABSTRACT

We developed a CuO/AgX (X = Cl, Br, or I) nanocomposite with visible-light photoactivity and antimicrobial properties using heterogeneous photocatalysis of semiconductors. The composite was derived from the calcination of Cu-BTC, a copper-based porous MOF, with incorporation of silver halide. The deposition of silver halide over the MOF provided high halide dispersion in the CuO matrix, resulting in a tight and effective heterojunction. Photodegradation studies of methylene blue and 4-chlorophenol under visible light and antimicrobial studies against *E. coli* and *S. aureus* under dark and visible-light conditions demonstrated the significant impact of reactive oxygen species, particularly hydroxyl and superoxide anion radicals, for the photocatalytic ability of the nanocomposites. Besides, the leaching of Cu and Ag ions has resulted in the activity dark-mode antibacterial activity of the nanocomposite. Our new synthetic pathway offers a promising approach for synthesizing biocompatible nanocomposites with superior heterojunctions and intimate component dispersion.



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F 077

Synthesis of Multifunctional Brownmillerite KBFO Nanofibers using Electrospinning method

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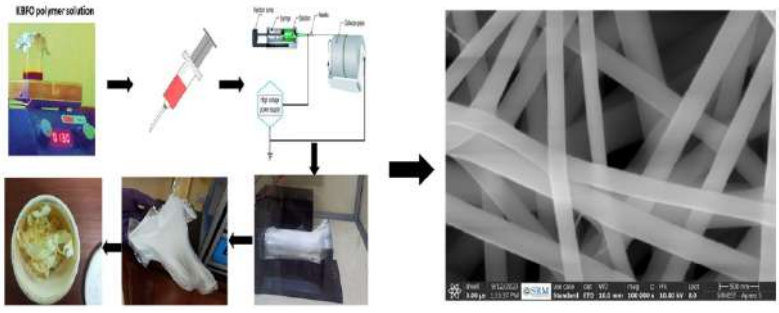
ABSTRACT

The multifunctional $KBiFe_2O_5$ (KBFO) is an oxygen deficient perovskite belonging to brownmillerite family. In this work, KBFO fibres have been synthesized using sol-gel combined electrospinning method for supercapacitor applications. The pure phase of KBFO was obtained after calcinating the electrospun fibres at 650 ℃ for 60 minutes. The phase formation, crystallinity, band gap, composition, and morphology of KBFO was obtained using XRD, FT-Raman, UV-Vis and HRSEM. The XRD pattern confirmed the monoclinic structure of KBFO and the absence of impurity phases. The crystalllite size was found to be 42nm. The optical band gap was calculated to be 2.3 eV. The morphology of the obtained KBFO fibres had diameters between 200 to 700 nm. The electrochemical properties of KBFO were analysed using cyclic voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) in acidic media. The CV results exhibited the pseudocapacitive nature of KBFO fibres. These investigations support the feasibility of exploration of KBFO fibers for advanced energy storage applications.

Keywords: KBFO, brownmillerite, electrochemical

Graphical abstract



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F 078

Evaluation of Nitrogen Doped Fluorescent Carbon Dots from Bamboo Stems for Sensing Applications

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ABSTRACT

Carbon dots have shown great potential for various chemical and biomolecule sensing due toes its diverse composition and surface properties. These properties can easily be tuned based on raw materials used and its synthesis conditions. Doping of carbon dots have recently been used to modify its composition and to improve its fluorescent quantum yield. Nitrogen-doped carbon dots (NCDs) were synthesised from bamboo stems using simple hydrothermal method, where bamboo and citric acid were used as carbon source and ethylenediamine was used as nitrogen source. The as-synthesized carbon dots were characterized to study it optical, structural and morphological properties. Under 365 nm UV light, the NCDs displayed strong blue fluorescent emission with a quantum yield of 50.89% which is much higher when compared to bamboo derived carbon dots with a quantum yield of 3.46%. The NCDs not only demonstrated high water solubility but also great stability. The surface functional groups were studied by FTIR spectroscopy which many consists of hydroxyl and carboxyl groups. Zeta potential of the carbon dots was found to be -36mV. Further its composition and size were analysed using XPS and HRTEM imaging. These primary studies indicate that the nitrogen doped carbon dots can be used for sensing applications.

Keywords: Nitrogen-doped carbon dots, fluorescence, sensing

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F 079

Ameliorating Oxygen Evolution Reaction Over $La_{1-x}Sr_xCo_{1-y}Ni_yO_3$

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ABSTRACT

Perovskite oxides (ABO_3) with rare-earth cations in the A-site and first-row transition-metal cations in the B-site have emerged as a potential catalytic material to overcome the sluggish kinetics of oxygen evolution reaction. In this study we have synthesized $La_{1-x}Sr_xCo_{1-y}Ni_yO_3$ by solution combustion synthesis method and thoroughly explored the structural, surface and electronic properties of the synthesized materials. The optimal aliovalent doping of Sr in La sites and Ni in Co sites have significantly improved the kinetics and efficacy of oxygen evolution reaction in $La_{1-x}Sr_xCo_{1-y}Ni_yO_3$. The detailed introspection of mechanistic studies indicated the importance of high covalency and surface oxygen vacancy tailored by aliovalent doping to ameliorate the catalytic oxygen evolution reaction in $La_{1-x}Sr_xCo_{1-y}Ni_yO_3$. The particular work serves as a bellwether to correlate the electronic and surface descriptors to probe the mechanistic aspect of oxygen evolution reaction over perovskite materials.

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F 080

Influence of Fuel on Phase formation of Ni^{2+} ions on $CoFe_2O_4$ ($CoFe_{2-x}Ni_xO_4$) Nanoparticles by Mild Solution Combustion Technique for Photocatalytic Applications

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ABSTRACT

Nanostructured spinel ferrites have been widely used in environmental degradation of organic pollutants such as dyes involved in the textile and food processing industries. Ni doped Cobalt ferrite nanoparticles were prepared by self-propagating solution combustion technique. The prepared Ni-Co ferrite nanoparticles have the chemical formula $CoFe_{2-x}Ni_xO_4$ (where x = 0.2, 0.4 and 0.6). Pristine $CoFe_2O_4$ and Ni substituted $CoFe_2O_4$ ($CoFe_{2-x}Ni_xO_4$) were synthesized using glycine as a fuel with precursors in the required molar ratios. X-ray diffraction data indicates the formation of pure phase cubic spinel structure with space group of $Fd\bar{3}m$and it has been confirmed with the JCPDS data (# 01 – 076 – 2496). The Raman spectrogram confirms the formation of metal-oxide formation (M-O) using tetrahedral and octahedral confirmation. FE-SEM analysis revealed the surface morphology of Nickel substituted cobalt ferrite nanoparticles. VSM confirms the magnetic behavior with reference to the coercivity, retentivity and saturation magnetization. The photocatalytic degradation kinetics and mechanisms were analyzed. X-Ray diffraction reveals that lattice parameter is decreasing with increasing concentration of Nickel ions in the lattice. This is attributed due to the smaller ionic radius nickel ions replacing cobalt ions. Raman spectrum confirms the existence Ni^{2+} ions in the octahedral sites and replaces the Fe^{3+} ions to tetrahedral sites. It shows the good removal efficiency against the methylene blue dye under UV light for a short duration and very stable for photocatalytic applications.

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F 081

Enhanced effects of Ni-doped CeO_2 Nanoparticles on Dye Degradation and Anti-Fungal Properties Via Green Synthesis Method

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ABSTRACT

Technology in the twenty-first century necessitates the downsizing of high-performance gadgets into nanometre (109 m) sizes. Nanotechnology is defined as the design, manufacturing, and application of nanostructured materials. Cerium's most stable oxide is known as ceria (CeO_2), cerium dioxide, or ceric oxide. Ceria has an extensive record in materials science. This study aimed to prepare Ni-CeO_2 nanoparticles (NPs) utilizing Pedalium Murex. L leaf extract as a surfactant in a cost-efficient way. The sol-gel technique was used to synthesize both CeO_2 and Ni-doped CeO_2 NPs in a bio-synthesis method. XRD, FTIR, UV-DRS PL, and TGA were applied to characterize the nanoparticles. XRD pattern showed a face-centered cubic fluorite-type structure for both CeO_2 and Ni-doped CeO_2 samples. It also revealed a peak shift towards the lower 2θ angle for Ni-doped samples. FTIR shows a characteristic absorption peak band at 949 cm^{-1} for Ce-O. The absorption peaks of Ni-CeO_2 NPs originated from 200-800 nm from UVDRS, in which the band gap is calculated. The photo-catalytic dye degradation was performed under methylene blue and was kept under UV- light and Sunlight. Using the agar well-diffusion method, the antifungal activity was assessed against the fungus *candida albicans Aspergillus niger* for Ni-CeO_2 NPs.

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F 082

Hydrothermal synthesis of $CuMnS_2$ Nanoflakes as an Effective Electrocatalyst for Oxygen Evolution Reaction in Alkaline Medium

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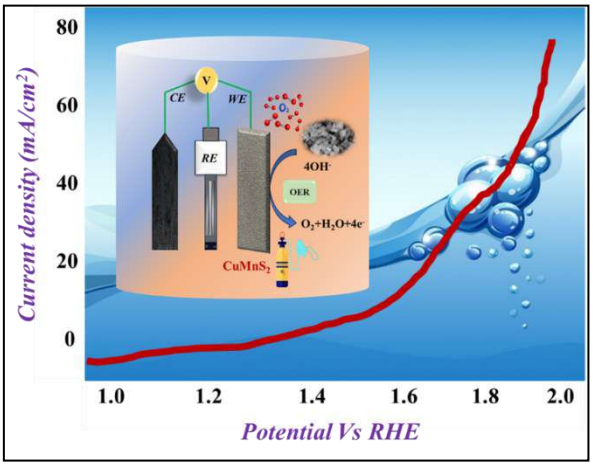
ABSTRACT

The ongoing use of outdated fossil fuels has posed significant challenges that threaten society's ecological health; although a deal is currently attained on the future growth of green energy technologies, huge-scale applicants still need to be expanded because of the intermittent nature of this sort of energy. The water-splitting process, which potentially overcomes this obstacle through the conversion of renewable energies to the chemical energy form, is currently attracting interest. Although this technique, involves two half reactions of hydrogen evolution (HER) and oxygen evolution reaction (OER), though OER is more complex compared to HER owing to delayed kinetics and low efficiency issues. The utilization of expensive metal-based materials was advanced as the competent electrocatalyst for OER; thereby, the creation of affordable and high activity catalysts is vital and crucial. Under these scenarios, the transition metal sulfides (TMSs) have been deemed to be viable OER electrocatalysts owing to their tremendous inherent activity, superior electrical conductivity and outstanding durability. Herein, $CuMnS_2$ nanoflakes were synthesized via a hydrothermal method to construct a novel electrode for OER. Phase purity, composition and morphological features of the samples were analyzed with the help of XRD, FTIR, XPS, SEM and TEM. In an alkaline medium, $CuMnS_2$ only needs 315 mV to get 10 mA/cm^2 current density and achieves a Tafel slope value of 404 mV/dec. According to our findings, $CuMnS_2$ produced hydrothermally may effectively increase OER activity, enabling alkaline water splitting.



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F 083

Effective Promotion of Oxygen Reduction Reaction Activity by 'Co' doping in $PrMnO_3$ at B-site

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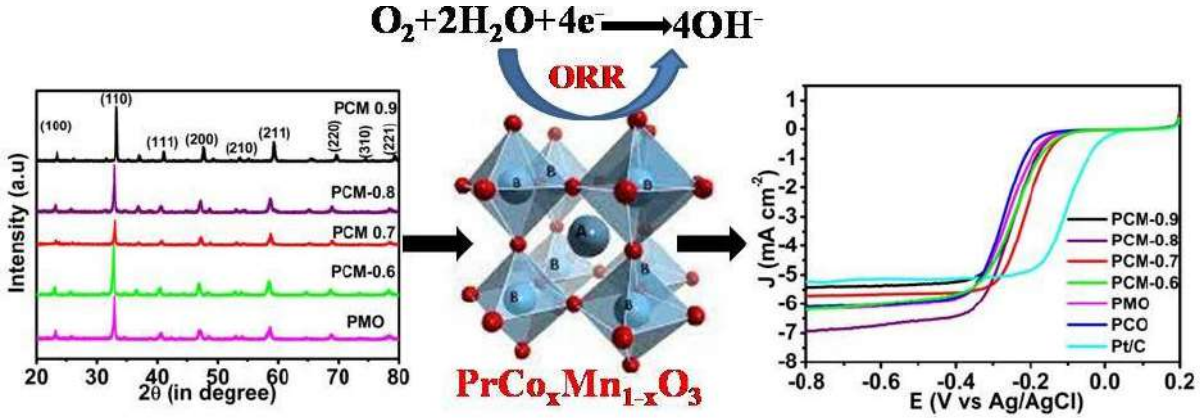
ABSTRACT

$PrMnO_3$-based materials are promising oxygen reduction reaction (ORR) electrocatalysts with high activity and stability. The cation of the Mn site in $PrMnO_3$ is changed to "Co" in this study, and sol-gel samples of the composition $PrCo_xMn_{1-x}O_3$ (x = 0.1, 0.2, 0.3, and 0.4) are produced with the indications PCM-0.9, PCM-0.8, PCM-0.7, and PCM-0.6. XRD, SEM and TEM are used to investigate the structural characteristics and morphology of the as-prepared catalysts. The synthesized catalysts' oxygen reduction reaction (ORR) activity in alkaline medium are reported. The most active ORR is found to be PCM-0.7, with onset and half wave potentials of -0.07 V and -0.21 V Vs Ag/AgCl and a limiting current density of -5.69 mA/cm^2 among the produced catalysts. Furthermore, the PCM-0.7 catalyst's lower tafel slope validates its increased catalytic activity. The electrocatalytic test findings demonstrate that the electrocatalytic activities of the samples depend on the Co concentration, with PCM-0.7 exhibiting the greatest ORR performance and stability at the same time. The results of X-ray photoelectron spectroscopy demonstrate that the addition of Co may greatly boost the amount of highly active Mn^{4+} and Co^{3+}. This result, as well as the enhanced electrical conductivity demonstrated by charge transfer resistance data, can explain why the oxygen catalytic activities were optimized.



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F 084

One Pot Colloidal Synthesis of Highly Emitting InP/ZnSe/ZnS Core Shell Quantum Dots and Formation of Self Assembled Flower Like Nanostructure

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ABSTRACT

For the past two decades, indium phosphide (InP) colloidal quantum dots (QDs) have drawn a lot of interest as a potential non-toxic substitute for cadmium-based QDs. However, in spite of several studies focused on improvement of optical and structural properties, yellow emitting InP based QDs are not much explored. In this study one pot synthesis of highly emitting, nearly monodispersed, non-toxic, highly stable colloidal InP/ZnSe/ZnS core shell QDs are reported. Further, as fabricated nanostructures and their self-assembled flower like highly crystalline 3D nanostructures are reported and investigated. Limited Ligand Protection (LLP) growth [1-3] plays the key role for evolution of nanoflower morphology. The synthesized large sized QDs exhibit bright yellow emission (570 nm) with very high photoluminescence Quantum Yield (PLQY) of 87 % which is the highest reported to date in yellow emitting InP based QDs [4-5]. The reason behind this high PLQY and self-assembled flower like morphology has been investigated in detail. The heavy metal free highly emitting InP based QD's size and composition tunability and their ability of forming superstructures may be highly beneficial for development of new solution-processable building blocks for QD based superstructures with superior and well controlled physical, optical and chemical properties.

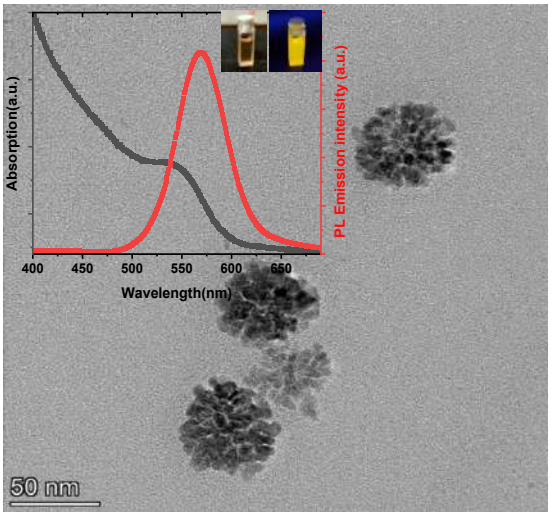

Fig 1: TEM image of synthesized InP/ZnSe/ZnS QDs and their emission, absorption spectra, photo under day light and UV light in inset.

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F 085

Impedance Spectroscopy and Electrical Conductivity Studies of Zinc Oxide Nanoparticle Reinforced Silicone Elastomer Nanocomposites.

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ABSTRACT

Silicone elastomer (SiR) nanocomposites have been prepared using different concentrations (1, 3, 5 and 7 wt%) of Zinc Oxide (ZnO) nanoparticles through mechanical mixing and compression moulding. Dielectric relaxation behavior of silicone elastomer nanocomposite samples has been studied as a function of ZnO nanoparticles concentration in a wide frequency range (10^{-1} –10^{6} Hz). The effect of ZnO nanoparticles concentration on the real and imaginary parts of impedance is distinctly visible. The significant changes in the impedance spectra have been explained on the basis of interfacial polarization in a heterogeneous medium and relaxation dynamics of polymer chains. The capacitance of the nanocomposites is expressed in terms of dielectric permittivity and explained on the basis of polarization of the ZnO nanoparticles in the silicone matrix. The effects of ZnO concentration on dielectric loss and electrical conductivity have also been studied. The dielectric behavior of the nanocomposites strongly depends up on the extent of ZnO nanoparticle concentration. The scanning electron photomicrographs (SEM) shows agglomeration of the ZnO nanoparticles above 5 wt% concentrations and formation of a continuous network structure. The same has also been observed through dielectric and electrical conductivity studies. Hence percolation threshold of ZnO nanoparticle in SiR nanocomposites has been confirmed at 5 wt% concentration.

Keywords: Silicone elastomer, Zinc Oxide, Nanocomposite, Impedance, Dielectric, Electrical Conductivity, Percolation.

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F 086

Comparative study of Polypyrrole/$CoFe_{1.9}RE_{0.1}O_4$ (RE = Sm^{3+}, Gd^{3+}, Yb^{3+}) Nanocomposites for Electromagnetic Interference shielding

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ABSTRACT

The work investigates the change in behavior of pure cobalt ferrite on doping it with rare earth (RE) metal ions such as Sm^{3+}, Gd^{3+}, and Yb^{3+} and further their nanocomposites with polypyrrole (PPy). These multiphasic organic-inorganic materials are applicable in high-frequency devices used for EMI shielding and stealth technology. The injection of larger ionic radii rare earth ions into the cobalt ferrite lattice changes the nature of interactions from Fe - Fe to RE - Fe which has changed the properties of the ferrites which acted as magnetic fillers in polymer matrix. The nanocomposites possess both the conductive and magnetic nature required to interact with electromagnetic radiation. Ferrites were synthesized by chemical coprecipitation method and corresponding nanocomposites were prepared by in situ chemical oxidative polymerization. XRD patterns confirmed the nanomaterial synthesis showing peaks of both amorphous (PPy) and crystalline (ferrites) phases. FTIR spectra in the 4000 – 400 cm^{-1} range have supported the material formation. The morphology of the prepared samples was examined. The room temperature magnetic properties were studied by VSM. The non-magnetic nature of the polymer was transformed into ferromagnetic after the incorporation of ferrites which made them suitable for EMI shielding.

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F 087

Trichromatic Branched Nanoribbons with Quantum Dots for White Light Source

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ABSTRACT

Hybridizing mono-color (like yellow), bi-color (like green/yellow and red), and multi-color (like cyan, green, yellow, & red) CdSe-based quantum dots (QDs) on blue-emitting LEDs is currently the commercial process for creating QD-white light emitting diodes (QD-WLEDs). However, the combination of two or more group of QDs typically introduces various decay rates among the differing emission wavelengths, which causes the device performance to deteriorate over time. In this regard, a lot of work has been done on developing synthesis procedures replacing the hybridization method, for example by onion like CdSe/ZnS/CdSe [1], $Zn_xCd_{1-x}Se$/ZnS/$Zn_yCd_{1-y}Se$/ZnS [2] and ZnSe/CdSe/CdS/CdSe/CdS/ZnS [3] heterostructures. Also, direct synthesis of stable bimodal QDs has also been carried out [4]. However, the visible spectral coverage of the presented onion-like and bimodal QD systems to date was still insufficient to generate white emission due to a substantial spectral deficiency [1-4]. Here, we report the synthesis of branched nanoribbon trichromatic CdZnSe/ZnS-CdSe-CdS based nanomaterials. The emission from these nanomaterials covers the whole visible spectra ranging from 495 nm to 656 nm. CdZnSe/ZnS QDs were first fabricated, which covers emission from red to deep red region (620 nm - 656 nm) of visible spectrum. Further, CdSe nanoribbons having emission in green to orange region (530 nm-600 nm) have been grown on CdZnSe/ZnS QDs followed by a growth of CdS non-emitting branches, and a second branch of CdSe nanoribbons having emission in blue to green region (495 nm - 530 nm). Also, a facile one-pot synthesis of trimodal QDs having three distinguished emission peaks has been developed. Further, their photophysics and formation mechanisms have been studied. Such nanostructures after further optimization can be a good replacement for complex white light emitting RBG QD mixture systems.

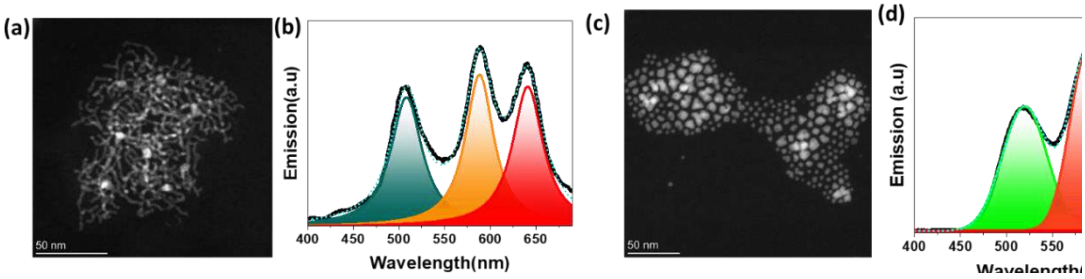

Fig: (a)STEM image of branched nanoribbon grown over QDs & its emission(b); (c)STEM image of one pot synthesized trimodal QDs & its emission

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F 088

Synthesis, Structural Analysis and Characterization of Tin Sulfide Nanoparticle

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ABSTRACT

We report a simple method for synthesizing monodispersed, crystalline and size-tunable tin sulfide nanoparticles for use in environmentally friendly next generation solar cell. Recently, tin sulphide (SnS) nanoparticles have drawn a lot of attention because of their special qualities. Due to its inexpensive cost, non-toxicity, and good natural abundance, it is starting to be considered for use in future multipurpose devices, especially those involving light conversion. In the present work, Synthesis, structural analysis and characterization of tin sulfide nanoparticles has been studied with the help of XRD analysis and Raman spectroscopy. The synthesized sample is verified as Tin Sulfide nanomaterials with the help of the given value of JCPDS card number (83-1758). The XRD spectra revealed hexagonal and orthorhombic phases of tin sulfide nanoparticles. The average crystalline sizes of the sample were found 1.9147 nm, which shows good agreement with the available result (9). Along with a few faint intensity modes, the Raman modes for SnS nanoparticles are seen at 315.11 cm^{-1}, 808.353 cm^{-1}, 1244.866 cm^{-1}, and 2325.83 cm^{-1}. Phonon confinement was observed to cause the Raman modes of SnS nanoparticles to shift towards the lower wavenumber side.

Keywords: Tin Sulfide nanoparticles; Synthesis, Characterization

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F 089

Improved Optical Thermometry through Non-Thermally Coupled Levels in $GdPO_4:Tm^{3+}/Yb^{3+}$ Phosphor Via Codoping of Li^+ ions

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ABSTRACT

The solid state reaction technique was used to produce the $GdPO_4$ phosphor codoped with Tm^{3+}/Yb^{3+} and $Tm^{3+}/Yb^{3+}/Li^+$ ions. The X-ray diffraction analysis validates the pure monoclinic phase, and the field emission scanning electron microscope reveals micro-sized particles resulted from high temperature synthesis. Excitation with a 980 nm laser diode results in three upconversion emission bands with centre wavelengths of 478, 648, and 692 nm. These bands originate from the $^1G_4 \rightarrow {}^3H_6$, $^1G_4 \rightarrow {}^3F_4$, and $^3F_3 \rightarrow {}^3H_6$ transitions of the Tm^{3+} ion, respectively. Li^+ ion codoping modifies the local crystal environment surrounding the dopant ions, resulting in the enhancement of the observed emission bands. The applicability of synthesized phosphors in optical thermometry employing non-thermally coupled levels was investigated using the fluorescence intensity ratio approach. Thermal stability, color coordinate studies, and anti-counterfeiting applications were also explored.

Keywords: Upconversion, optical temperature sensing, anti-counterfeiting, thermal stability.

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F 090

A Facile Single-Step Synthesis of Boron Nitride Nanoparticles and Its Applications in Label-free Optical Biosensing Using Surface Plasmon Resonance Ellipsometry

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ABSTRACT

We present a label-free, real-time, rapid, non-invasive optical biosensing platform with enhanced sensitivity and higher precision using the Surface Plasmon Resonance (SPR)-enhanced Ellipsometry (SPRE) technique. It has the advantage over SPR by providing amplitude (Ψ) along with sensitive phase (Δ) information [1]. Due to unique physiochemical properties, which include their large surface area, nontoxicity, higher band-gap, higher optical absorption, and prevention of oxidation in aqueous media, boron nitride nanoparticles (BN NPs) have recently attracted much attention in the medical and biological domains [2]. The sensor chip was prepared by modifying a bimetallic Ag/Au thin film with chemically synthesized BN NPs. The FESEM of the coated sample and PL spectra of synthesized BN NPs are illustrated in fig.1a. The bulk sensitivity was obtained around 2006°/RIU (R^2 0.97) for the bilayer Ag/Au (45/5nm) sensor chip by varying concentrations of ethanol-water solution (0-28%). The standard Bovine Serum Albumin (BSA) protein adsorption experiment was performed using our in-house-built SPRE setup to compare the sensitivity for bare and BN-coated samples. The coated sample shows higher sensitivity, as shown in Fig (b,c).

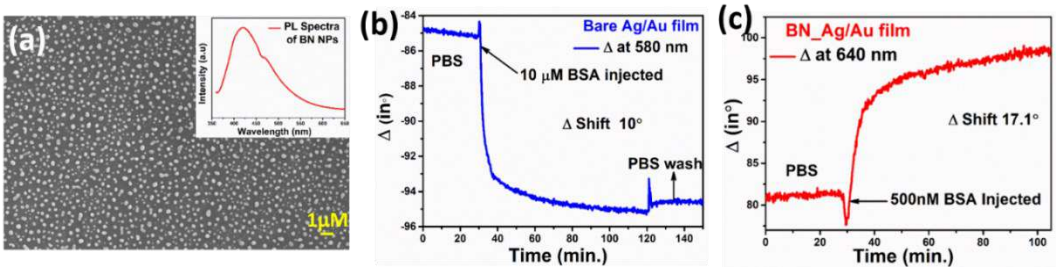

Fig.1.(a) FESEM of BN nanoparticles coated sample, inset shows the Photoluminescence (PL) spectra of BNNs. (b,c) Real-time Δ response for bare and coated samples while introducing 10µM and 500nM BSA.

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F 091

Development of a Paper Analytical Device for the Fluorescent Detection of Copper Ions

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ABSTRACT

Copper is an essential metal ion in the human body, playing a vital role in the biological process. Elevated copper levels in body fluids lead to an increased risk of cardiovascular diseases, gastrointestinal problems, liver damage, and Wilson's disease which affects the neurological systems. A paper analytical device (PAD) was developed for the fluorescence detection of copper ions in human serum samples. An amino-functionalized N and S co-doped carbon dot was synthesized using a hydrothermal method. The synthesized carbon dot showed a bright blue fluorescence with the maximum emission at the excitation wavelength of 340 nm. Interference studies revealed that there was negligible interference from the other ions tested. The developed PAD is a promising affordable tool for detecting copper ions.

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F 092

Development of Graphene oxide/Polyvinyl alcohol (PVA) based Temperature Sensor for battery housing application

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ABSTRACT

Temperature monitoring plays a critical role in battery management, particularly in battery housing applications. It plays a crucial role in ensuring the safety, performance, and longevity of battery systems by enabling real-time temperature measurement, prediction, and management. The integration of flexible temperature sensors in such as applications can lead to a versatile and customizable solution for temperature monitoring with advantages in terms of flexibility, low cost, and better sensing performance. This paper presents a development of graphene oxide/PVA based nanocomposite temperature sensors. The graphene oxide has been synthesized by oxidizing and exfoliating micronized natural graphite in the presence of traditional reagents (H_2SO_4, $KMnO_4$, and H_2O_2) at a relatively low temperature during exfoliation and graphene oxide preparation (H_2O addition). The nanocomposite based on graphene oxide/PVA sensors were synthesized using a solution mixing approach, and a drop casting technique was used to fabricate the temperature sensors, resulting in the dimension and thickness of the sensor being 1 cm × 1 cm and 80 -90 µm, respectively. The sensors show better linearity and temperature coefficient of resistance (TCR) greater than 1.07 %/°C with a hysteresis effect corresponding to an energy loss of less than 3\%. In order to ensure the reproducibility and repeatability of the developed sensors, ten sensors were fabricated with the same processing conditions and subjected to repeated temperature measurements over 50 cycles. Sensors show a small variation in TCR value of 0.016 %/°C among ten sensors for 50 cycles of repeated temperature measurements from 20 to 90 °C.

F 093

Alkyl Chain Functionalized *h*-BN-MoS_2 Heterostructure as a Highly Dispersible Additive for Lubrication Application

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ABSTRACT

In machineries, high friction and wear are accountable for energy and material loss, leading to the failure of machinery parts, high fuel/energy consumption, and environmental pollution. The minimization of friction and wear is crucial for enhancing service life, and operational efficiency of the mechanical system and reducing environmental pollution. Two-dimensional layered nanomaterials such as hexagonal boron nitride (*h*-BN) and molybdenum disulfide (MoS_2), show immense potential for lubrication because of their lamellar structure and high mechanical strength. The weak Van der Waals interaction between lamellae facilitate sliding along the basal plane and furnish low interfacial friction. However, the poor dispersion stability of these 2D nanomaterials in liquid lubricants has been a major challenge for lubrication applications. Various approaches have been made to improve the dispersion stability of 2D materials in liquid lubricants. The combination of two different nanomaterials is gaining large interest as an additive because of incommensurate contact in all sliding directions owing to their crystal lattice mismatch and reducing the friction significantly [1-3]. Herein, the *h*-BN-MoS_2 heterostructure was synthesized by hydrothermal method using cetyltrimethylammonium bromide (CTAB) as a surfactant. The CTAB was used as a dispersant to prevent the restacking of the *h*-BN-MoS_2 heterostructure and facilitate the long-term dispersion stability in lubricating oil. The lubrication performance of *h*-BN-MoS_2 nanosheets was evaluated using their dispersions in engine oil for steel tribopair.

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F 094

Tuning the surface oxygen vacancies of Bi_2O_3 varying the reaction parameters with rGO by building block designed and its effect on photocatalytic activity and morphology

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ABSTRACT

A novel graphene oxide intercalated with oxygen vacant Bi_2O_3 as pillars and photocatalysts, was fabricated through a mixed-dimensional assembly strategy. In this study, various calcine temperatures were used to create a variety of Bi_2O_3 and designed a building block photocatalysts with rGO. There aren't many reports, though, on how calcine temperature affects Bi_2O_3 photocatalyst morphology. series of Bi_2O_3 photocatalysts were prepared at different Calcine temperature (250, 300, 400, 500, and 550˚C). The structural, morphological and optical, properties of as-synthesized materials were characterized by various characterization techniques. Photocatalytic activity of the as-prepared The Bi_2O_3/rGO nanosheets composite was examined using Norfloxacin and Ciprofloxacin mixed (Nor+CIP) aqueous antibiotics experimental solutions under UV–visible light irradiation for 60 min under visible irradiation. Photocatalytic regeneration, and pollutant degradation by ·OH and $\cdot O_2^-$ radicals are proposed as effective cooperation mechanisms.

Keywords: Calcine temperature, morphology study, photocatalytic activity, antibiotics.

F 095

Synthesis and characterization of perovskites ($CaTiO_3$) for environmental applications

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ABSTRACT

Among the materials most developed today are ceramics based on mixed oxides, specifically perovskites.[1] They are families of compounds with a crystalline structure of the general formula ABO_3.[2.] It is the most versatile ceramic host. They can accommodate most of the elements of the periodic system and exhibit a wide variety of properties,[3] which is why they have gained enormous attention in recent years from the scientific community for their potential application in the environmental area. In this research, we synthesized calcium titanate ($CaTiO_3$) using the solid-state method. The particles were characterized by several physicochemical techniques: X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and diffuse reflectance spectroscopy (DRS). It was found through XRD and Raman that the crystal structure is orthorhombic with the *Pbnm* space group. The synthesized $CaTiO_3$ particles have an average diameter of ≈ 2 µm. Furthermore, the value obtained for the energy gap (E_g) was 3.41 eV; it also presents a low energy step at a value of 2.66 eV, which may correspond to the gap electronic states. Therefore, developing $CaTiO_3$ particles is a viable alternative for energy storage, with potential uses in applications for air, soil, or other areas of interest.

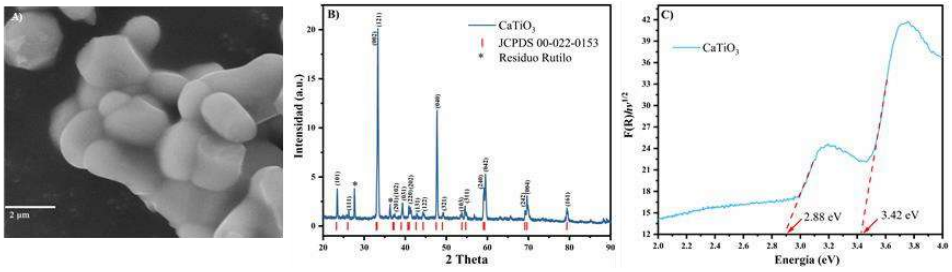

Figure 1. $CaTiO_3$ particles synthesized with an orthorhombic system: A) micrograph, B) diffractogram, and C) spectrum $[F(R)]hv^{1/2}$].

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F 096

Catalytic Potential of Copper Ferrite Nanoparticles and Its Synthesis

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ABSTRACT

.In this study, we present a method for the synthesis of copper ferrite nanoparticles by Co-precipitation technique. Copper ferrite, a promising material for various applications, was successfully prepared by Co-precipitation using copper and iron precursors. The reaction parameters including pH, temperature, reaction time were systematically optimized to obtain well defined nanoparticles with controlled size and morphology. The synthesized copper ferrite nanoparticles were characterized using techniques such as XRD and UV-Visible Spectroscopy to confirm crystal structure. The result indicates the formation of cubic phase copper ferrite nanoparticles. Various applications of Copper ferrite nanoparticles as catalysts in different organic processes like reactions of dehydrogenation, alkylation, oxidation are reviewed. So, we can say it provides valuable insights into the synthesis of copper ferrite nanoparticles by coprecipitation, paving the way for their widespread applications as catalyst and many more.

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F 097

Tuberculosis Sensor based on 1D Topological Photonic Crystal Mirror Heterostructures

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ABSTRACT

In this paper, we present a biosensor based on the photobiological characteristics of one-dimensional (1D) topological photonic crystals. Two photonic crystal structures (Phc1 and Phc2) made of dielectric layers Si and SiO_2 have been combined to create a topological structure. These two, Phc1 and Phc2, differ in terms of the thickness of these dielectric materials. When the 1D-topological PhC-mirror heterostructure and its mirror-image structures are stacked together, the sensor becomes more efficient for analyte detection. Tuberculosis can be detected by introducing the sensing layer into the 1D topological photonic crystal mirror heterostructure photonic crystals. The sensing process is based on the refractive indexes of the analytes in the sensor layer. Photonic media witness notable blue shifts due to the analytes' variations in refractive index. The transfer matrix approach is used to compute the numerical results of the sensor. Effective results are achieved by optimizing the thicknesses of the sensor layer and dielectric layers. In normal incident light, the proposed sensors have a high sensitivity of 1125nm/RIU with a very low detection limit and high-quality factor.

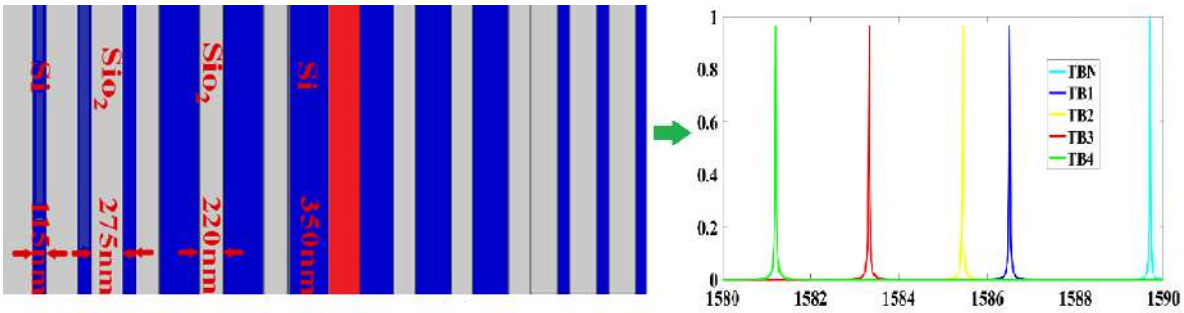

Figure: Schematic and Transmission spectra of proposed Tuberculosis sensor

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F 098

Synthesis and characterization of titanite using the ball milling technique

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ABSTRACT

Titanite is a common constituent of several mineral rocks and ceramics with excellent mechanical and thermal stability properties.[1] Titanite has been used as nuclear waste disposal, luminescent materials, and pigments because of its ability to incorporate many elements into its crystal lattice.[2,3] The literature has reported titanite synthesis by various methods such as sol-gel, combustion, and hydrothermal.[4] In this research, the synthesis of titanite was carried out by the ceramic route. The synthesized titanite was subjected to grinding using a ball mill (BM),[5] varying the sphere size and cycle number (0.5 h) to examine the effect of crystallite size reduction. Several physicochemical techniques were used to characterize the titanite. The morphology of the material was studied by scanning electron microscopy (SEM). The elemental chemical composition was determined by energy dispersive spectroscopy (EDS). The crystalline nature was studied by X-ray diffraction (XRD) and the Rietveld refinement. The structure and identification of the crystalline phase was complemented by Raman spectroscopy. The optical properties were determined by diffuse reflectance spectroscopy (DRS). The ceramic route successfully synthesized monoclinic titanite; BM reduced its particle size, and their physicochemical characterizations were conducted, acquiring relevant results. This study gives a complete description of the effects of milling on the physicochemical properties of titanite, indicating a range of possible environmental applications.

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F 099

A novel synthesis of surfactants assisted Bi_2WO_6 nanocatalysts for boosting the photocatalytic activity of RhB dye degradation under visible light irradiation

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ABSTRACT

In this study, the surfactants-assisted Bi_2WO_6 nanostructure photocatalysts have been prepared through a simple hydrothermal route. Organic compounds like Polyvinylpyrrolidone (PVP), Cetyltrimethylammonium bromide (CTAB), Sodium dodecyl sulfate (SDS), and polyethylene glycol (PEG) are taken as Surfactants to create different structured Bi_2WO_6 catalysts. The X-ray diffraction (XRD) technique characterizes the phase purity of prepared samples. The different morphological images of the samples are analyzed by Field emission Scanning electron Microscopy (FESEM). The surface area and pore size distribution of samples are characterized by BET analysis. The band shift and bandgap energy of prepared samples are measured by UV-visible spectroscopy. The photoluminescence and photocurrent density spectra measured the rate of recombination of charge carriers. The photocatalytic activity of the prepared catalysts has been observed through the degradation of Rhodamine B. The Trapping test confirmed the $\cdot OH^-$ radicals plays a significant role in the photodecomposition of RhB. The photocatalyst exhibits excellent photostability and reusability after four consecutive tests.

Keywords: Surfactants, hydrothermal, Bi_2WO_6 photocatalyst, RhB, visible light

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F 100

Multiphase Tin oxides Nanocrystals: Enhancing alloyed material properties

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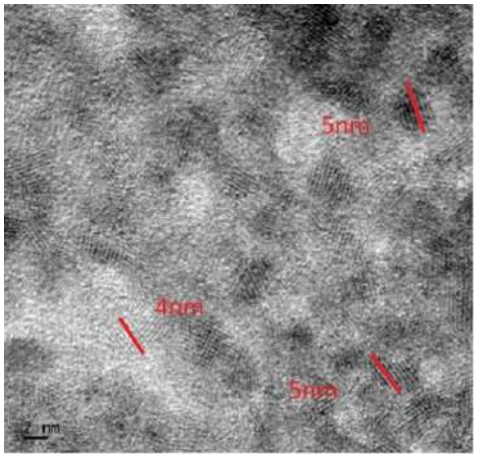
ABSTRACT

Recent research studies have highlighted the significance of incorporating multiphase alloyed materials to enhance the optical properties for photovoltaic applications. In this particular study, innovative tinoxide nanocrystals with multiple phases were successfully synthesized using precipitation techniques. An X-ray diffraction(XRD) analysis of the material revealed the presence of the multiphase composition of finding intermediate oxides, including SnO, SnO_2 and Sn_3O_4 a finding consistent with earlier work by Batzil et.al.[1]. Further examination of these nanocrystals through Transmission Electron Microscopy (TEM) indicated a crystalline size of approximately 5nm. Subsequent UV-Vis absorbance characterization displayed a single absorbance peak at around 271nm. This data was used to construct a Tauc plot, revealing a band gap of 3.38eV, suggesting the prevalence of SnO_2 crystals within the multiphase structure which is thermodynamically stable than other intermediate oxides. Photoluminescence analysis showed that when excited at 368nm the multiphase tin oxide had emission 431 nm and 735nm. Notably, the 735nm emission peak, which had not been reported, may be attributed to some unique metastable characteristic of multiphase material. Similar outcomes were observed in earlier reports on double phased stannous and stannic oxide. Additionally, the chromaticity coordinates were determined using absorbance results, showing a blue emission, with values of (0.27,0.27)



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F 101

Phytochemical Profiling and GC-MS Analysis of Bioactive Compounds and Biosynthesis of Silver Nanoparticles using *Annona Muricata* Bark and its Antioxidant and Antistress Activities

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ABSTRACT

Screening of phytochemicals is a precious stair in the detection of bioactive principles present in particular medicinal plant and may lead to novel drug discovery. In present study aimed to investigate the preliminary phytochemical screening, fluorescence, spectroscopic characterization, and GC MS analysis in the bark of *Annona muricata*. The qualitative analysis of different extracts like aqueous, hexane, ethanol, hydro-ethanolic and methanol extracts of *Annona muricata* bark were investigated. Among the various extracts, the hydro-ethanolic extract of *Annona muricata* bark contains a higher concentration of phytochemicals than other extracts and is used for subsequent studies. Quantitative analysis revealed that the *Annona muricata* bark has contain significant amount of phenol, flavonoids, saponin, tannin and alkaloids were present. Histochemical analysis further confirmed the presence of phytochemicals in *Annona muricata* bark. UV-VIS spectral analysis had confirmed that the presence of tannins and flavonoids. FTIR analysis had confirmed the presence of alcohol, phenol, aromatic, carboxylic acid and aliphatic amines. Twenty-five phytocompounds were identified in the hydro-alcoholic extract of *Annona muricata* bark by GC-MS analysis. The prevailing compounds are Allene, Trans.beta.ionon5,6epoxide, Propanedioic acid, Hexadecenoic acid and 9,12-Octadecadienoic acid. Results of the study concluded that rich source of phytochemicals in *Annona muricata* bark is responsible for their therapeutic effects. Here demonstrated that the bark of *Annona muricata* is capable of production, AgNPs extracellularly by rapid reduction of silver ions. By characterization studies confirmed that the appearance of functional group, size, and peaks of the compounds in the extract and shows the responsibility for the reduction, capping, and stabilization of the newly formed nanoparticles. Among the tested samples synthesized silver nanoparticles of *Annona muricata* has significant Antioxidant and Antistress activity than the hydroethanolic extract of bark of *Annona muricata*.

Keywords: *Annona muricata* bark, Phytochemicals, Histochemical, Fluorescence, UV visible spectrum, FTIR, GC-MS, Silver Nanoparticles, Antioxidant, Antistress.

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F 102

Synthesis and Characterization of TiO_2 nanoparticles and Their enhanced Photocatalytic activity

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ABSTRACT

The pure anatase phase of TiO_2 nanoparticles was prepared by simple sol-gel(SG) method and annealed at 400°C. Titanium tetra-isopropoxide was used as TiO_2 precursor. The powder was characterized by X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM and TEM), UV–vis absorption spectra and Raman spectroscopy. X-ray diffraction analyses (XRD) and Raman spectroscopy both confirm the pure anatase phase. By UV spectroscopy study, the optical band gaps were estimated. Transmission electron microscopy used to estimate the size of the prepared nanoparticles. The photocatalytic activity of prepared nanoparticles was investigated by degradation of methylene blue aqueous solution under visible light irradiation.

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F 103

Green Synthesis of Titanium Dioxide Nanoparticles for Antibacterial and Photocatalytic Activity using Justicia Adhatoda Leaf and Cissus Quadrangularis Extract

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ABSTRACT

Multidrug-resistant bacterial strains have emerged as a result of the widespread use of antibiotics, raising concerns for human health and food safety. Metal oxide nanoparticles have drawn attention as novel antibacterial materials. In particular, titanium dioxide (TiO_2), being an affordable, non-toxic, and chemically stable material, has been viewed as a desirable antibacterial component because of its photocatalytic properties. In this work, TiO_2 was synthesised using *Justicia adhatoda* and *cissus quadrangularis*. The synthesized TiO_2 nanoparticles were characterized using ultraviolet–visible spectroscopy (UV–Vis), fourier transform infrared spectroscopy (FTIR), X-ray difraction analysis (XRD), field emission scanning electron microscopy (FESEM) and energy dispersive X-ray spectroscopy (EDS) for their optical, structural, morphological and compositional analysis. Further, these synthesized TiO_2 nanoparticles were studied for their antibacterial activity against multi-drug resistant microorganisms like Staphylococcus aureus (Gram-positive) and Escherichia coli (Gram-negative). Since TiO_2 is a well-known photocatalyst, methylene blue dye has been used for the investigation of photocatalytic activity.

Key words: TiO_2 nanoparticles, Justicia adhatoda, cissus quadrangularis, Antimicrobial activity and photocatalytic activities.

F 104

Effect of Temperature on Structural, Morphological, Compositional and Electrical Conductivity Study of ZnS and ZnO Nanoparticles Prepared by Chemical Co Precipitation Method

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ABSTRACT

Zinc sulphide and zinc oxide is one of the most promising materials for solar cells and of great interest for their practical applications in up to electronics and photonics. The physical and chemical properties of zinc sulphide and zinc oxide nano particles are found to be size depended. In the present work describes preparation and characterization of zinc sulfide and zinc oxide using chemical co precipitation techniques at room temperature. The prepared Zns and ZnO powders were further treated with different temperature (200^0 C and 400^0C). The crystallite sizes (hkl) of zinc sulfide and zinc oxide nano particles were estimated from the peaks of XRD. FT IR spectral studies revels the presence of functional groups. The optical properties of the prepared ZnS and ZnO samples were estimated by UV- visible spectroscopy. Microstructural analysis using scanning electron microscope (SEM) supplemented with EDS were carried out for the sample to find grain size as well as chemical composition. AFM study shows the above prepared nano particle will have a particle size of 70 (nm). Electrical conductivity study exhibits the semiconducting property of ZnS nanoparticles. Results will be discussed in detail.

F 105

Photoelectrochemical Performance of Nanostructured $BiVO_4$/C/FeOOH Photoanode for Solar Water Splitting Application

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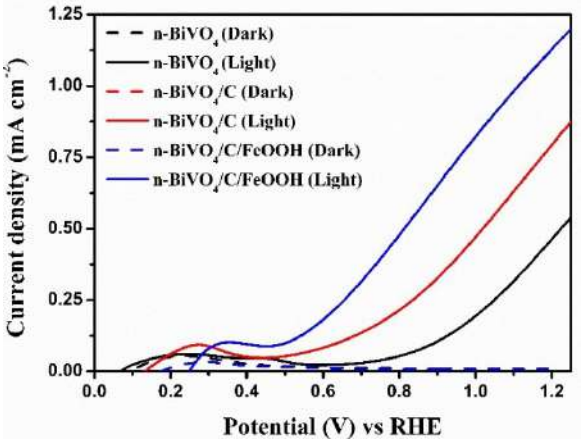
ABSTRACT

Slow water oxidation kinetics and recombination is a serious concern for the $BiVO_4$ photoanode. Nanostructure in $BiVO_4$ (n-$BiVO_4$) [1] photoanode is beneficial as it increases the surface-to-volume ratio and provide better minority charge migration [2]. The recombination can be reduced by adding thin carbon layer on top of the nanostructured n-$BiVO_4$. So, the photoanode was loaded with thin carbon layer. In order to improve the water oxidation kinetics, ultrathin FeOOH cocatalyst was loaded on the photoanode by simple impregnation method. The photoanodes were tested in 0.2 M phosphate buffer solution (pH 8). The modified photoanode n-$BiVO_4$/C/FeOOH reached a maximum current density of 1.178 mA cm^{-2} at 1.23 V vs RHE. This higher current density is because of increased surface-to-volume ratio, efficient charge transfer and reduced overpotential which was obtained by nanostructuring, addition of thin carbon layer and deposition of ultrathin FeOOH cocatalyst respectively. Finally, n-$BiVO_4$/C/FeOOH photoanode was tested for stability and photoanode was stable for the stability test of 3000 seconds.



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F 106

Synthesis of Co-doped TiO_2 nanobelts with Secondary Titania Nanoparticles for Degradation of Industrial Azo Dye

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ABSTRACT

The release of industrial wastewater from textile manufacturing plants poses a serious threat to the quality of our water resources, as it introduces hazardous pollutants into the environment. In the realm of textile industry effluents, azo dyes stand apart as a group of synthetic dyes that exhibit remarkable tenacity in aquatic environments, which are found to be very much toxic to all living organisms. Hence it is highly desired to eliminate the harmful substance by making in use of nanomaterials which can absorb the dye to have a clean and healthy environment. In this regard here we propose an efficient hierarchical growth of TiO_2 nanobelts with a secondary growth of titania nanoparticles via solvothermal and chemical bath deposition to enhance the active sites with efficient catalytic performance. Though TiO_2 being an excellent photoactive material it limits due to its wide range band gap and absorption towards UV spectrum. Therefore, here we have modified the surface and structural properties by co-doping with N and S with the intention of enhancing the visible-light photocatalytic performance by expanding the absorption in the visible-light region and improving the quantum efficiency of the photocatalytic reaction towards the degradation of hazardous dye methyl orange. The morphologies, crystal structures, surface state, microstructure, and photocatalytic activity were characterized by scanning electron microscopy, transmission electron microscopy, X-ray diffraction, Raman spectroscopy, UV−vis spectroscopy and X-ray photoelectrons spectroscopy, respectively. The surface modified doped samples exhibited excellent visible light activity and the synergistic effects of N and S was responsible for improving the photocatalytic activity.

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F 107

Effect of g-C_3N_4 Heterostructure with $ZnCr_2O_4$ for Photocatalytic Degradation of Methylene Blue

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ABSTRACT

Achieving optimal performance in solar photocatalysis demands the efficient separation of photogenerated charge carriers, coupled with their swift transportation to the semiconductor interface. The interplay between bulk and surface properties of the semiconductor substantially influences the mechanisms and kinetics of charge separation, as well as interfacial/interparticle charge transfers (CT). Emphasizing the significance of surface properties is crucial, as they play a pivotal role in driving interfacial Charge transfer and consequently, facilitating effective photocatalysis. In this manner, making heterostructure influences the charge carrier transfer. ZnCr2O4 is a spinel oxide that has a cubic crystal system and agglomerated particle morphology. In this work, the heterostructure is formed between $ZnCr_2O_4$ and g-C_3N_4. The structural and morphological characterizations of the prepared samples were examined using XRD, HRSEM and HRTEM analysis respectively. From the HRTEM analysis, it can be observed that the formation of heterostructure. This heterostructure decreases the recombination rate of the photoexcited electrons and thus increases the photocatalytic performance of the catalyst. Compared with the bare $ZnCr_2O_4$, the composite samples exhibit increased photocatalytic performance. From the scavenger analysis, it can be concluded that the electrons play a major role in the overall photocatalytic degradation.

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F 108

Formulation and *in Vitro* Evaluation of Topical Naproxen Sodium Loaded Nanosponge-Based Gel for the Treatment of Rheumatoid Arthritis

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ABSTRACT

In the present study, nine formulations (NNS1-NNS9) of Naproxen sodium loaded Nanosponges (NS) were fabricated by emulsion solvent evaporation technology, using 3^2 full factorial design. Different concentration of ethyl cellulose (EC) and polyvinyl alcohol (PVA) as a rate retarding polymer and surfactant, respectively. Prepared NS were characterized for particle size (PS), zeta potential (ZP), entrapment efficiency (EE) and drug loading (DL). It was evaluated for physicochemical characterizations; FTIR, DSC, XRD, TEM and SEM. Selected NNS3 and NNS4 composed of Naproxen sodium, EC and of PVA, PS (13 ± 0.01 nm), ZP (−4.01 ± 0.02 mV), %EE -(0.87 ± 98.12%), respectively. Fabricated NS also revealed; polymer-drug compatibility, drug-encapsulation, non-crystalline state of the drug in the spherical NS as per the physicochemical evaluations. Optimized NNS with equivalent amount of (1%, w/w or w/v) Naproxen was incorporated into the (1%, w/w or w/v) Carbopol gel. Naproxen loaded NS based gel was then evaluated for viscosity, spread ability, flux, drug diffusion, stability and skin irritation studies. NNS4 based topical gels exhibited a flux rate of 0.18 (mg/cm^2.h), drug diffusion of 91.42% in 24 hr in Franz cell diffusion following excellent drug release. The NNS3 based-gel could be effective against Rheumatoid arthritis.

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Studies on Magnetron Sputtered Flexible MoO_3 Electrochromic Electrode for Smart Window Applications

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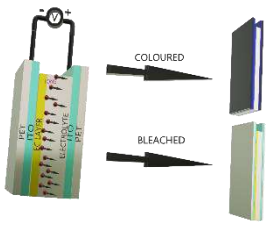
ABSTRACT

The ability to switch between different transmissive states upon application of electric potential in certain materials is termed “Electrochromism”, which has gained traction due to its application feasibility in multiple avenues as Electrochromic devices (ECD), starting from smart windows to E-displays [1]. Transition metal oxide-based flexible thin films are our study of interest, particularly intervening on the physicochemical properties of MoO_3 thin films deposited onto the ITO/PET substrates using RF reactive Magnetron sputtering for flexible smart window application [2]. The preconditioning part of the work includes opting the suitable sputtering power and duration. After scrutinising different powers and durations it has been fixed that the duration of three hours under 75 W sputtering power is a conducive parameter. The films fabricated under this condition remained unblemished on the bendability tests. The X-ray diffraction pattern is predominantly matched with the MoO_3 phase and the elemental presence is strongly supported by energy-dispersive analysis of X-rays (EDAX). The smooth surface morphology is confirmed by SEM imaging with comparatively fewer cracks obtained through the films coated in higher powers. Resistance is estimated by a simple two-probe method for the coated films. From the transmittance data, the energy band gap values of the films are determined which showed a sharp decrease with increasing power and duration of deposition. The electrochemical analysis performed on the films shows that the films can be effectively used for enhanced electrochemical applications.



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F 110

Visible light photocatalytic activity of spray pyrolyzed Ga and Al doped ZnO thin film electrodes

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ABSTRACT

Spray deposited Ga and Al doped ZnO thin film electrodes are explored for the degradation of methylene blue dye. X-ray diffraction unveils both the films to have highly textured growth along (002) plane could be attributed to the lowest surface energy density [1]. The surface morphology is found to be near spherical and near rectangular particles for Ga and Al dopants, respectively. Photoluminescence emission study reveals that both the films to have visible light emissions in the violet, blue and green regions due to oxygen vacancy defects. The deposited films exhibit a reasonably higher transmittance of 89 and 77 % with a mobility of 30.5 and 29.6 cm^2/Vs for Ga and Al doping ZnO, respectively. Based on these suitable optoelectronic properties the electrodes are explored for the degradation of methylene blue dye with significant efficiency [2].

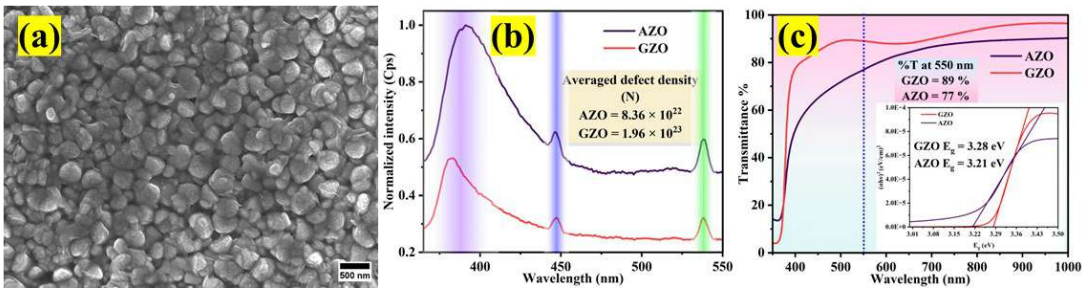

Fig. 1. (a) FESEM micrograph of Ga doped ZnO, (b) Photoluminescence emission spectra, and (c) transmittance spectra and band gap from Tauc plot (inset)

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Development and Experimental Investigation of Graphene Oxide and Silicon Carbide Nanoparticles as Lubricant Additives in Modified Waste Sunflower Oil

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ABSTRACT

The demand for alternate lubricants has increased in recent years due to the economic and environmental consequences of conventional mineral-based lubricants in the manufacturing industry. The disadvantage of mineral-based lubricants is replaced with vegetable-based lubricants but pure vegetable oils are not economically feasible. So, the use of waste cooking oil, which is considered to be a pollutant is used for green lubricant development. In this work, the waste sunflower oil (WSO) is chemically modified by esterification and then epoxidized to develop lubricant oils and experimentally investigated the tribological, rheological, and physiochemical properties. The Graphene oxide nanoparticles (GO) and Silicon Carbide (SiC) nanoparticles were dispersed with optimum concentration to the esterified epoxidized waste sunflower oil (EEWSO) as a lubricant additive. From the experimental results, it is observed that the double-stage chemical modification of WSO improves the lubricant properties. Also, the effect of GO and SiC nanoparticles shows that they can be used as anti-wear and antifriction additives in lubricants.

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Study of the Interaction of Nanotube with Anticancer-Targeted Drug Therapy for Breast Cancer by using First Principles

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ABSTRACT

Breast cancer is a major ongoing health issue that has developed over the past decades. Therefore, the current clinical chemotherapy processes are invasive, low specificity and toxicity-induced severe side effects. In this regard, sustained innovative nanoparticulate-based encapsulated targeted drug delivery approaches call for tumor targeting and accumulation of drugs in the tumor to play promising opportunities for cancer treatment. This work approaches SWCNT (10,10), the cargo, as a carrier encapsulating the drug thiotepa in treating breast cancer. Density functional theory (DFT) and *ab initio* molecular dynamics simulation have been used to optimize and stabilize the structures and their corresponding electronic structure. Our study includes the differentiation of SWCNT (10,10) with defects in the same regard. The targeted drug delivery demands the adsorption and desorption energy concept, which the paper satisfied. Further remaining work by molecular dynamics will confirm the insertion and transportation pathway with the adsorption energy as a function of the distance in terms of stability.

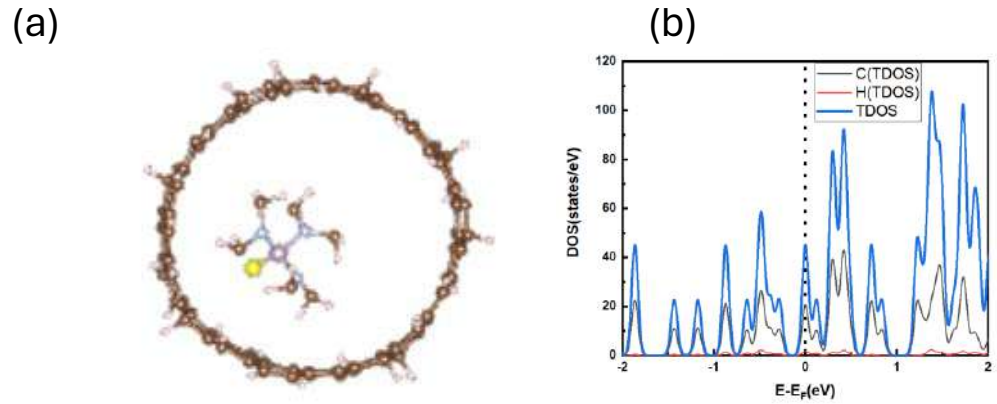

Figure (a): Encapsulated drug thiotepa inside SWCNT (10,10) (b) DOS calculation of SWCNT (10,10) with hydrogen passivation

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Ferromagnetic Properties of Zinc and Magnesium Ferrite Prepared by MOD Technique

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ABSTRACT

Zinc ferrite ($ZnFe_2O_4$: ZFO) is known for antiferromagnetic materials and Magnesium ferrite ($MgFe_2O_4$: MFO) is known for ferromagnetic materials at room temperature[1)], however, the sputtering technique or PLD technique have reported the possible preparation of ferromagnetic ZFO at room temperuture[2,3)]. The ferromagnetic ZFO or MFO are an attractive material for new magneto-optical devices because they show transparency in short wavelength region of the visible light. This property compensates the poor transparency of magnetic garnet materials in the short wavelength region. In this report, we have investigated the preparation of ferromagnetic ZFO, MFO and their mixed crystal with the metal organic decomposition (MOD) technique and have compared the detail magnetic properties depending on crystalizing conditions. The thicknesses of the prepared the films were approximately 250 nm and the spinel single phase was confirmed by the XRD analysis. The saturation magnetizations Ms of the ZFO films were depend on both the annealing temperatures and the annealing time, whereas the coercive force Hc indicated approximately 700 Oe for the all ZFO specimens. The valence of the Fe ions in ZFO was confirmed only 3+ by the Mossbauer spectroscopy. The Curie temperature was estimated to be of approximately 190 K. The hysteresis magnetic curves showed that the MFO films were ferromagnetic at room temperature. Both Ms and Hc of the films depend on the annealing temperatures and time and they have trade-off relation. The Hc of the film annealed at 510 degreeC was approximately 2 kOe and the film annealed at 900 degreeC was approximately 60 emu/g.

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F 114

Synthesis of Magnetic Polystyrene Nanoparticles Using Amphiphilic Ionic Liquid Stabilized RAFT Mediated Miniemulsion Polymerization and Application in Knoevenagel Condensation

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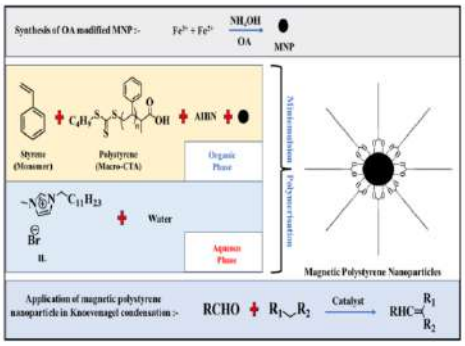
ABSTRACT

Polymer magnetic composite (PMC) nanoparticles draw significant attention due to their wide biological applications in magnetic resonance imaging, nucleic acid purification, enzyme immobilization, drug delivery, etc.[1] Miniemulsion polymerization (MEP) is one of the most effective methods to synthesize MEP. Surface modification of hydrophilic magnetic nanoparticles (MNP) (e.g., Fe_3O_4) is one of the essential requirements in this process. In this regard, oleic acid (OA) is used most frequently. In this process, the use of surfactant is very important to avoid homogeneous and micellar nucleation which could form pure polymer nanoparticles.[2] To avoid the loss of MNP during MEP due to insufficient encapsulation some interaction between MNP and polymer chain is introduced. In our present investigation, we chose a carboxyl functionalized polymer that can interact with MNP. To synthesize functional polymer RAFT polymerization method was selected. Monocarboxyl-functionalized polystyrene, synthesized by bulk RAFT polymerization, was used as a macro chain transfer agent (macro-CTA) as well as a non-volatile hydrophobe in miniemulsion polymerization of styrene for the synthesis of PMC particles. Imidazole-based amphiphilic ionic liquids (ILs) were used as surfactants in MEP due to their amazing properties like wide liquid range, excellent thermal stability, high ionic conductivity, low volatility, and ease of modification of their chemical structure. The materials have been analyzed by NMR, GPC, DLS, SEM, and TEM. The resultant PMC can be used in low temperature Knoevenagel aqueous phase reactions with high efficiency.

Keywords: Polymer magnetic composite, miniemulsion polymerization, RAFT polymerization, ionic liquids, Knoevenagel condensation.



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$BiVO_4/AgFeO_2$ Heterostructure with Antibacterial and Photocatalytic Properties

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ABSTRACT

Photocatalysis deals with the alteration of the kinetics of a chemical reaction with the aid of light. Monoclinic scheelite $BiVO_4$ has a relatively narrow band gap (approx. 2.4eV) and is a well-exploring catalyst due to its stability and less toxic nature. While forming heterostructures, photogenerated electrons and holes will separate thus reduction and oxidation will occur in separate materials in the heterostructure, which will effectively reduce the recombination. This work primarily aims to fabricate a $BiVO_4/AgFeO_2$ heterostructure with antibacterial and photocatalytic properties synthesized by hydrothermal & precipitation methods, for the effective decomposition of Cr (VI) and bacteria *Staphylococcus aureus*. $AgFeO_2$ photocatalyst has antibacterial properties, with a band gap of ~1.9eV. So, on the illumination of light, electron-hole pairs are formed, and the photogenerated electrons move from the conduction band of BiVO4 to the valence band of $AgFeO_2$, forming a Z-scheme mechanism. Those electrons will interact with atmospheric oxygen and undergo reduction to form superoxide radicals, holes in the valance band will interact with moisture to form hydroxyl radicals. These radicals will break down the organic molecules into nontoxic products. The material confirmation, optical property measurements, morphology analysis, etc. are done by XRD, RAMAN spectroscopy, PL absorbance spectra, SEM & TEM analysis. The heterostructure showed enhanced activity towards degradations compared to pure $BiVO_4$.

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Quasi-Periodicity in Fuzzy Fibonacci Arrays on Nanomaterials

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ABSTRACT

Fibonacci words are important in combinatorial theory because they have unique combinatorial features such as aperiodic behaviour. Apostolico and Brimkov studied array repetitions by extending Fibonacci words to Fibonacci arrays. The study of formal languages, number theory and quasicrystals using Fibonacci are widely used in wave propagation, signal processing, image processing and so on. Periodicity is a trait that is used in various domains, including string searching algorithms, data compression, and the study of coding properties of sets of words and sequence assembly in computational biology. However, multidimensional periodicity has not been formally investigated in pattern matching. The lack of periodicity can result in fascinating features such as extraordinary optical transmission and amplified transmission resonances. Aperiodic order can be artificially imposed during sample fabrication and can be precisely controlled. These features have paved the way for the development of technologies based on aperiodic structures. Optoelectronic devices based on multimode effects, which can be created by aperiodic order, have received a lot of attention due to their possible uses in optical communication, energy harvesting, nanoantennae, and other fields. To examine light localization, Kohmoto et al proposed dielectric multilayers in the Fibonacci sequence and demonstrated that the transmission coefficient exhibits a multifractal spectrum due to its non-periodic long-range order. These findings sparked interest in optical applications as well as theoretical aspects of light transmission in quasiperiodic media, pointing to the possibility of light localization because of the quasiperiodic order. In this paper we aim to extend the concept of Fibonacci Arrays to Fuzzy Fibonacci Arrays by introducing membership grades within and define Fuzzy Fibonacci languages. Also, we study some of the operations such as union, intersection, concatenation and Kleene closure, closure properties and their applications and functions of Quasi-Periodicity in Fuzzy Fibonacci Arrays on Nanomaterials.

Keywords: Fibonacci arrays, Membership grades, Fuzzy languages, Quasi-periodicity, Nanomaterials

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Synthesis and Characterization of $CuMn_2O_4$ Nanoparticles for Photocatalytic Degradation of Wastewater

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ABSTRACT

In the present study, highly proficient visible light active photocatalyst, copper manganese oxide ($CuMn_2O_4$) nanoparticles were synthesized via solid-state method. Powder X-ray diffraction (XRD) revels that $CuMn_2O_4$ nanoparticles is face centred cubic structure and optical properties were determined from Ultraviolet-visible (UV-Vis) spectroscopy. FTIR, XPS and SEM were used to identify elemental composition, functional groups and morphological features of the $CuMn_2O_4$ nanoparticles. Photocatalytic performance of, $CuMn_2O_4$ nanoparticles was evaluated against Methylene blue and the study revealed that $CuMn_2O_4$ nanoparticles exhibited very good efficiency against the Methylene blue dye removal in the water.

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CuBTC MOF-derived Porous Carbon Electrocatalyst for Oxygen Evolution Reaction

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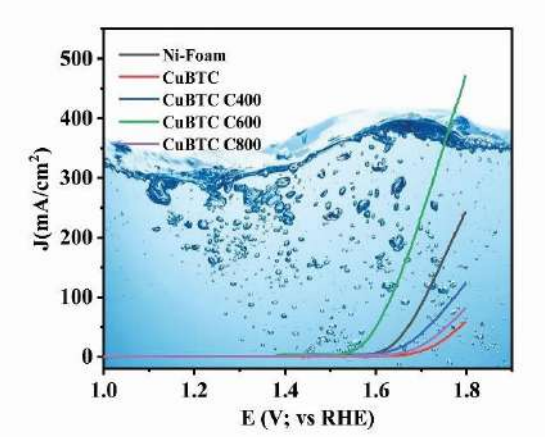
ABSTRACT

Oxygen evolution reaction (OER) plays a vital role in the field of water splitting, which has a promising way to achieve high efficiency and clean energy. However, the efficiency of the water splitting is limited by the sluggish kinetics and large overpotential. Thus, effective electrocatalysts are required to make OER more practicable. In this communication, we report a metal-organic framework (MOF) carbonization path to develop Cu-BTC MOF and its derived nanomaterials that were highly efficient and superior electrocatalysts for OER in an alkaline electrolyte condition. The Cu-BTC MOF-derived electrocatalyst enhances the electrocatalytic activity and the conductivity towards the OER. The obtained Cu-BTC C600 material shows a low overpotential of 310 mV @10 mA/cm^2 and Tafel slope (80 mV dec^{-1}), as well as excellent long-term stability. The present work shows a facile strategy to design and synthesize a Cu-BTC based electrocatalyst, which offers superior electrocatalytic performance towards water electrocatalysis.



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Enhanced photocatalytic performances of g-C_3N_4/$MnFe_2O_4$ Composites for degradation of organic pollutants

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ABSTRACT

In the present study, g-C_3N_4/$MnFe_2O_4$ nanocomposites were prepared by using simple co-precipitation method. The structural, optical and morphology of the synthesised materials were studied using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), UV-Vis spectroscopy, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The photocatalytic performance of g-C_3N_4/$MnFe_2O_4$ was evaluated through the degradation of rhodamine B (Rh B). It was found that the prepared photocatalyst exhibited a maximum removal efficiency of 82% of Rh B within 150 min. And the as prepared nanocomposites did not show any major loss of activity and becomes more stable even after four consecutive cycles during the stability analysis. This may be attributed to large surface area and low electron hole recombination rate of the g-C_3N_4/$MnFe_2O_4$ composite.

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Efficient Photocatalytic Hydrogen Evolution Utilizing Sb-Doped SnS_2 Hexagonal Nanosheets

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ABSTRACT

In the present world, it's crucial to prioritize eco-friendliness and clean energy. Hydrogen, with its high energy density and non-harmful byproducts, plays a major role in achieving these goals. The collaboration between hydrogen production and photocatalysts is significant as these catalysts efficiently convert light into energy, providing a cleaner alternative to traditional sources. At present, Platinum (Pt) and other noble materials are recognized as cutting-edge photocatalysts for hydrogen generation. However, the high cost and limited availability of Pt group photocatalysts make their practical use for this purpose nearly impractical. This situation underscores the need to explore alternative materials that are both low-cost and abundant in rare-earth elements for efficient and cost-effective hydrogen generation. In pursuit of this objective, researchers have explored compound semiconductors such as metal oxides, metal sulfides, and chalcogenides as promising catalysts for photocatalytic hydrogen production. In our research, we created nanostructures made of crystalline hexagonal sheets containing Sb-doped SnS_2 using a hydrothermal method. The effective substitutional doping of Sb into the SnS_2 lattice led to enhancement in surface area, as observed from Scanning Electron Microscopy (SEM). Furthermore, the doping induced a change in the Fermi level within the semiconductor, resulting in an increased concentration of free electrons. This in turn, improved conductivity and modified electronic properties, as verified by X-ray photoelectron spectroscopy (XPS) analysis. The SnS_2 with 6% Sb doping demonstrated the highest hydrogen evolution rates (214.39 mmol g^{-1} h^{-1}) and improved stability compared to pure SnS_2 (92.95 mmol g^{-1} h^{-1}). The improvement can be mainly attributed to the enhanced light absorption properties due to Sb doping, as confirmed by UV-visible spectroscopy. The findings promise to be invaluable for the research community, offering significant contributions towards advancing cleaner and more efficient energy production.

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Comparison of Structural, Thermal, Electrical, Optical, and Magnetic Properties of Various Polyaniline/Metal Oxide Nanocomposites and their Photocatalytic Activity

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ABSTRACT

Polyaniline-metal oxide nanocomposites i.e. PANI/$M_{0.01}Ni_{0.99}O$ (M=Li, Na, and K) [LP, NP, and KP], synthesized using in-situ chemical polymerization. The structures, bonds and compositions affirmed with X-ray diffraction, Fourier transform infrared spectroscopy and energy dispersive X-ray spectroscopy. The average crystallite size found to be around 21nm, 25nm, and 29nm for LP, NP, and KP. The nanocomposites have nanofibrous morphology. Thermogravimetric analysis showing composites strengthens because of stronger interaction between oxides and PANI matrix, makes these suitable for thermal applications. The absorbance spectra consist of two spectrum peaks. The room temperature photoluminescence showing multiple emission peaks. The room temperature AC conductivity follows trend: LP<NP<KP. The frequency dependence of the real & imaginary parts of the impedance analysis and electrical modulus, Nyquist plots, and equivalent circuit parameters values for composites analyzed at the room temperature. The hopping charge carriers are responsible for enhanced conductivity. The nanocomposites showed superparamagnetic behavior & presence of multi magnetic domain. These have applications for opto-electronic, electronic devices, and nanodevices. Photocatalytic activities performed using these nanocomposites on methylene blue dye, and found to have higher degradation percentage, photostability and reusability.

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Extraction of Cellulose Nanocrystals from Natural Fibres for Energy Storage Applications

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ABSTRACT

The extraction of nanocellulose from agro-industrial wastes is feasible due to the significant amount of cellulose in these natural fibres. In this work, cellulose nanocrystals (CNC) were synthesised by acid hydrolysis method from natural fibres. The Extraction of cellulose was carried out in a two-step procedure: the first treatment to the production of holocellulose by the gradual removal of lignin, while the ensuing sulphuric acid hydrolysis process allowed obtaining cellulose nanocrystals in an aqueous suspension. The cellulose from okra and the effects of the hydrolysis of different acids on the morphology, structure, and properties of the resultant cellulose and cellulose nanocrystals were investigated. Morphological characterization through scanning electron microscopy (SEM) clearly showed the formation of rod-shaped CNS's. The physiochemical analysis was done via Fourier Transform Infrared (FTIR), and needle-shaped CNC's were observed from Transmission electron microscopes (TEM). Owing to higher quality of CNCs obtained from efficient and modified techniques, these can find potential usage in nanocomposites for energy storage applications.

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Melamine Assisted Synthesis of Hollow Porous MgO Cubes as a Fluorescence Probe Materials for Detection of Antibiotics

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ABSTRACT

The development of fluorescence-based materials is attractive for research in biological and environmental science applications due to detection/degradation of antibiotics. However, the excess antibiotic residues in any product will pose hazards in terms of physical or environmental contamination. In these regards, we synthesized three-dimensional nanostructures of hollow porous MgO cube- like material as probes for the detection of antibiotics. As-prepared samples are well characterized with various spectroscopy and microscopy techniques. Here, it shows an interesting opto-electronic property of fluorescence intensity interacting on antibiotics molecules to select/sensing solid-state photoluminescence characteristics. Moreover, a plausible mechanism for these detections has been realized, and possible mechanisms have been discussed.

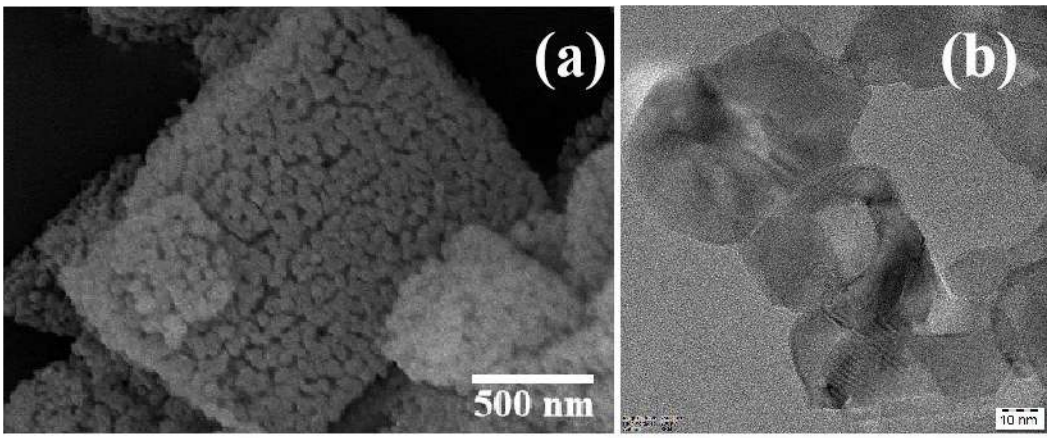

Figure 1. (a) SEM and (b) TEM images of hollow porous MgO cube-like morphology.

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Preparation and use of Agglomerated Metal Nanoparticles Decorated Glass Substrates in Achieving Enhanced Light Absorption in Sb_2Se_3 Solar absorber Thin films

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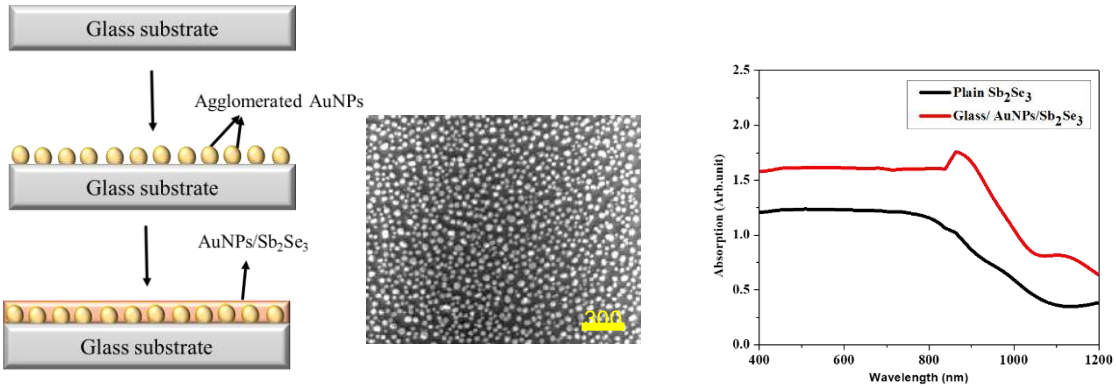
ABSTRACT

In this work, agglomerated Au nanoparticles (AuNPs) were prepared on the glass substrates through post deposition vacuum annealing of thermally evaporated ultrathin Au films having a thickness of ~5nm. Post deposition annealing was done at 250 ℃ for 2 hours to achieve agglomeration resulting in uniformly distributed AuNPs having a particle size of ~33nm. The surface morphology of the agglomerated AuNPs were examined using scanning electron microscope. These substrates were used for the deposition of binary semiconducting Sb2Se3 solar absorber thin films and the optical properties were compared with the films deposited on a plain glass substrate. The observed results showed a significant increase in the optical absorption values for the films grown on substrates with agglomerated AuNPs, indicative of plasmonic effects that improves overall light absorption.



(a) (b) (c)

Figure: (a) Process flow of preparation of Sb2Se3 thin films on glass substrate with agglomerated AuNPs, (b) SEM image of agglomerated AuNPs and (c) absorption spectra of Sb_2Se_3 thin film grown on plain and agglomerated AuNPs covered glass substrates

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Studies of Two- Dimensional Multilayered MXene Structural Properties and Applications

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ABSTRACT

MXenes are the Two-dimensional (2D) layered materials composed of transitional metal carbides, carbonitrides, and nitrides that were first discovered in 2011. $Ti_3C_2T_x$ MXene is a specific type of Multilayered MXenes are often derived from parent MAX phases through selective etching processes. Multilayered MXenes $Ti_3C_2T_x$ were synthesized by selectively etching Al atoms layers from Ti_3AlC_2 Titanium Aluminium Carbide MAX phase and the resulting impact on the stacking order and morphology of the MXene layers. The multilayered nature of MXenes introduces intriguing properties that differ from their single-layer counterparts. Surface terminations, such as hydroxyl and fluorine groups, exhibit layer-dependent variations, influencing hydrophilicity, electronic structure, and chemical reactivity. Each single MXene phase was confirmed by X-Ray Diffraction Analysis (XRD). Further, subjected to Raman and HRSEM analysis. Compared with Raman Spectroscopy results, XRD shows similar patterns for MXenes Layers with different structures. In HRSEM analysis, the MXene samples exhibited a distinct multilayered structure with observable interlayer spacing and well-defined surface terminations. The images revealed a prevalence of hydroxyl groups on the surface, consistent with the expected functionalization. The tailored properties of multilayered MXenes open up new avenues for applications. The multilayered structures also exhibit unique catalytic properties, impacting their potential use in various chemical reactions. As research on MXenes progresses, the understanding of multilayered structures continues to evolve.

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Fabrication and characterization of Ba_{1-x} La_xTiO_3 (x = 0.2–0.8) Nanocomposites for Energy Storage Applications

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ABSTRACT

The sample preparation of Lanthanum doped barium titanate using the Hydrothermal method. The structural, morphological, optical, and dielectric properties of $Ba_{1-x}La_xTiO_3$ (x = 0.2, 0.4, 0.6,0.8) nanoparticles are explored. Diffraction patterns and a comparison to the corresponding standard JCPDS pattern has been verified the structure of the current samples. Average crystallite size (Dp), theoretical density (ρx), porosity (P), dislocation density (ρd), strain (ε), and lattice constant (a) deduced from X-ray diffraction pattern. Morphology studies done by SEM measurements. The optical characterization done by FTIR and UV-vis. Subsequent research on the dielectric behaviour revealed frequency-dependent dielectric characteristics, the space charge effect, and the dynamics of dielectric relaxation. Impedance and dielectric modulus formalization were used to clarify the microstructure, polarization, and electrical properties.

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Effect of varying Ti/V ratio on Synthesis, Thermal Behavior, Optical Band Gap, and Electrical Properties of $(Ti_xV_{1-x})_2AlC$ Max Phase

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ABSTRACT

Bimetallic layered solid solution MAX phases have attracted significant interest because of their tunable properties. Easy machinability, relatively low densities, high elastic constants, catalytic activity, etc., make $(Ti, V)_2AlC$ MAX phase an appreciable candidate for different mechanical, electrical, and electrochemical based applications. Earlier reported synthesis methods of bimetallic MAX phases are not economical due to high temperature, high pressure, an inert atmosphere, etc. Herein, we present an alternative route, modified molten salt shielded synthesis, to produce $(Ti_xV_{1-x})_2AlC$ MAX phases with varying Ti/V ratios. X-ray diffraction shows the shift in main peak positions with varying Ti/V ratios. Post oxidation XRD of the MAX phase constituents shows that increasing the Ti / V ratio increases the peak intensity of TiO2 and reduces the intensity of V_2O_5. UV-vis spectroscopy data illustrate that increasing the Ti/V ratio enhances the optical band gap. Calculated thermodynamic parameters like activation energy, entropy, enthalpy, and Gibb's free energy manifest the reaction kinetics of the oxidation behavior of the MAX phases. Electrical resistivity measured at room temperature decreases with increasing Ti/V values. The outcome of this present systematic and meticulous work provides greater insight into the synthesis of the solid solution based $(Ti_xV_{1-x})_2AlC$ MAX phase and its thermal, optical, and electrical behavior with varying Ti/V ratios.

Keywords: MAX phase; Layered materials; Oxidation; Bandgap; Electrical resistivity.

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F 128

Impact of Chitosan Coating on Hyperthermic Behaviour of Magnetite Nanoparticles

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ABSTRACT

A lot of interest has been shown in magnetite nanoparticles as a potential therapeutic agent for the treatment of cancer due to their superparamagnetic behaviour, biocompatibility, smaller sizes and heat generation upon applying an alternating magnetic field. Surface modification of magnetite nanoparticles is considered necessary for probing magnetite to the desired shape, size, better colloidal stability, and improved dispersion in various solvents. Chitosan is a hydrophilic, biocompatible, biodegradable, natural polymer which can serve better colloidal stability and *in vivo* blood circulation for magnetite nanoparticles on incorporation with chitosan. Herein, chitosan-stabilized magnetite nanoparticles were synthesized using the coprecipitation method. Different concentrations of chitosan (0-2_wt%) were employed for coating, and its impact on the structural chemical and magnetic properties was examined via X-ray diffraction, High resolution transmission electron microscopy, Energy dispersive X-ray spectroscopy, Fourier transform infrared spectroscopy, thermogravimetric analysis, and vibrating sample magnetometry. XRD analysis depicts the average crystallite size of prepared samples ranges from 9.51 to 11.13 nm upon the increase of chitosan concentration, induction heating of these nanoparticles showed better self-healing properties for 1.5wt% chitosan-coating with Specific absorption rate 36.76 W/g and Intrinsic Loss Power 1.148 nHm^2/kg

Keywords: Hyperthermia, magnetic nanoparticles, chitosan, specific absorption rate, intrinsic Loss Power, coprecipitation.

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Photocatalytic Selective Oxidation of Aromatic Alcohol

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ABSTRACT

The selective oxidation of alcohols to its corresponding aldehydes has been a crucial interest in industrial forums. Out of variety of alcohols present, oxidation of Benzyl alcohol to Benzaldehyde in low cost is a challenging task. Hence, we in this work are inclined to engineer an outrageous semi-conductor photo catalyst with an elevated yield and upmost selectivity. Semi-conductor photocatalyst materials are highly promoted since they can easily be retrieved after the reaction and can be reused. Amongst wide range of photocatalytic material, Bismuth Vanadate ($BiVO_4$) reigns as a promising material for benzyl alcohol oxidation due to its suitable band edge position, ability to captivate visible light and high stability in chemical reactions. Further its performance was improved extremely by addition of silver nanoparticles over its surface. Due to surface plasmon resonance (SPR effect), the decorated samples showed enhanced optoelectronic properties. The band edge positions shifted to higher energy levels profitably paving the way for the production of superoxide radicals ($\bullet O_2^-$) effectively and a righteous yield was procured.

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F 130

Modified Molten Salt-shielded Synthesis of Layered Transition Metal Ternary Borides: WAlB and Mn_2AlB_2

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ABSTRACT

Nowadays, the layered transition metal ternary borides, commonly known as MAB phases are the focus of scientific exploration for their excellent covalent-ionic properties i.e. good thermal shock resistance[1], high electrical and thermal conductivity[2], oxidation resistance[3] and, excellent wear resistance[4]. Synthesis of these MAB phases requires high temperature, prolonged heating time and, an inert atmosphere to prevent oxidation. The commonly used synthesis methods are hot isostatic pressing, spark plasma sintering, arc-melting, self-propagating high-temperature synthesis, etc which are time-consuming and costly. So the motivation of this work was to synthesize WAlB and Mn_2AlB_2 MAB phases at lower temperatures and shorter times with high purity using a newly developed and optimized molten salt-shielded synthesis (MS^3) method. This MS^3 method is a proven tactic to synthesize oxidation-prone materials in a cost-effective and eco-friendly pathway by reducing the heating temperature and heating time[5]. So far, MoAlB, Fe_2AlB_2 and, Cr_2AlB_2 MAB phases are synthesized using molten salt assisted method. Mn_2AlB_2 has been synthesized using the KBr salt, but under the long heating time of 10 hours which increases its risk of oxidation. According to our best knowledge, this work is the first report on the successful synthesis of high-purity WAlB and Mn_2AlB_2 using MS^3 method. The optimized synthesis temperatures for WAlB and Mn_2AlB_2 are 900° C and 1000° C respectively with two hours of heating time for both.

Fig. 1: Modified Molten Salt Shielded Synthesis (MMS^3) method for WAlB (a-c) and Mn_2AlB_2 (e-h) samples. (a,e) Green pellets of WAlB and Mn_2AlB_2 with salt kept in the alumina crucible. (b,f) Green pellets of WAlB and Mn_2AlB_2 covered with NaCl-KCl mixture of salt placed inside the alumina crucible. (c,g) Alumina crucible after heating in the box furnace. (d,h) WAlB and Mn_2AlB_2 sample with solidified salt after heating and breaking the crucible.

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Insights into the Phase Formation of Iron Oxynitride ($Fe_xO_yN_z$) Systems and its Magnetic Field-Dependent Photocatalytic Properties towards Water Splitting

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ABSTRACT

Besides metal oxides, other anionic systems like metal chalcogenides and metal oxyhalides have been widely studied for photocatalytic applications. Metal oxynitrides, with their unique properties, have sparked interest in photocatalysis research. In this regard, an iron oxynitride ($Fe_xO_yN_z$) system is developed from iron nitride (Fe_xN) through solid-state annealing at relatively low temperature of ~400°C. The oxynitride phase formation is facilitated by the partial substitution of lattice nitrogen with oxygen, as confirmed by new peaks in the XRD patterns and Rietveld refinement analysis. XPS analysis indicates that the oxynitride phase is stabilized via the N^{3-}-$Fe^{3+/2+}$-O^{2-} network in the system. The structure-property relationship of the formed iron oxynitride phase has been examined using various optical (UV–vis, PL, and TRPL), photoelectrochemical (CV, LSV, EIS, photocurrent, Mott–Schottky), and surface (BET) analysis techniques. The results suggest that the iron nitride counterpart in association with oxide counterpart synergistically contributes to the overall enhancements in the properties of the resulting oxynitride phase. The photocatalytic properties of the developed iron nitride, oxide, and oxynitride systems have been studied for H_2 generation under solar irradiation with and without the presence of a magnetic field. The application of an external magnetic field enhanced the rate of photocatalytic H_2 production, revealing the influence of magnetic properties on the redox reactions of the oxynitride photocatalyst. Moreover, the improved magnetic properties and photo-stabilities of the synthesized $Fe_xO_yN_z$ system enabled its easy recovery and reusability according to the post-characterization studies. This study provides insights into the phase formation of an atypical iron oxynitride system through various characterizations and experimental studies. It also explores the influence of magnetic fields on enhancing photocatalytic efficiencies, leveraging the inherent magnetic nature of the system.

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Synthesis of m-PEG Functionalized Manganese Iron Oxide Nanoparticles by using Thermal Decomposition Method in Magnetically Activated Hyperthermia Therapy

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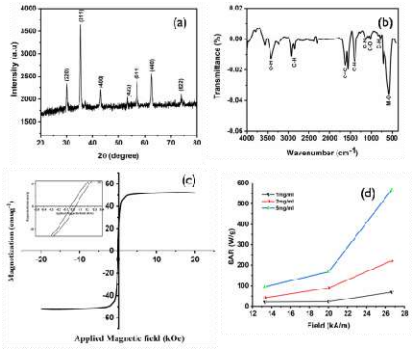
ABSTRACT

Magnetic hyperthermia, which involves using magnetic nanoparticles (MNPs), holds significant promise as an additional therapy for cancer treatment. This is due to the inherent ability of MNPs to generate heat when exposed to an alternating magnetic field (AMF). In this study, manganese iron oxide nanoparticles were synthesized using the thermal decomposition method. The resulting nanoparticles exhibited a cubic spinel structure, as confirmed by X-ray diffraction, Transmission electron microscopy, Fourier transform infrared spectroscopy, and vibrating sample magnetometry. The synthesis pathway successfully produced monodisperse $MnFe_2O_4$ nanoparticles with average size in the range of 20.84 nm, displaying excellent cubic morphology. The observed specific absorption rate (SAR) and intrinsic loss power of the nanoparticles are 154.67 W/g and 3.37 nHm^2kg^{-1} at the maximum clinical field of 352.2 Oe and under a frequency of 277 kHz. We experimentally provide evidence of the enhanced magnetic heating efficiency of m-PEG functionalized manganese iron oxide nanoparticles. After functionalization, its SAR increased at the same field of 566.54W/g and 5.11 nHm^2kg^{-1}. This finding presents new possibilities for advancing hyperthermia as an alternative approach to conventional cancer therapies.



Keywords: Magnetic hyperthermia, Magnetic nanoparticles, Nanoclusters, Thermal decomposition etc.

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F 133

Different Ways to Produce Low-Lost Carbon Nanofibers-A Mini Review

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ABSTRACT

Carbon Nanofibers have high potential market as they are useful in a variety of applications, including filtration, tissue engineering, automobile, aerospace, and energy storage etc. So far, electrospinning is the most used method for producing carbon nanofibers. In electrospinning, factors like polymeric source of carbon, requirement of high power supply, high temperature for stabilization and carbonization increases the ultimate of produced carbon nanofibers. This hinders the wide-spread commercial use of carbon nanofibers and shows the demand to explore ways to produce low cost nanofibers. In this quest, various ways to produce low cost carbon nanofibers such as biomass based carbon nanofibers, hydrothermal carbonization are coming as solution. In this paper, different ways to produce low-cost carbon nanofibers using hydrothermal carbonization, flame retardant doping, biomass based nanofiller and biomass based carbon nanofibers production are discussed. This paper also focuses on real time applicability, challenges and future prospects of these methods.

F 134

Sol-Gel Synthesis of NiMnO Nanoparticles for Photocatalytic Methylene Blue Degradation

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ABSTRACT

NiMnO nanoparticles have been successfully prepared through the sol-gel method. The effects of different factors without (CTAB) and in the presence of the chelating agent. The size of the peak broadening in FWHM which impacts crystalline size without CTAB is 4.56nm and with CTAB is 4.88nm. UV-Vis diffuse reflectance spectroscopy was used to investigate the optical properties of the anticipated products, finding an estimated band gap for the product of roughly 3.78 and 4.04 eV. The validated band gap estimation implies that this product might be used as a photocatalyst. As a result, a photocatalytic evaluation was carried out, which involved the photooxidation of dyes under visible light irradiation while using NiMnO nanoparticles. The results showed that after a 180-minute exposure to the visible light source, MB degradation was roughly 66% and 71%. As a result, the effectiveness of the synthesised compound as a viable photocatalyst is confirmed.

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Structural, Morphological and Optical Properties of upflourescent EuF_3: Holmium @ glycine nanoparticles

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ABSTRACT

EuF_3: Ho nanoparticles have been synthesized in presence of glycine as surface modifier using chloride route. The nanoparticles were subjected to XRD, SEM, TEM, EDAX, SAED, FTIR, FT-Raman, UV-Vis and PL spectroscopy analysis. XRD profile indicates hexagonal phase with average size of 43 nm with lattice parameter a = b = 6.920 A^0, c = 7.085 A^0 in agreement with JCPDS card no 32-0373. SEM analysis shows formation of flakes. TEM studies show presence of hyperboloid, rod and globular shaped structures. Formation of EuF_3 is confirmed by EDAX spectra. Three prominent rings in SAED pattern remain confined with planes in XRD studies. UV-Vis spectrum shows multiple absorption peaks due to quantum dots below 400 nm and a transparent window above indicates its applications in optoelectronic devices. Emission peak at 653 nm (red) in PL spectra suggests its applications in biological field.

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F 136

Cost-effective X-ray Imaging Potentials of Copper Doped Cesium Silver Iodide Scintillator

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ABSTRACT

Scintillator emits visible light if it interacts with ionizing radiation such as X-rays[1]. Since, Cu-doped Cs_2AgI_3 exhibits attenuation coefficient at X-ray photon energy of 70 KeV is 5.1 cm^2/g, quick response time, high light yield, and low toxic nature[2]. Single phase Cu-doped Cs_2AgI_3 sample was prepared coated on plastic substrates in four different thickness using doctor blade technique. Then its X-ray imaging potentials were recorded for different coating thicknesses using a customized system with a USB camera interfaced with a mobile phone using an OTG cable. The material displays scintillation under 70 KeV photon energy X-rays exposures and the interfaced camera records the resulting real-time image. This imaging potential demonstrates the effectiveness of Cu-doped Cs_2AgI_3 as a cost-effective material for X-Ray imaging applications.

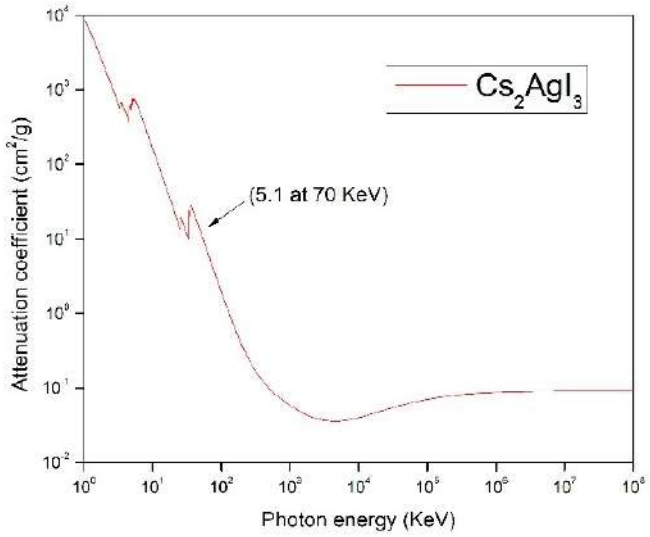

Figure: Energy dependent attenuation behaviour of Cs_2AgI_3

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F 137

Microwave assisted synthesis of Carbon Quantum Dots for selective fluorescent sensing of Mg^{+2} ions

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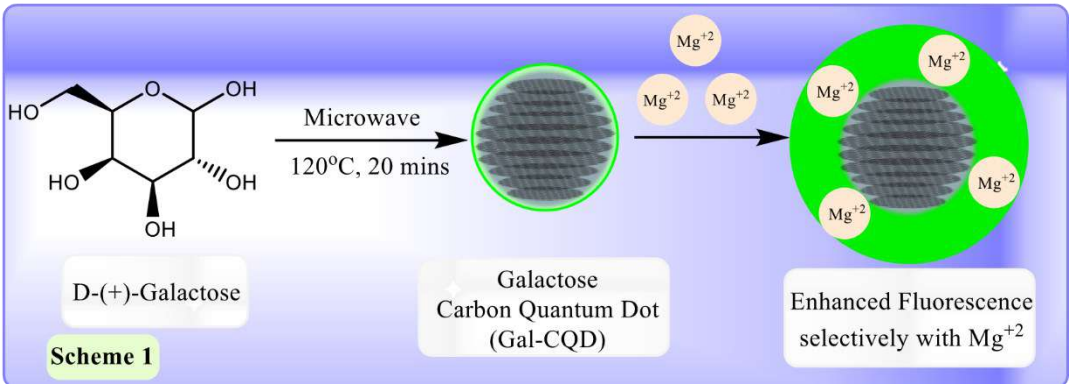
ABSTRACT

Carbon dots are being extensively studied in recent years.[1] The gaining interest is due to the unique properties exhibited such as bright fluorescence[2], excellent photostability[3], tuneable fluorescence emission[4], biocompatibility, low toxicity, and good water dispersibility. Carbon dots with a well-tuned surface can be used for applications such as catalysis[1], bioimaging, biosensing, etc. In this work, a single step microwave assisted CQD synthesis was developed using D-(+)Galactose as the sole reactant (Scheme 1). The Gal-CQD has good water dispersibility, excellent photostability and an excitation-dependent fluorescence emission. The metal sensing of the GalCQD was studied. It was seen that in the presence of Mg^{+2} ion solution the fluorescence emission was enhanced, while the fluorescence was quenched in presence of other metal ions. The enhancement of fluorescence emission was due to the formation of a complex between Gal-CQD and Mg^{+2} ions .[5]



Scheme 1

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F 138

Averrhoa carambola Fruit Extract Mediated Synthesis, Characterization of Cu/Cu_2O Nanoparticles and Evaluation of their Antioxidant, Anticancer and Catalytic activities

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ABSTRACT

The distinct properties of Cu_2O NPs like large surface area, moderate band gap and as p-type semiconductors are useful in both the scientific and industrial fields. In the present study, the green synthesis of Cu/Cu_2O from copper sulphate pentahydrate using *Averrhoa carambola* fruit extract is described and the extract acts as a capping and reducing agent. The prepared Cu/Cu_2O nanoparticles were characterised by different spectroscopic and microscopic techniques. Cu/Cu_2O nanoparticle synthesis was observed by UV-visible spectrophotometry and two absorbance peaks were observed at 290 and 350 nm. The average hydrodynamic size is 24.5 nm and the Zeta potential is 23.4 mV by DLS method. In the XRD spectrum, both cubic metallic copper and FCC Cu_2O peaks appeared, and the average crystallite size is found to be 40.4 nm. The XPS spectrum two main peaks at 934.5 eV and 954.5 eV are corresponding to the spin-orbit split of Cu $2p_{3/2}$, Cu $2p_{1/2}$ components of Cu and Cu_2O and The Oxygen 1s peak appears at around 530.5 eV. EDX spectrum had high-intensity copper metal peaks including oxygen. The SEM micrograph have a dominant hexagonal particle which belongs to metallic Cu NPs and spherical particles which are related to Cu_2O NPs. The HR-TEM image indicated spherical nanoclusters of an average size of 150-200 nm. The antioxidant ability of NPs showed good free radical scavenging activity against DPPH and NO with the percentage of inhibition values at 54.6% and 57.6%, respectively. The synthesized NPs moderate cytotoxic effect on the lung cancer cell lines at 100 µg/mL and exhibit 55.7% of cell viability. The photocatalytic studies of synthesised nanoparticles reveal that they act as a suitable catalyst for the degradation of yellow food dye, The 43.5% of dye degradation is observed at 45 minutes of solar irradiation. The research successfully demonstrates a simple way of employing plant extract to produce Cu/Cu_2O nanoparticles in a given method and the potential ability of these nanoparticles in diverse applications.

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Synthesis and Characterization of Stannic Oxide thin films and their application in Quantum Dot Sensitized Solar Cells

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ABSTRACT

The Stannic Oxide (SnO_2) is the wide gap semiconductor and due to its excellent transport properties it is having potential application in solar cells as photoanodes, also it is used in the UV detectors, gas sensors, transparent electrode etc. In the current work the SnO_2 is synthesized by chemical bath deposition technique and used as photoanode to study the application in Lead Sulphide Quantum Dots sensitized Solar Cells. Lead Sulphide with tunable bandgap and high absorption coefficient in near infrared region is useful as efficient light absorber. The thin films are characterised by X-ray diffraction, UV-visible absorption spectroscopy, scanning electron microscopy to analyze structural and optical properties. The photo electrochemical performance through J-V measurement is performed.

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F 140

Lead-free Piezoelectric Nanomaterials and their Piezo-Photocatalytic Activity

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ABSTRACT

Ferro-/piezo-electric bulk materials have found wide applications in traditional fields such as sensing, actuation and memory devices. Recently, piezoelectric nanostructures have been demonstrated to exhibit piezocatalytic activity, i.e., in situ electrochemical reaction driven by piezoelectric effect under the excitation of mechanical vibration such as ultrasound via dispersing piezoelectric nanomaterials in solution. In this work, we studied several piezoelectric nanocomposite materials such as nanoparticles, nanocubes, nanowires, and nanofilms for piezo-photocatalytic applications. We used a piezoelectrochemical method to realize the selective deposition of Ag nanoparticles on the positively polar end of {001}-enclosed $BaTiO_3$ nanocubes/cuboids. The BTO nanocubes/cuboids with selectively-deposited Ag nanoparticles show approximately 2 times higher piezocatalytic activity than those with randomly-loaded Ag nanoparticles, and much higher than pure BTO nano-cubes/cuboids. It is believed that the Ag nanoparticles deposited on positively polar end act as “fast lanes” for electrons to transfer to catalysts/solution interfaces, while those loaded on negatively polar end serve as holes trappers hindering ·OH formation and pollutant degradation. The vertically standing BTO nanosheets grown on the top of TiO_2 nanorod arrays prepared on fluorine-doped tin oxide glass substrate exhibited superior piezocatalytic performance as well as piezo-electrochemical property. The finite element method simulation shows that a stronger piezoelectric filed can be built in BTO nanosheets because of their easier deformation, and thus can lead to a higher piezocatalytic degradation efficiency. Our work presented here is expected to provide a potential route for the nanoengineering of thin-film piezocatalysts and clarify the catalytic mechanism for substrate-fixed piezocatalysts.

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F 141

Copper Nanowire-immobilized substrates for use as Antibacterial coatings

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ABSTRACT

Inanimate surfaces play an important role in the spread of infectious diseases, particularly in closed environment with high microbial burden like hospitals.[1] Bacteria are deposited on these surfaces either by settling of infectious droplets or transferred by touch. Once attached, they quickly colonize the surface and can survive for days even under ambient indoor conditions.[2] These bacteria are then transmitted to others via touch. In this context, antibacterial coatings placed over some "high-touch" areas in the hospital can break this loop of pathogen transmission.[3] In this work, we have fabricated copper nanowire (Cu NW)-immobilized coatings that possess good antibacterial activity and can be deposited over any substrate. Cu NWs were synthesized via environmentally-friendly and facile chemical reduction method using glucose as the reducing agent and hexadecylamine as the capping agent.[4] The coatings were fabricated via a two-step process. First, a thin layer of polydopamine was deposited over the substrate followed by immobilization of pre-synthesized Cu NWs. The amount of Cu loaded onto the coatings was optimized and the resulting coated substrates demonstrated excellent antibacterial activity against *E. coli*. The results demonstrate the promising use of Cu nanomaterials for antibacterial applications.

Keywords: Nanowire, copper, antibacterial, mussel-inspired, surface functionalization

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F 142

Electrochemical Exfoliation of Graphite into Graphene in Aqueous Solutions of Inorganic Salt: Effect of Concentration Variation of H_2O_2

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ABSTRACT

A two-dimensional sheet of Sp^2 hybridized carbon is known as graphene. Other significant allotropes are fundamentally constructed from its enlarged honeycomb network. Graphene hasn't been widely adopted despite a great deal of interest and ongoing experimental progress. This is mainly because it is challenging to produce high-quality samples consistently, especially in a scaled way. Since performance is influenced by both the number of layers present and the general crystal lattice quality, the difficulty is actually 2-fold. In this study, a one-step, cost-effective, simple, and highly productive process for generating high-quality graphene is presented. The electrochemical exfoliation method used in the current study to create graphene in aqueous media with different H_2O_2 concentrations. At standard reaction conditions, the suggested system is capable of generating high-quality, anodic few-layer graphene nanosheets. H_2O_2 plays a critical part in the exfoliation of graphite, as evidenced by the control experiment employing inorganic salt and water. A potential exfoliation mechanism is suggested. Highly nucleophilic peroxide ions (O_2^{2-}), which are produced when H_2O_2 reacts with hydroxyl ions (OH^-), are essential for the exfoliation of graphite by electrochemical potential-assisted intercalation and significant expansion of graphite sheets. The synthesized graphene is evaluated using XRD, FESEM, EDS, UV-Visible, FTIR, Raman spectroscopy, TGA, and other methods. With changes in H_2O_2 concentration, the number of defects which may be edge defects or oxygen functional groups decreases. The nucleophilicity of OH^- and O_2^{2-} can account for this.

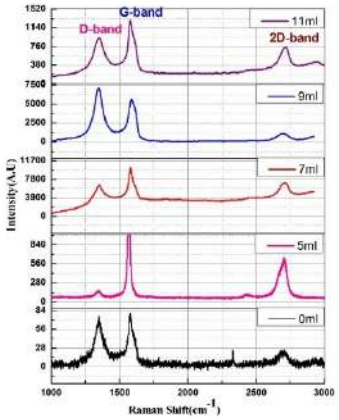

Fig.1. Raman spectra of graphene specimen at different concentration of H_2O_2

F 143

Synthesis of ZnO/Bi_2O_3 Nanocomposite Photocatalyst for Visible Light-Assisted Degradation of Synthetic Dyes and Energy Storage Application

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ABSTRACT

Nanocomposites play a pivotal role in various fields owing to their unique properties and versatile applications. These materials exhibit enhanced mechanical, electrical, thermal, and optical characteristics compared to their individual counterparts. Presently, research focus has been devoted to prepare metal oxide based nanocomposites for possible application in photocatalysis and energy storage applications. This study reports the preparation of ZnO/Bi_2O_3 nanocomposites by co-precipitation method. The role of this nanocomposite in the photodegradation of synthetic dyes like methyl orange (MO) and Congo red (CR) has been investigated. Further, energy storage ability of the above nanocomposite has been tested by electrochemical measurements. The structural characteristics of the materials have been studied using X-ray diffraction (XRD) which shows the successful formation of the binary composite. To elucidate the morphological properties, scanning electron microscopy (SEM) study was performed which displays the formation of nanosheet like structure. The optical absorption study was performed which helped in estimating the band gap of the materials. Fourier transformed infrared (FTIR) measurement showed the vibrational properties of the materials. The photocatalytic activity of the ZnO/Bi_2O_3 nanocomposite was evaluated for the degradation of synthetic dyes under visible light irradiation. The results demonstrated enhanced photocatalytic performance of 92% compared to individual ZnO and Bi_2O_3 counterparts, showcasing the synergistic effects of the composite. The visible light absorption capability of the nanocomposite was attributed to the narrowed band gap resulting from the coupling of ZnO and Bi_2O_3. The kinetic model suggests the degradation pathway obeys pseudo-first order kinetic and the degradation property of the photocatalyst was evaluated with varying dye concentration, loading concentration of photocatalyst and pH. Electrochemical Impedance Spectroscopy (EIS) study was performed and explained in detail. The above study shows the effective energy storage properties of the nanocomposite.

Keywords— Environmental remediation, adsorption isotherm, heterojunction, electrochemical Impedance Spectroscopy (EIS)

F 144

Unleashing the Photocatalytic and Antimicrobial Performance of $Mo_2/ZnS/Bi_2O_3$ Nanocomposite Prepared by Ultrasound Assisted Wet-Chemical Method

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ABSTRACT

Nanocomposites have become a subject of great interest in the scientific community, thanks to their exceptional properties and wide range of applications. These materials exhibit superior mechanical, thermal, and electrical, optical properties when compared to their individual counterparts. Ternary nanocomposites, which consist of multiple distinct material components, exhibit remarkable synergistic effects that result in exceptional performance characteristics. In this work, highly efficient $MoS_2/ZnS/Bi_2O_3$ nanocomposites were successfully prepared by sonochemical technique. The as-synthesized nanocomposite was studied to characterize and test its photocatalytic and antimicrobial efficiency. The structural, optical, morphological, chemical composition and specific surface area of as-prepared $MoS_2/ZnS/Bi_2O_3$ hybrid nanocomposite was investigated by different characterization tools. The photo-degradation efficiency of as-prepared $MoS_2/ZnS/Bi_2O_3$ photocatalyst over aqueous methylene (MB) dye degradation was evaluated under visible-light irradiation. The ternary nanocomposite exhibits photocatalytic activity about 93.29 %, which is higher than other as-prepared samples. Also, the $MoS_2/ZnS/Bi_2O_3$ hybrid photocatalysts showed excellent degradation activity and excellent cycling stability even after five successive recycles. The above performance of the $MoS_2/ZnS/Bi_2O_3$ catalyst might be due to the increased visible-light absorption ability, lower band gap values, and effective charge separation along with the faster migration properties. The results also suggested that the nanocomposite has shown good antimicrobial activity against different human pathogenic bacteria (*Escherichia coli and Staphylococcus aureus*).

Keywords— Nanocomposite, visible light absorption, photocatalyst, antimicrobial activity

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MoS_2 Based ZnS/g-C_3N_4 Ternary Nanocomposite for Enhanced Visible Light Driven Photocatalytic Performance and Bacterial Assassination

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ABSTRACT

Nanocomposites, a novel class of materials, have garnered significant attention due to their remarkable properties and versatile applications. These materials offer enhanced mechanical, thermal, and electrical, optical properties compared to their individual counterparts. Nanocomposites comprising of more than two distinct material components often termed as ternary nanocomposites and show synergistic effects, leading to superior performance characteristics. In the present work, MoS_2 based ZnS/g-C_3N_4 ternary nanocomposites were successfully synthesized by a facile ultrasonic dispersion method. The crystalline structure and morphology of the nanocomposites were characterized by X-ray diffraction (XRD) and scanning electron microscopy (FESEM). The crystallite size was found to be 62nm for composite which higher than single and binary catalyst. The optical property of the as-prepared nanocomposites was studied by UV-visible and photoluminescence (PL) techniques. It could be observed from the FESEM image that the MoS_2 and g-C_3N_4 nanosheets along with ZnS nanoflakes were formed and well combined together in the sample. Moreover, the photocatalytic activity of MoS_2-ZnS/g-C_3N_4 composites was evaluated by the removal of o-nitrophenol and p-nitrophenol under visible light irradiation. The experimental results show degradation of 83.4 % for the nanocomposite which is higher than the single photocatalysts. A possible photocatalytic mechanism for the MoS_2-ZnS/g-C_3N_4 nanocomposites with enhanced photocatalytic activity could be ascribed to the hetero-structure of MoS_2, ZnS and g-C_3N_4. The nanocomposites of MoS_2-ZnS/g-C_3N_4 possessed significant stability and recyclability up to six consecutive cycles which is beneficial to minimize the cost. The improved photo-efficiency is due to the increase surface area, and high charge separation in ternary heterojunction which helps in environmental remediation. Their antibacterial property was assessed against *E. coli* bacteria and nearly 85.5 % of gram negative bacteria were killed by using ternary photocatalyst as determined by CFU method. The improved antibacterial efficiency helps in food packaging application.

Keywords— Environmental remediation, o-nitrophenol; p-nitrophenol, heterojunction Photocatalyst, antibacterial efficiency

F 146

Highly Efficient and Reusable ZnO/CuO Nanocomposite for Photocatalytic Removal of Malachite Green Dye

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ABSTRACT

This study explored the synergistic effects of combining ZnO and CuO at different ratios to enhance the degradation of malachite green dye (MG), a cationic dye, under UV light. ZnO/CuO composites at 1:4, 1:1, and 4:1 ratio was successfully synthesized by chemical co-precipitation method. X-ray diffraction (XRD), Scanning Electron Microscope (SEM), UV-Visible absorption, Fourier Transform Infra-Red (FTIR) and Photoluminescence (PL) spectroscopy were employed to assess the properties of synthesized materials. The PL results indicated a significant reduction in charge recombination in the composite samples compared to pure ZnO, leading to enhanced MG dye degradation. Notably, the ZnO/CuO composite at 4:1 ratio exhibited the highest efficiency, degrading 99% of MG within 3 hours under UV irradiation. Optimal conditions for the 4:1 composite was determined with a catalyst load of 0.3 g/L, an initial dye concentration of 4 ppm, and a pH of 8 which reduced the irradiation time to 50 minutes. Scavenging experiments identified hydroxyl radicals as the primary contributors to the degradation process. Reusability test shows that the composite samples exhibit high stability even after 3-4 consecutive runs suggesting that the samples have potential for large scale use in this field.

F 147

Exploring Multifunctional Properties of Tetragonal Tungsten Bronze Structured Materials

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ABSTRACT

This study explores the multifunctional capabilities of Tetragonal Tungsten Bronze (TTB) structured multiferroic materials doped with ferroic-phases inducing elements. Various TTB multiferroics, including Tetragonal Tungsten Bronze/Barium Hexaferrite ($Ba_2SmFeNb_4O_{15}$ with the presence of $BaFe_{12}O_{19}$ secondary magnetic phase) multiferroic composite ceramics, Eu-substitution-induced TTB $Ba_4(Eu_xLa_{1-x})_2Fe_2Nb_8O_{30}$ multiferroics with x=1, TTB $Ba_4Nd_2Fe_2Nb_8O_{30}$ (N_2 annealed), high-density TTB $Ba_4Sm_2Fe_2Nb_8O_{30}$ (BSFN) ceramics [1][2]. The study also delves into their synthesis methods, structural analysis, and phase identification. Notably, Polarization and magnetization measurements at ambient temperature exhibit distinct characteristics that delineate the effect of ions occupation across different sites of the TTB multiferroic skeletons, and the distortion of BO_6 corners [3]. This effect changes the ferroic behaviors of the ceramics. The examination sheds light on the diverse functional properties of the materials and positions itself for practical applications, especially in devices like semiconductor memories, transducers, sensors, spintronics, etc

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Carbon quantum dots-DNA nanocomplex for non-viral gene delivery and bioimaging applications

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ABSTRACT

Carbon quantum dots (CQDs) was synthesized and confirmed via various spectroscopic and microscopic characterization techniques such as UV-Vis spectroscopy, fluorescence spectroscopy, High resolution transmission spectroscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FT-IR). CQDs was used for potential application as non-viral gene carriers. The electrophoretic mobility confirmed the electroneutral nature of CQD-DNA nanocomplex. The cytotoxicity study was carried out on human endothelial kidney cells (HEK-293) and breast cancer cells (MCF 7). The cytotoxicity study revealed that there was no obvious inhibition of cell viability with high concentration. The prepared CQD-DNA nanocomplex has potential in live cell bioimaging applications.

Keywords: Bioimaging; Carbon quantum dots; Cell viability; DNA transfection

F 149

Effect of Size of Rod Shaped Zinc Oxide Particles on the Random Lasing Action of a Weakly Scattering System

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ABSTRACT

The effect of size of zinc oxide rods on the performance of random laser system of a weakly scattering system containing Rhodamine B dye and Zinc Oxide rods with ethanol as the solvent was studied. It was observed that the size of the rods greatly effects the random lasing performance. For the same particle density of the scatterers, the scattering mean free path was calculated and for particles having larger dimensions the scattering mean free path is smaller which favours multiple scattering events and thus better random lasing performance.

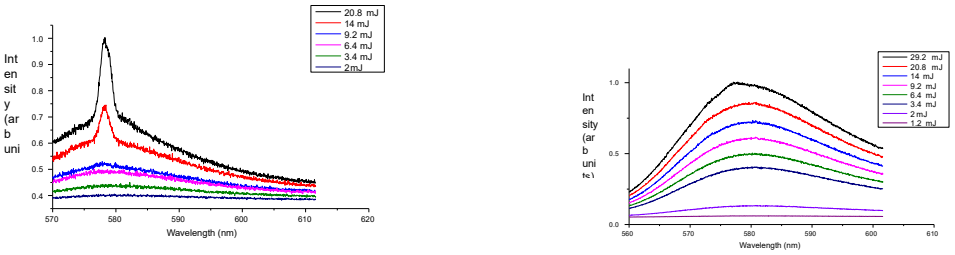

Figure: Emission spectrum of Rhodamine B/Zinc Oxide colloidal system with larger and smaller sized scatterers (zinc oxide rods).

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F 150

Characterization of Carbonized TiO_2 Nanotubes for Improved Supercapacitance

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ABSTRACT

The usage of energy storage devices to meet the demand for energy consumption has been increasing daily. Supercapacitors have drawn attention and have become one of the leading research topics in energy storage devices for their potential to have high energy and power density. Areal capacitance plays a significant role in designing supercapacitors as a power source for an electronic device. TiO_2 is a promising anode material for supercapacitor application as it is naturally abundant, non-toxic, and environmentally friendly [1]. TiO_2 nanotubes (TNT) offer the advantage of unidirectional electron transport, high surface area, and porosity, which are essential for good supercapacitor anode material. However, some setbacks in such metal oxide anode materials must be addressed, such as inherently suffering from inferior rate performance and poor cyclability due to low ion conductivity and slow ion diffusion [2]. Various strategies are being employed to address these issues; doping is one such method. Introducing impurity to the pure structure is believed to develop defects often exhibiting prominent effects that could lead to substantial advancement. Therefore, TNT with a defective structure could enhance electric conductivity owing to the plentiful oxygen vacancies. Combining carbon in TiO_2 enhances the capacitance of the material [3]. It can improve electronic conductivity, reduce oxygen deficiency, and increase the contact area with electrolytes, promising features for a superior electrode. This study prepared the electrodes by single-step anodizing titanium foils in Ammonium fluoride-based electrolytes at 40 volts, followed by carbonization. The carbonized TNT is characterized for supercapacitor applications. We observed an area capacitance of 3.67mF/cm_2 when the weight percentage of carbon is 10.

KEYWORDS: Doping; Electronic Conductivity; High surface area; Oxygen vacancy; TiO_2 nanotubes

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F 151

Structural, Morphological and luminescence Properties of Sm^{3+} ion doped Cadmium Magnesium Phosphate Nano powder for W-LED applications and Display Devices

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ABSTRACT

Samarium-doped cadmium magnesium phosphate (CMP) nanopowder was prepared by a well-known and frequently used solid-state reaction technique. The prepared sample was analyzed by using a variety of analytical techniques, including Powder X-ray diffraction (P-XRD), FESEM with EDX, Diffuse Reflectance Spectroscopy (DRS), Fourier Transform Infrared Spectroscopy (FTIR) and Photo Luminescence (PL). The P-XRD results reveal that the produced nanopowder has a crystalline size 30 nm and also indicate the CMP nanopowder has a monoclinic structure. The Morphological studies of FESEM results suggest that the nanopowder has a flower-like structure with the presence of elements Cd, Mg, Sm, P, and O [1]. The DRS spectrum of Sm3+ ion doped CMP nanopowder exhibits five prominent peaks, with wavelengths of 287 nm, 459 nm, 946 nm, 1086 nm, and 1243 nm which are located in the UV to IR region. The PL spectrum studies examined four sharp peaks attributed to the wavelengths 564 nm, 598 nm, 648 nm, and 707 nm were observed in the emission spectra upon excitation at 403 nm and five sharp peaks attributed to the wavelengths 360nm, 375nm, 403nm, 415 nm,432 nm, and 475nm were observed in the excitation spectra upon emission at 598 nm. The calculated values of color purity, CRI, and CCT confirm that the CMP nanopowder coordinates were found in the orange region. This prepared nanopowder was suitable for the applications of W-LEDs and display devices. The prepared nanopowder's ions associated with the phosphate group were confirmed by FT-IR [2].

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rGO Mixed PDMS Microtip Device for Highly Efficient Intracellular Delivery Activated by Infrared Light Pulses

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ABSTRACT

Nanoparticles-mediated photoporation has emerged as a universal intracellular delivery tool due to its efficient and uniform delivery. However, the direct interaction of nanoparticles and cells hampers its clinical translation. Here, we report a novel massively parallel intracellular delivery platform that transfects more than a million cells within a few seconds and avoids the direct contact of nanoparticles and cells, thereby improving cell viability. Our platform consists of a microfabricated device (1.5 cm × 1.5 cm) with an array of polydimethylsiloxane (PDMS) pyramidal microtips containing reduced graphene oxide (rGO) nanoflakes, which are densely distributed at the apex and the base included plain PDMS. Individual microtip have ~15-17 µm height, 5-8 µm apex width and 20-30 µm base width, and the gap between two tips is ~ 40 µm (edge to edge). Upon infra-red light pulse irradiation, due to the photothermal enhancement of rGO, cell membrane pores are generated and diverse sizes of biomolecules are delivered. In addition, the presence of rGO mixed PDMS at the apex enables safe delivery with an ultra-low laser fluence (0.9 mJ/cm2) and 5 seconds of exposure time. Using this delivery platform, we have achieved the delivery of small to very large cargo (668 Da to 465 kDa) in various mammalian cells and cancer cell lines. The best results were achieved for the¬ 465-kDa enzyme with a transfection efficiency and cell viability of ~ 97% and 98% in SiHa cervical cancer cells. The highly efficient cargo delivery tool demonstrated in this work will facilitate a safe and effective approach to basic biological research, drug screening, cell therapy, and diagnosis.

Keywords: rGO-mixed PDMS microtip device, photoporation, ultra-low intensity light pulses, hard-to-transfect cells, transfection efficiency, cell viability

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F 153

A study on the Evolution of Hydrothermally Synthesized MoS_2 on Thermal Annealing and Development of Novel MoS_2-MoO_3 Hybrid Nanostructure for Supercapacitor Applications

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ABSTRACT

The electrochemical capacitor also known as supercapacitor is a high-performance energy storage device with exceptional properties. For fabricating fully efficient supercapacitors based on nanomaterials a better understanding of parameters affecting supercapacitor performance, such as the morphology, structure, composition, and surface area of the electrode materials is necessary. We report the evolution of supercapacitor properties of MoS_2 with phase change on thermal annealing along with its structural, morphological, compositional, and optical characteristics. In this study, the pristine MoS_2 was synthesized via the hydrothermal method at 200^0C and the material was annealed in the presence of air at 250^0C, 300^0C, and 350^0C. The sample annealed at 300^0C has shown $MoO_{3-x}MoS_{2-y}$ coexistence phase and a complete transition from MoS_2 to MoO_3 is observed at an annealing temperature of 350^0C. The study revealed that the 300^0C annealed sample with a $MoO_{3-x}MoS_{2-y}$ coexistence phase possesses a maximum charge-discharge time and a high areal capacitance. 2D MoS2 is widely recognized as a supercapacitor material with excellent electrical and mechanical properties and MoO3, on the other hand, is a pseudocapacitive material with high specific capacitance and good rate capability. The evolution of MoS_2 on annealing and its phase dependent properties was studied using XRD, Raman, thermo gravimetric analysis (TGA), FESEM, UV-Vis spectroscopy, and XPS. Electrochemical analysis was employed to study the supercapacitative nature of the materials.

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F 154

Evaluation of Cytotoxicity of Amino modified Nb_2CT_x MXene in normal and Cancer Cell lines.

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ABSTRACT

Here, we have explored the functionalization of Nb_2CT_x MXene with various amine-terminating groups and evaluated their biocompatibility. To introduce amine groups on the surface of Nb_2CT_x, the surface of MXene was modified using ethylene diamine (EDA) and 3-aminopropyl triethoxy silane (APTES). The SEM and XRD analysis confirmed the formation of Nb_2CT_x and FTIR confirmed the presence of functional groups and the modification at each stage. Cytotoxicity of the amino-functionalized Nb_2CT_x was checked using MTT assay in the HUH-7 cell line and ARPE-19 cell line. It was found that both the amino-functionalized Nb_2CT_x were non-toxic in both cell lines. Non-functionalized MXene was seen to form non-uniform aggregates in the cell culture medium, however, the functionalized Nb_2CT_x formed aggregates but they were uniform in nature. This shows that despite amino functionalization of the Nb_2CT_x is not toxic to cells; the modification with amino groups will enable us to manipulate the MXene surface for various biological applications like drug delivery systems and photothermal therapy.

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F 155

A comprehensive Novel Study on Structural, Morphological and Vibrational Characteristics of Pr^{3+} doped Magnesium Cadmium Pyrophosphate Nanopowders

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ABSTRACT

Solid State Reaction (SSR) method was used to prepare undoped and Pr^{3+} ions doped magnesium cadmium pyrophosphate (MCP) nanopowders. Various analytical and spectroscopic techniques viz. X-ray diffraction (XRD), Field emission scanning electron microscopy (FE-SEM), Energy dispersive spectroscopy (EDS), Fourier transform infrared spectroscopy (FT-IR) and Raman spectroscopy were used to determine the structural, morphological and vibrational characteristics of prepared samples. Based on the X-ray diffraction (XRD) studies, the samples exhibited a high degree of crystallinity with average crystallite sizes around 63 nm and 70 nm when calculated by using the Debye-Scherer's formula and W-H plot method respectively. The surface morphology of prepared samples displays a grouped pattern resembling of stones. Vibrational modes of pyrophosphate group were found when the samples were analyzed by using FTIR Spectrophotometer in the 400–4000 cm^{-1} range. The peak detected around 715 cm^{-1} in FTIR spectra is related to the symmetric P-O–P bridge vibrations and the peak observed around 1060 cm^{-1} is related to the symmetric stretching vibrations of the P–O bonds. The same were confirmed by Raman spectral analysis [1], [2].

Keywords: SSR Method, XRD, Nanopowder, Debye-Scherer's formula, Vibrational modes.

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F 156

Hydrothermal synthesis of WS_2 and WS_2/WC composite for Electrocatalytic Application

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ABSTRACT

For a decade, transition metal dichalcogenides (TMDC) have attracted the scientific community due to their availability of band gap and 2D layered structure, which find application in switching devices, sensing, electrocatalysis, storage devices, etc. To cater to the growing energy demand, electrochemical water splitting using WS_2 and its composites can be used since hydrogen is the most promising fuel due to its high gravimetric energy density and cleanliness. In this work, we suggest a hydrothermal method to synthesize pristine WS_2 (*p*-WS_2) and WS_2/WC composite (c-WSC) maintaining the temperature at 220˚C for 24 hours. The prepared samples were characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), X-ray photoelectron spectroscopy (XPS), and Raman studies. The XRD studies for p-WS_2 revealed the existence of metallic 1T as the predominant phase with the characteristic (002) peak at 9.40˚. The presence of 1T phase was further confirmed by Raman spectra. The XRD studies on c-WSC show the coexistence of both WC and the 1T phase of WS_2. The morphological studies using FESEM manifested a flower-like structure for p-WS_2 and a similar structure for c-WSC with the WC strongly adhered to the WS_2 flowers. The XPS analysis of p-WS_2 showed the co-existence of 1T phase with peaks for W at 31.7 eV and 33.8 eV, 2H phase with peaks for W at 32.3 eV and 34.7 eV, and amorphous tungsten oxide. Linear sweep voltammetry (LSV) measurements for the glassy carbon electrodes modified with the as prepared p-WS_2 and c-WSC nanostructures, used separately as the catalysts, exhibited better performance for the c-WSC with an onset potential of -0.16 V and an overpotential of -0.36 V at a current density of 10 mA/cm^2.

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F 157

ReS_2 decorated Nb_2CT_x Nanosheets for Highly Efficient Photothermal Cancer Therapy in the NIR I region

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ABSTRACT

Cancer therapy is still being developed and improved to increase survival rates and minimize side effects of the treatments. Photothermal therapy (PTT) is one of the recent advancements in cancer treatment, which offers the key merits including the capability for deep tissue penetration and high selectivity with minimal effect of surrounding normal cells. Here we have utilized ReS_2 decorated Nb_2CT_x MXene (ReS_2-Nb_2CT_x) nanosheets as an efficient photothermal agent at NIR-I region for the photothermal therapy of cancer. A notable improvement in the photothermal efficiency was observed by the incorporation of ReS_2 into the Nb_2CT_x MXene. The biocompatibility and hydrophilicity of the ReS_2-Nb_2CT_x composite is enhanced by the PEGylation of the composite. The FTIR spectrum exhibits distinct peaks at 970 cm^{-1} and 600 cm^{-1}, providing clear evidence for the existence of ReS_2 in the composite. The UV-Visible absorption spectrum of Nb_2C-ReS_2 composite shows a maximum absorption at 808 nm. The thermal imaging study displayed an average temperature rise of 55 ± 5°C after 5 minutes of irradiation with 808 nm NIR laser. The cytotoxicity of composite was evaluated using the MTT assay in which HeLa and HepG2 cells were exposed to the composite at different concentrations of 1, 10, 25, 50, 100, 150 and 200 µg/mL for 24 hours. A relatively low toxicity was shown in both cell lines at concentrations of up to 200 µg/mL. Additionally, the cytotoxicity analysis of the cells after the laser treatment showed the clear cytotoxic nature which reveals the suitability of the Nb_2CT_x-ReS_2 composite for the photothermal therapy. The Nb_2CT_x-ReS_2 composite has shown promising results in increasing the efficacy of cancer therapy through its efficient photothermal properties.

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F 158

Photocatalytic degradation of Hazardous Congo Red Using Hydrothermally Synthesized Sodium Bismuth Titanate and Iron-doped Sodium Bismuth Titanate

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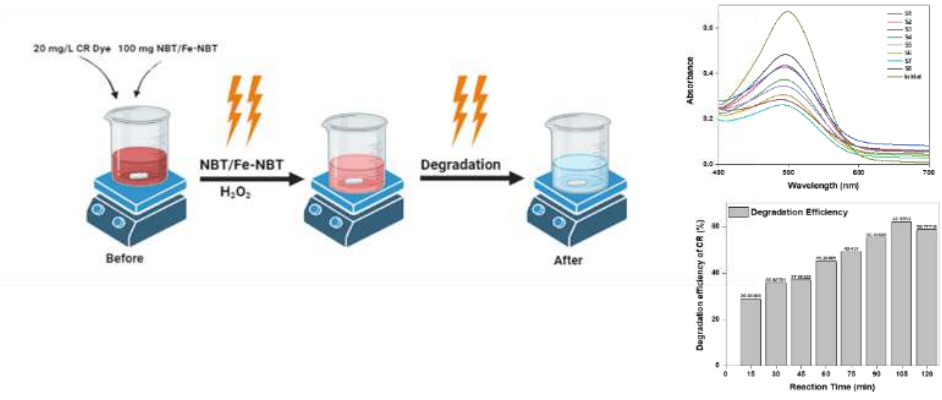
ABSTRACT

Ceramics-based mixed metal oxides have been explored for photocatalytic dye degradation studies. In this work, the photocatalytic degradation of Congo Red (CR) dye was investigated using Sodium Bismuth Titanate (NBT, band gap energy of 3.25 eV) and Iron Doped Sodium Bismuth Titanate (Fe-NBT, band gap energy of 2.45 eV) perovskites, synthesized via simple hydrothermal method. The crystal structure of pristine NBT and Fe-NBT was characterized using X-ray diffraction (XRD) and confocal Raman spectroscopic analysis, and morphologies were analyzed using field emission scanning electron microscope (FESEM) and high-resolution transmission electron microscope (HRTEM). The NBT nanoparticles showed better degradation of CR dye (20 mg/L) within 120 min of radiation under Ultraviolet Radiation. It is found that the degradation efficiency is further enhanced by the addition of H_2O_2. Doping of iron to NBT NPs is further found to improve the photocatalytic degradation efficiency of Congo Red Dye. This investigation reveals the potential use of mixed metal oxides based on ceramics, specifically Fe-NBT, as effective photocatalysts for the breakdown of dangerous dyes, offering a sustainable method of treating wastewater. The results highlight Fe-NBT's potential to address environmental issues associated with textile dye contamination and promote environmentally friendly photocatalytic technology.



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Ferrocene Clutched Azomethine Probe Fc-DNP for Colorimetric, Fluorometric and Electrochemical Detection of Cyanide Ion

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ABSTRACT

A highly selective, multiple ways of cyanide ion detection has been achieved by Fc-DNP, an azomethine functionalized ferrocene clutched compound. The synthesized probe has been systematically characterized and the final confirmation was obtained through SC-XRD. Fc-DNP crystallizes in a monoclinic crystal system with a P-1, 21/C1 centrosymmetric space group. The probe has shown excellent photophysical properties, and AIE property makes it an appropriate material for real-time sample analysis. The incorporation of the active redox mediator "ferrocene" in Fc-DNP imparts remarkable redox behaviour to the probe. Henceforth, Fc-BPy has been deployed selective detection of cyanide in various methods, including naked eye colorimetric, fluorometric, and electrochemical approaches. The probe demonstrates a substantial color change upon introduction of cyanide ion, along with significant fluorescence quenching proportional to cyanide ion concentration. The potential shift of Fc-DNP in DPV with each addition of cyanide ion signifies the interaction-based detection. The detection mechanism was further validated through NMR titration. Henceforth, Fc-DNP emerges as a cost-effective, simpler probe for cyanide ion across different analytical techniques.

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F 160

Synthesis and characterization of Dy^{3+} ion doped $MgGa_2O_4$ nanophosphor.

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ABSTRACT

$MgGa_2O_4$ (Magnesium gallate) is an excellent host matrix for the doping of many RE and TM ions, since it is one of the stable ultrawide bandgap oxide semiconductor materials. It has high chemical and thermal stability, which exhibits stable optoelectronic properties. In this study we synthesized Magnesium gallate ($MgGa_2O_4$) and rare earth ion Dy^{3+} doped nanophosphors by solution combustion method. The PXRD of the synthesized nanophosphors are well matched with the JCPDS data (10-0113). $MgGa_2O_4$ belongs to the space group Fd3m, having a cubic structure. Using the PXRD data and Scherrer formula, the average crystallite size was determined and found to be around 30 nm. The SEM micrographs revealed the surface morphology of the sample with occurrence of spherical, agglomerated and porous particles of non-uniform distribution. The band gap of the pure and Dy^{3+} doped $MgGa_2O_4$ were determined by Tauc plot varies between (4.61-3.59 eV). The photoluminescence spectra of the pure $MgGa_2O_4$ reveal a broad emission band in the range of (625–800 nm) with the sharp peak at 696 nm and weaker peaks at 467 nm and 577 nm under 356 nm excitation the observed luminescence originates from the intrinsic defects in the host. The PL emission peaks are observed at wavelengths 482, 577 and 668 nm respectively at excitation wavelength of 356 nm in the doped phosphors. The emissions of Dy^{3+} are caused by the transitions of $^4F_{9/2}\rightarrow{}^6H_{15/2}$,, $^4F_{9/2}\rightarrow{}^6H_{13/2}$, $^4F_{9/2}\rightarrow{}^6H_{11/2}$,respectively, which shows that $MgGa_2O_4$ phosphors doped with Dy^{3+} ions have the potentiality to be applied for white LEDs applications.

Key Words: Solution combustion synthesis, Energy band gap, Emission and excitation wavelength, Photoluminescence, LED applications.

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Unlocking the Bifunctional Application of Vanadium Oxide Modified Nanotitania: Utilization of the Nanocomposite in Photodegradation of Industrial Dyes and as a Labelling Agent for The Visualization of Latent Fingerprint Analysis in Forensic Investigation

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ABSTRACT

In search of the treatment of dye-contaminated water using a suitable photocatalyst, TiO_2-V_2O_5 nanocomposites are found to be a suitable candidate, as evidenced from the present study. The prepared nanocomposites are also explored for the visualization of latent fingerprints in forensic analysis and it is found that the visualized patterns exhibit well-defined ridge characteristics, high sensitivity, high adherence to the substrate surface and low background interference proving its efficiency in forensic application. Microstructural analysis of the sol-gel synthesized nanocomposites has been performed by XRD, FESEM-EDX and FTIR. The optical spectroscopic analysis showed a shift in the absorption edge towards the longer wavelength region and thus a decreasing trend in the energy band gap as the concentration of V_2O_5 in the nanocomposite increases. The photoluminescence study conducted on the synthesized samples revealed the impact of V_2O_5 on the recombination rate of electron-hole pairs in the nanocomposite which has a direct influence in photocatalytic activity. Further study was carried out by selecting industrial dyes such as rhodamine blue and rose bengal under UV light irradiation and found that the synthesized nanocomposites are highly effective for photocatalytic dye degradation and thereby removing organic pollutants from contaminated water. In conclusion, our present study into dye photodegradation and visualization of fingerprints in forensic analysis provide valuable knowledge which highlights the potentiality of the synthesized nanocomposites in environmental remediation as well as forensic investigation at crime scenes.

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F 162

Carbon Quantum Dots in Zinc Oxide Eugenol Cement for Enhanced Detection and Removal of Dental Implant Cement Residues

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ABSTRACT

Marginal retention of dental cement during implant cementation procedure causes peri-implantitis. The removal of these cement residues before setting time is challenging. We aim to detect and remove cement residues by embedding Carbon Quantum Dots (CQD) in dental cement. A 2 nm CQD is synthesized via thermal decomposition using citric acid and diethylene glycol as precursors. Physicochemical characterization reveals that CQD incorporated zinc oxide eugenol (ZOE-CQD) consisted of cuboid, hexagonal prism, thin rods, near-spheroid, and irregularly shaped particles. Zinc oxide particles are crystalline, and the hexagonal wurtzite phase of zinc oxide was observed in ZOE-CQD. The Infrared (IR) band at 3375 cm^{-1} is observed due to the extensive O-H stretching of eugenol and CQD. The absorption peak at 376 nm was accredited to the n-π* transition of the C=O band and π-π* transition of the conjugated C=C band of the CQD. Four different concentrations of CQD were tested with ZOE, namely 12, 16, 20, and 30 mg/ml. ZOE with 20 mg/ml CQD concentration exhibited greater luminescence. A quenching effect was observed in the CQD concentration above 20 mg/ml due to the chemical interaction between Zn^{2+} metal ion and CQD. The overlapping of the absorption and emission spectra of zinc oxide, eugenol, and CQD leads to the inner filter effect. Therefore, a CQD concentration of 20 mg/ml can be used for detecting cement residues. In conclusion, this research demonstrates that incorporating fluorescent CQD into ZOE cement can significantly aid in the detection of cement residues when compared to conventional zinc oxide cement.

Keywords: Carbon quantum dots, dental cement, peri-implant disease, fluorescent agent, nanoparticles, cement residues

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Development of Magnetically Retrievable Heterogeneous Nanocatalysts for Diverse Applications

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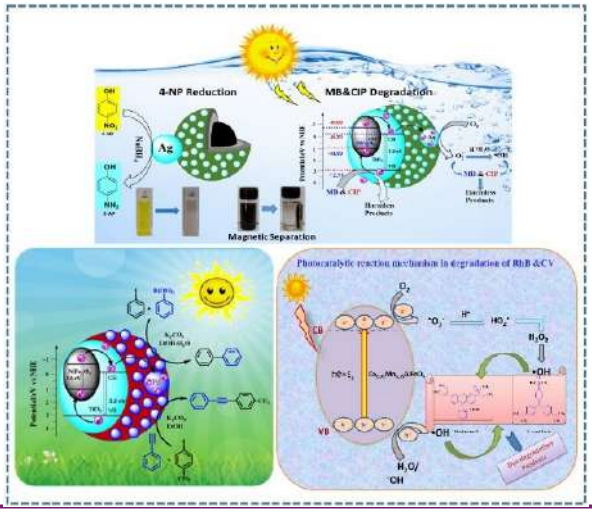
ABSTRACT

Over the past few years, heterogeneous nano catalysis has become a growing field of study. In the direction of sustainability there is a great demand for reusable catalysts in the field of catalysis. To achieve this, the recovery of the catalyst after completion of the reaction by simple means is vital. Recovery of the catalyst by centrifugation, filtration is tedious process. Best alternate method is magnetic recovery of the catalyst with the aid of an external magnet for which the catalyst must be magnetic in nature. To address this we have developed few ferrite based heterogeneous magnetic nanocatalysts by simple method with unique features and will be discussed in this presentation. Their applications were explored in diverse fields for organic transformations particularly in synthesizing pharmaceuticals, agrochemicals, fine chemicals and photocatalytic applications in degradation of toxic dyes, antibiotics, etc. In these catalysts, mixed spinel ferrites were used as catalysts as such or can be used as a catalyst support for further functionalization with active metal nanoparticles (NPs). To accommodate active metal NPs without agglomeration on the catalyst support, the supports are coated with different linkers such as polymers to hold the metal NPs. Basically spinel ferrites are semiconductors with band gap falling in visible region so that they can be used as photocatalysts. To avoid the recombination of e^- - h^+ pairs and to tune the band gap, spinel ferrites can be combined with other semiconductors to form heterojunctions or composites to develop visible light active photocatalysts. In this work, ferrite based nanocatalysts such as Aluminium doped Co-Mn mixed ferrite, active metal NPs immobilized PDA coated ferrite composites for coupling reactions, catalytic reduction of nitrocompounds, photocatalytic degradation of toxic dyes and antibiotic colorless pollutants will be discussed.



F 164

Thermal and Chemical Reduction of Graphene Oxide: Effect of Temperature and Concentration of Reducing Agent on the Purity of the Reduced Graphene Oxide

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ABSTRACT

Graphene oxide (GO) is a single layer of carbon atoms arranged in a hexagonal lattice obtained from the oxidation of graphite flakes using the modified Hummers' method. In the Hummers' method, graphite is treated with a mixture of sulfuric acid, sodium nitrate, and potassium permanganate, leading to the insertion of oxygen-containing functional groups, such as epoxides, hydroxyls, and carboxyls, onto the graphene layers. The resulting graphene oxide is hydrophilic and possesses excellent dispersibility in water. Further reduced graphene oxide (RGO) can be obtained from GO by chemical method using different reductants like L-Ascorbic acid and sodium borohydride or by thermal reduction. The degree of oxidation and the purity of the obtained RGO were investigated by Scanning electron microscopy, Electron dispersive spectroscopy, Raman Spectroscopy, and Ultraviolet–Visible Spectroscopy methods. Both methods of reduction have shown a higher carbon-to-oxygen ratio, but high-quality RGO can be obtained by thermal reduction with a temperature of around 350 ˚C at atmospheric pressure.

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F 165

Synthesis of Nickle Sulphide on a Nickle-Iron Layered Double Hydroxide (NiFe-LDH) Matrix for Electrocatalytic Water Splitting

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ABSTRACT

Our study introduces a novel electrocatalyst for the bi-functional application (OER+HER) comprised of Nickel sulfide[1] (NiS) supported on a Nickel-Iron Layered Double Hydroxide (NiFe-LDH) matrix[2]. The composite material, synthesized through a facile hydrothermal method, exhibits well-defined structural features. Characterization using XRD, SEM, TEM, XPS and EDS confirms successful integration, highlighting the crystallinity and surface area of the catalyst. Electrochemical evaluations reveal superior OER as well as HER performance for the NiS/NiFe-LDH composite, displaying reduced overpotential and enhanced stability compared to individual components. Synergistic effects between NiS and NiFe-LDH contribute to optimized charge transfer kinetics and increased active sites. EIS analysis indicates improved electron transport, making the composite a promising candidate for efficient HER and OER applications in energy conversion systems.

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Effect of Biaxial Strain on Transport and Magnetoresistance in $La_{0.5}Pr_{0.2}Ba_{0.3}MnO_3$ Manganite Thin Films

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ABSTRACT

A series of $La_{0.5}Pr_{0.2}Ba_{0.3}MnO_3$ (LPBMO) manganite thin films were deposited on (100) $SrTiO_3$ substrate by pulsed laser deposition. The manganite films are biaxially strained due to positive substrate lattice mismatch. Decrease of the metal-to-insulator transition temperature T_p with increasing lattice distortion ε_{bi} has been observed. Furthermore, the magnetoresistance of the manganite films was found to strongly increase with increasing film thickness. An anomalous upturn of resistivity in the low-temperature regime (T<50 K) has been detected, which is attributed to enhanced Coulomb interaction of the charge carriers resulting from disorder due to the lattice distortion. Our analysis clearly demonstrates the importance of biaxial strain and Jahn-Teller-type lattice distortions for the physics of the LPBMO manganite thin films.

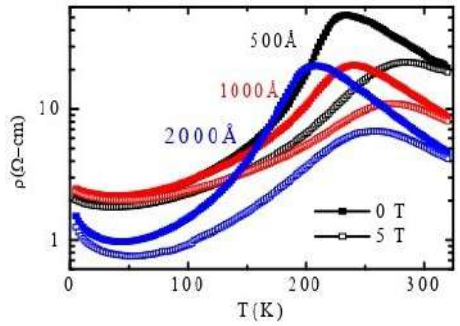

FIGURE 1. Resistivity (ρ) (Ω-cm) vs. Temperature (K) plots for LPBMO/STO thin films

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F 167

Schottky Barriers To Self-Organized Quantum Dot CdS Films

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ABSTRACT

Self-organized nanocrystalline and bulk CdS thin films have been deposited through wet-electrochemical technique. The optical, structural and morphological properties were studied thoroughly. A clear blue shift in the energy gap from 2.40 to 3.30 eV is observed for bulk to nanocrystalline CdS. Schottky diodes have been fabricated with bulk and nanocrystalline CdS with the configuration Au/bulk CdS/ITO and Au/Q-CdS/ITO. The thermionic emission model has been used to calculate device parameters. The value of series resistance (Rs), diode quality factor (n) and the barrier height (Φ_b) for Q-CdS diode are 750 Ω, 5.62 eV, and 0.39 eV were calculated from current voltage (I-V) curve. The carrier concentration, diffusion voltage, width of space charge layer and the electric field have been calculated from Capacitance-Voltage (C-V) measurement.

Keywords: *CdS thin films, self-organized Q-Dots, Schottky diode, X-ray diffraction, UV-vis spectroscopy*

F 168

Study of Near Band Edge Emission Spectra and Conductivity Transformation in Fe doped Cadmium Telluride Nanoparticles for the Light Emitting Diode Applications

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ABSTRACT

The research work discussed here explains about the photoluminescence (PL) and electrical properties of the Iron (Fe) doped Cadmium Telluride (CdTe) Nanoparticles (NPs) synthesized by hydrothermal method. The P-XRD analysis is done to calculate the size and lattice constant of the undoped and Fe doped CdTe NPs. The XPS spectra clearly shows the successful doping of Fe in the CdTe QDs and also the orbital state of Fe in CdTe. The EDAX spectra is taken to trace the elements present in the synthesized nanoparticles. From the UV visible absorption spectrum, the band gap is found to decrease when doped with Fe in different concentrations A near band edge emission property is observed for the Fe doped CdTe NPs when doped with different Fe concentrations. The van der Pauw Hall measurement technique is employed to study the electrical properties such as conductivity, carrier concentration, mobility and Hall coefficient of the undoped and Fe doped CdTe nanoparticles. The consistent p-type conductivity is observed for the undoped CdTe nanoparticles till the time duration of 45 minutes of synthesis. When doped with Fe in 30% concentration, the type of conductivity is found to trans form from p-type to n-type. Such nanoparticles can be employed in the fabrication of light emitting diode applications.

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Chitosan Modified nZVI Nanocomposites for Treatment of Textile Wastewater: OptimizationThrough RSM-CCD

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ABSTRACT

In recent years, there has been a growing emphasis on addressing the environmental impact of textile wastewater, posing a significant threat to aquatic ecosystems and local communities. This study explores the efficiency of a chitosan modified nanoscale zero-valent iron composite (CS@nZVI) in treating textile wastewater, employing the RSM-CCD model. The structural and morphological characteristics of CS@nZVI were analyzed using XRD, FTIR, FESEM, and EDX. CS@nZVI demonstrated notable adsorption capabilities in removing COD, color, and various physico-chemical parameters from textile wastewater. The findings revealed the remarkable efficiency of CS@nZVI in COD and color removal from textile wastewater. Under optimized conditions (pH 6, contact time 60 min, and 1.84 g of CS@nZVI), COD removal reached a maximum of 85.53%, with a decolorization efficiency of 89.73%. The quadratic model, indicated by high R2 (0.98) and AIC (269.75) values, proved to be the best-fitted model for optimizing process parameters in COD removal. Moreover, the physico-chemical parameters were found to be within permissible limits after treatment with CS@nZVI. The influence of coexisting ions on COD removal followed the order $PO^{3-} > SO^{2-} > Cl^{-} > Na^{+} > Ca^{2+}$. Kinetics data aligned wellwith the pseudo-first-order reaction, indicating physisorption as the primary mechanism. Thermodynamic analysis revealed the endothermic nature of the removal process. Reusability tests demonstrated that spent CS@nZVI maintained significant regeneration capacity, retaining 71% effectiveness after five consecutive cycles. These results suggest that the prepared CS@nZVI nanocomposites could serve as a cost-effective, efficient, and environmentally friendly nanosorbent for treating textile effluents, holding substantial potential for commercial applications.

Keywords: *Textile effluent, Adsorption, RSM-CCD, Chitosan, Nanoscale zerovalent iron (nZVI).*

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Anti-Microbial Studies on Nano-Phased Lanthanum Doped Nickel Ferrites Prepared by Citrate Gel Auto-Combustion Method

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ABSTRACT

Lanthanum-doped nickel ferrites prepared by citrate gel auto combustion method. XRD patterns confirms the single-phased cubic spinel structure. No indications of secondary or impurity peaks are observed. Escherichia coli, Pseudomonas aeruginosa, and Staphylococcus aureus are the chosen microorganisms used to assess the antibacterial properties of the lanthanum-doped Nickel ferrite nanopowders. Disc diffusion susceptibility testing is used to determine whether nickel ferrites with lanthanum doping have antibacterial properties. Staphylococcus aureus exhibits a maximum zone of inhibition at all doses, while Escherichia coli exhibits a minimum zone of inhibition at x=0. For Staphylococcus aureus, the largest zone of inhibition is found at x=0, or 2.1 mm, whereas a comparatively lower zone of inhibition is reported for x = 0.01 and x = 0.05. Additionally, all samples exhibit efficient antibacterial activity at lower doses up to 100 g/ml because of their exceptional antibacterial capabilities against Escherichia coli, Staphylococcus aureus, and Pseudomonas aeruginosa, Lanthanum doped Nickel nano ferrites are an excellent source of disinfection in Polluted water bodies with effective qualities that promote microbe inhibition.

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F 171

Enhancing The Efficiency of Water Splitting Through Spin-Filtering Anodic Current Using Chiral Iron-Cobalt Oxide Thin Film Catalysts

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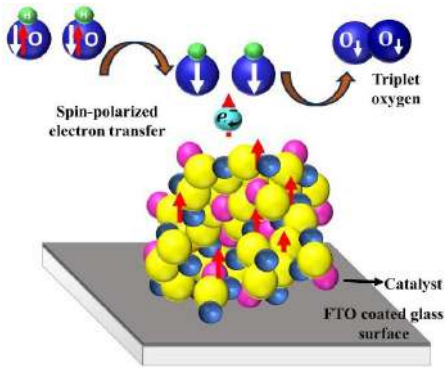
ABSTRACT

Water splitting is considered as an alternative way for a clean substitute for fossil fuels. Namely, it produces hydrogen without a carbon footprint. However, the sluggish oxygen evolution reaction (OER) hinders its extensive application.[1] Recent studies have shown that the chiral molecules manifest a preference for electron spin orientation which is known as the chiral-induced spin selectivity effect.[2] In this study, we demonstrate the enhancement of oxygen evolution reaction kinetics by spin filtering the anodic current by using electrochemically deposited chiral Fe-Co oxide. The overpotential for the OER process is revealed to be smaller for the chiral oxide with respect to the electrochemically deposited achiral Fe-Co oxide. The anodiccurrent density for the chiral oxide at 1.0 V (vs. Ag/AgCl) is almost 1.9 times higher than the achiral Fe- Co oxide. Besides, we experimentally shown the chemical selectivity of the chiral anode for product formation using a neutral electrolyte medium. Production of hydrogen peroxide as the byproduct at higherelectrochemical potential is reduced while using chiral oxide as an anode. This observation is attributed tothe formation of spin-polarized intermediates which help in promoting the oxygen evolution reaction and accounting for the observed outcomes.



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F 172

Synthesis of Silver Nanoparticles Using Bioactive Seaweeds Against Poultry Pathogens

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ABSTRACT

There is an increasing demand to create nanomaterials that are eco-friendly, non-toxic,and less expensive in relation to human health. In order to investigate the effectiveness of the marine macro algae silver nanoparticles against two specific poultry bacterial infections, methanol extracts of *Halimeda macroloba* (green), *Turbinaria conoides* (brown), and *Spyridia filamentosa* (red) were used. The zone of inhibition against the two bacterial pathogens as well as $AgNO_3$ as a control increases with an increase in the concentration of marine macro algae synthesized nanoparticles. The characterization by UV, FTIR, XRD, SEM and EDAX reveals the formation of silver nanoparticle through seaweeds and the LC-MS data reveals the presence of bioactive compounds which exhibit antibacterial activity. Thus the chemical compounds such as phyllophenone and phorbasterone present in the marine macro algae may be responsible for the antibacterial action of poultry pathogens such as *Staphylococcus aureus* and *Salmonella typhi* according to LC-MS characterizations.

Key words: *Halimeda macroloba- Turbinaria conoides- Spyridia filamentosa*, LC –MS characterization, *S. aureus*, *S. typhi*.

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F 173

Synergistic Enhancement of ZnO Nanoparticles with Carica Papaya Leaf Extract: Synthesis, Characterization, and Multifunctional Applications

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ABSTRACT

The comprehensive analysis of the ZnO and ZnO + CPLE composite reveals significant improvements in their structural, optical, and morphological properties. XRD analysis indicates changes in peak positions, intensities, and crystallite size, suggesting an interaction between ZnO and CPLE. FTIR analysis confirms the presence of organic functional groups from CPLE, impacting the surface interactions of ZnO. UV analysis demonstrates tunability in the band gap energy, opening avenues for tailored optical properties. SEM and EDAX analyses provide insights into the morphological variations and elemental composition, showcasing the successful incorporation of CPLE into ZnO. DLS analysis reveals a more monodisperse system in ZnO + CPLE, suggesting a size-modifying influence of CPLE. Antibacterial activity assays demonstrate a synergistic enhancement in ZnO + CPLE, particularly against S. aureus, B. subtilis, and E. coli. The MTT assay reveals promising anticancer activity of ZnO + CPLE against MCF-7 breast cancer cells.

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Polydopamine Modified Graphene Oxide Nanocomposite Membranes for Efficient Dye Removal from Water

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ABSTRACT

In recent years, industrialization has caused numerous adverse effects on environment. One of them is the water pollution caused by dyes waste from textile industries. Nanotechnology is playing a significant role in combating environmental issues [1]. Graphene, the most versatile material, has created a prominent place in research in the recent past [2]. Porous structure of Graphene Oxide (GO) laminates enables its use in separation and purification application [3, 4]. Studies demonstrate that micrometer thick graphene oxide membranes are utterly impermeable to gases, liquids while permitting unrestricted permeation of water [5]. Herein we report the synthesis of nanocomposite membranes of Graphene oxide (GO) with polyacrylonitrile (PAN) polymer via phase inversion method for dye removal application. Graphene Oxide has been synthesized via Hummer's method followed by the modification with polydopamine (PDA-GO). Dopamine polymerized to polydopamine (PDA) through oxidative polymerization is helpful in adhering to other surfaces. PAN membrane has been fabricated containing different ratios of PDA- GO(2, 5 and 10wt%) within the matrix. Membranes without PDA coated GO, pure PAN has been prepared for the comparison. Prepared membranes have been examined for water permeation and dye rejection performance. P-PDAGO5(5wt% PDA-GO) membrane shows the best water permeation performance among all prepared membranes. Membranes have been found effective towards Congo red dye rejection.

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SnSe Nanoparticles-Lysozyme Interaction: Study of Binding and Quenching with EnergyTransfer Process

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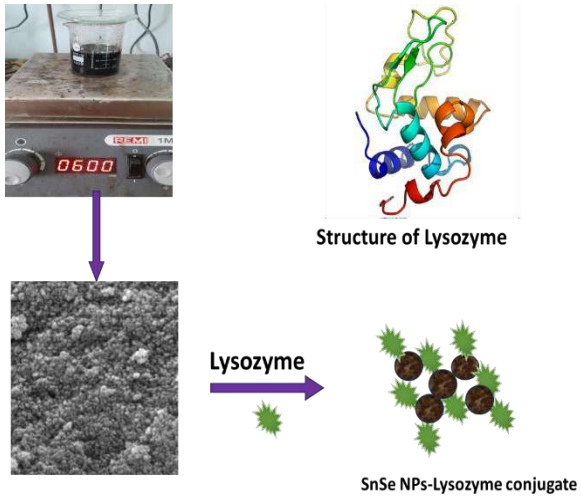
Abstract

Now a days Nanoparticles are widely being used in nano-based therapies and in the different field of biomedical applications. In this work, the interaction of Lysozyme with synthesized SnSe nanoparticles is studied. The SnSe nanoparticles are synthesized using chemical precipitation method at room temperature within 30 minutes of reaction. The crystal phase of grown SnSe is orthorhombic. The average size of the SnSe nanocrystal is ≈ 12.5 nm with spherical particle nature observed from XRD and FESEM, respectively. According to the optical spectroscopy analysis, there is a noticeable red emission and a band gap range of ≈2.2 eV. The interaction of the fabricated SnSe nanoparticles with Lysozyme showed formation of ground state complex. The visual image of the Lysozyme coronaaround SnSe NP has been observed from HRTEM image. The quenching of the Lysozyme during interaction has been observed from emission spectrum. Denaturation and energy transfer have been analysed. TCSPC study showed the variation of dose dependent life time of carrier SnSe Nanoparticles-Lysozyme bioconjugate.



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Metal-Organic Frameworks Based Triboelectric Nanogenerator as A Self-Powered Motion Sensor

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ABSTRACT

Self-powered sensors are gaining attention nowadays because of their flexibility in various applications. Wearable technology demands self-powered sensors drastically [1]. Self-powered sensors can be easily constructed using a Triboelectric nanogenerator, which works based on the principle of contact electrification and electrostatic induction. TENG converts mechanical energy into electrical energy [2]. Based on the difference in charge affinity, a triboelectric series is set up, which demands novel materials. Metal-Organic Frameworks are the novel materials getting added to this series. This paper discusses the triboelectric property of ZIF-8, a sub-class of MOF, and it can be employed as a self-powered tactile sensor [3]. The open circuit voltage obtained for the Z-TENG is 75 V, and the short circuit current of 12 µA. The device is used to power a display based on the touching activity of a human hand. Fig 1 denotes the exploded view of Z-TENG motion sensor and the simulated structure of ZIF-8 is also included.

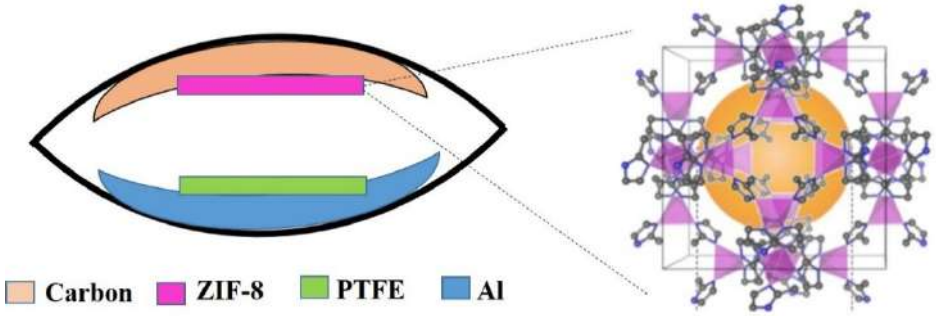

Fig 1. ZIF-8 based triboelectric nanogenerator as motion sensor

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Ce-Decorated Iron Boride-Based Bifunctional Electrocatalyst for Enhanced Green Hydrogen Production

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ABSTRACT

Electrochemical hydrolysis has emerged as the most promising and eminent alternative to deleterious hydrocarbon sources. Recently, the research community has been highly influenced by the amalgamation of rare earth metals and metal borides. Here, a detailed study of $Fe_{(1-x)}Ce_xB$ (x=0.02, 0.04, 0.06) anchored directly on Nickel foam (NF) using the chemical reduction method is utilized to investigate the bifunctional electrocatalytic activity in wide pH. The as-prepared electrode was characterized to evaluate structural and morphological characterizations using XRD, SEM, HR-TEM, XPS, and EDS. Moreover, the electrochemical study proved that the $Fe_{0.96}Ce_{0.04}B$ catalyst is highly efficient for hydrogen-oxygen evolution in water with an overpotential 239 mV vs RHE and 1.5 V, respectively at the current density of 10 mA/cm^2 along with lower Tafel slope value symbolizing improved chemical kinetics. Additionally, the long-term stability and durability for $Fe_{0.96}Ce_{0.04}B$ were confirmed at a high current density of 150 mA/cm^2 for over 15 hours. The present work shows the collaboration of native elements and metal borides to be a promising relationship for connecting the bridge between lab and industrial-scale energy production

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F 178

Binder Free Growth of V-Cu_2S 3D-Catalytic Network for Water Electrolysis at Industrial Scale

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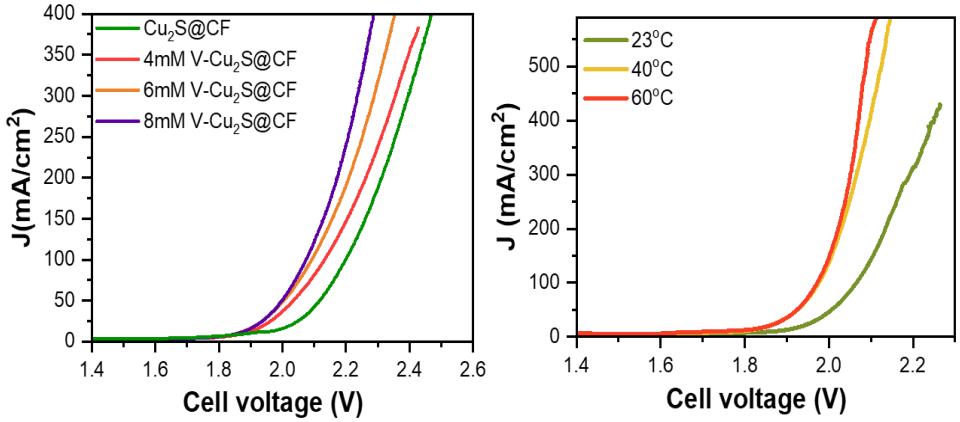
ABSTRACT

We report a facile synthesis of self-supported 3D-catalytic network composed of V-Cu_2S nanosheets on copper foam. This advanced and polymeric binder free catalytic network is intended for use in large-scale water splitting operations at industrial-level current densities. The incorporation of vanadium significantly enhances catalytic performance for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in an alkaline electrolyte, enabling the attainment of current densities surpassing 500 mA/cm^2. This improvement is ascribed to the reduction in charge transfer resistance, optimized intermediate adsorption/desorption processes, and an increased electrochemical surface area. The bi-functional alkaline water electrolyser demonstrates exceptional catalytic performance, realizing a current density of 100 mA/cm^2 at 2.07 V and 300 mA/cm^2 at 2.23 V in 1M KOH electrolyte. To meet the demands of industrial-scale hydrogen and oxygen production, the V-Cu_2S@CF electrolyzer attains a current density of 500 mA/cm^2 at a cell voltage of 2.12 V when operating at elevated temperatures and utilizing an industrial alkaline electrolyte (5M KOH). This development in catalytic efficiency and performance holds promise for the scalable production of hydrogen and oxygen in industrial settings, marking a significant step forward in sustainable energy generation.



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F 179

Development And Experimental Investigation of Graphene Oxide And Silicon Carbide Nanoparticles as Lubricant Additives In Modified Waste Sunflower Oil

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ABSTRACT

The demand for alternate lubricants has increased in recent years due to the economic and environmental consequences of conventional mineral-based lubricants in the manufacturing industry. The disadvantage of mineral-based lubricants is replaced with vegetable-based lubricants but pure vegetable oils are not economically feasible. So, the use of waste cooking oil, which is considered to be a pollutant is used for green lubricant development. In this work, the waste sunflower oil is chemically modified by esterification and then epoxidized to develop lubricant oils and experimentally investigated the tribological properties, rheological properties, and physiochemical properties. The Graphene oxide nanoparticles (GO) and Silicon Carbide (SiC) nanoparticles were dispersed with optimum concentration to the esterified epoxidized waste sunflower oil (EEWSO) as a lubricant additive. From the experimental results, it is observed that the double-stage chemical modification of waste sunflower oil improved the lubricant properties. Also, the effect of GO and SiC nanoparticles shows that they can be used as antiwear and antifriction additives in lubricant samples. The synergistic interaction of GO, SiC, and EEWSO demonstrates that adding 0.5 weight % GO and 0.04 weight % SiC nanoparticles to biolubricant samples increased their thermal conductivity by 9%, decreased wear scar diameter and coefficient of friction by 43.9%, and 51.3% respectively in comparison to waste sunflower oil.

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Substrate dependent fractal behaviors of Hot Wire Chemical Vapor Deposited Hydrogenated Silicon Thin Films

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ABSTRACT

This study is focused on the synthesis and experimental analysis of nc-Si:H films on various substrates. Herein, nanocrystalline hydrogenated silicon (nc-Si:H) films were synthesized by hot-wire chemical vapor deposition (HWCVD) process at a low substrate temperature of 250 ^{o}C on different substrates. The nc-Si:H films were investigated by various methods including X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), Fourier transform infrared (FTIR) spectroscopy, and Raman spectroscopy to probe the morphology, structural, vibrational and electronic properties. The deposition rate varied from 24.04 nm/min for the silicon substrate to 15.04 nm/min for the quartz substrate. The fractal dimensions of the nc-Si:H surface varied from 0.816 to 0.965 by using the power spectral density function (PSDF), partition function, cube counting and triangulation counting. Raman analysis shows the crystalline fraction varied from 43 to 63%. The hydrogen content remains <7-11 at.% with different substrates confirmed from the FTIR study. XPS data confirms the doublet formation in the glass substrate and the highest rate of Si-Si bond formation in Si substrate.

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Investigation on Barrier Layers of Pt/BT/Pt Based Thin Film Capacitors

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ABSTRACT

Barium titanate is a ferroelectric material used as a dielectric in thin film capacitors owing to its high dielectric constant. Barrier layers are utilized in these capacitors to improve the capacitors' performance by controlling the microstructure and creating thin resistive films. In this paper, zinc oxide and aluminium oxide are kept on both sides of Barium titanate as barrier layers in Pt/BT/Pt capacitors and different dielectric properties are studied. The performance parameters such as capacitance, leakage current, equivalent series resistance, dielectric loss and dielectric strength of Pt/BT/Pt thin film capacitors with barrier layers of different sizes are simulated using COMSOL Multiphysics modelling software. Aluminium oxide of 2nm thickness as a barrier layer gives optimal performance. The leakage current, dielectric loss, capacitance, equivalent series resistance and dielectric strength of Pt/BT/Pt capacitor are found to be 5.19×10^{-4}A, 9.62×10^{-12}, 4.32fF, 9.62kΩ, 10^8 V/m respectively whereas that of Pt/ALO/BT/ALO/Pt capacitor are found to be 1.56×10^{-18}A, 7.81×10^{-18}, 2.9fF, 9.01×10^{15}Ω, 5.05×10^9 V/m respectively. The low capacitance in Pt/ALO/BT/ALO/Pt capacitor is due to the low dielectric constant of aluminium dioxide barrier layer. The reduced leakage current and increased equivalent series resistance are due to the low conductivity of the aluminium oxide barrier layer. The use of aluminium oxide barrier layer between the conductive surfaces can reduce the electric field and increase the breakdown voltage, leading to improved dielectric strength and reduced dielectric loss.

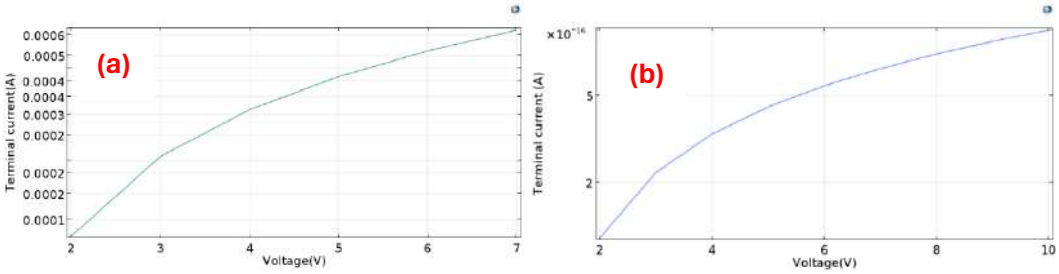

Figure 1: Leakage current of (a) Pt/BT/Pt and (b)Pt/ALO/BT/ALO/Pt thin film capacitors

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Effect Of Nitridation Temperature on the Synthesis of GaN Fibers by Electrospinning Method

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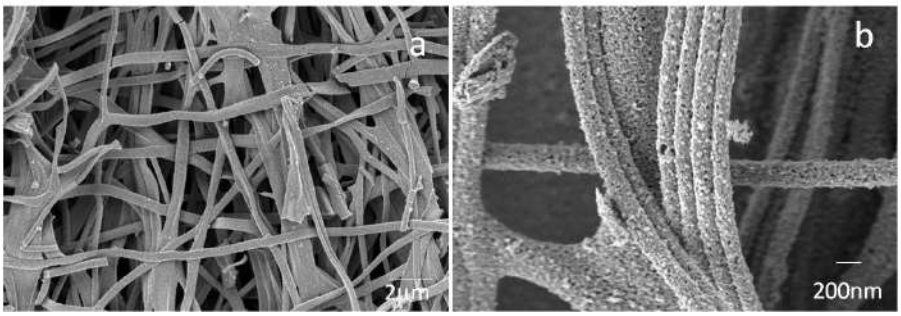
ABSTRACT

GaN fibers were prepared using facile electrospinning method and the effect of nitridation temperature on the structural and optical properties have been studied. Gallium nitride (GaN) is one of the most promising compound semiconductor materials among III-nitride family because of its excellent properties which comprise wide direct bandgap, high thermal stability, excellent electron mobility, high physical and chemical stabilities [1]. 1D GaN nanostructures like nanowire/nanofibers are receiving much attention because of their high surface area, excellent aspect ratio and effective electronic properties. Several methods were used to synthesis nano dimensional gallium nitride [2], the electrospinning technique is one of the simplest methods for the growth of one-dimensional continuous fibers in nanometer range[3]. The XRD analysis confirms the formation of gallium oxide fibers at 750ºC and highly crystalline wurtzite gallium nitride fibers at 850ºC. The optical phonon modes were determined from micro-Raman studies. The strong E_2 (high) phonon mode observed in the sample synthesized at 850ºC shows a sharp and intense peak at 568 cm^{-1}, which signifies the high crystalline nature of the GaN fibers. The additional peak at 273 cm^{-1} is attributed to phonon frequency at the 'k' point of the Brillion zone in wurtzite GaN fibers. SEM analysis shows smooth and continuous fibers like morphology of GaN with a diameter ranging from 100 to 400 nm. Diffuse reflectance spectroscopy spectra were used to calculate the band gap of the GaN fibers. These results exhibit that, the GaN fibers are a potential candidate for optoelectronic devices such as gas sensors and UV photodetectors.



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Thin-Film graphene/SnS_2/g-C_3N_4 Heterojunction Photocatalyst by CVD Method

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ABSTRACT

Artificial photosynthesis is a technology that uses sunlight to convert water and carbon dioxide into valuable solar fuels through photocatalysis and is attracting attention as a technology that simultaneously overcomes the problems of global warming and energy supply [1]. However, the rapid recombination of photogenerated electron-hole pairs in the process of photocatalysis has significantly reduced the efficiency of photoelectric conversion, limiting its practical application. In this study, we form sheet graphene/SnS_2/g-C_3N_4 stacked heterojunctions by using the CVD method. This method is expected to improve the photoelectric conversion efficiency and catalytic activity by securing a large junction area and facilitating charge separation at the junction interface. Graphitic carbon nitride (g-C_3N_4) has a band gap of 2.7 eV and a CB edge of -1.4 eV (vs. NHE, pH0), and has attracted attention as a photocatalyst with strong reducing power [2]. SnS_2 has a band gap of 2.18-2.44 eV and has attracted attention as a visible light absorption photocatalyst [2]. We grow graphene as a charge transport film on a synthetic quartz substrate, followed by SnS_2 and g-C_3N_4 to form stacked heterojunctions (Fig. 1). As shown in Fig. 2, the Raman spectra of each single thin film confirm the bands that characterize each, indicating that the crystals can be grown successfully. In addition, the graphene/SnS_2/g-C_3N_4 heterojunction photocatalyst shows enhanced D and G bands due to the six-membered rings compared to the single thin film, indicating epitaxial growth and successfully formed a heterojunction.

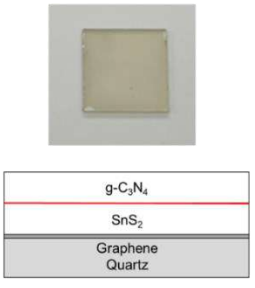

Fig. 1 graphene/SnS_2/g-C_3N_4 stacked heterojunction thin film

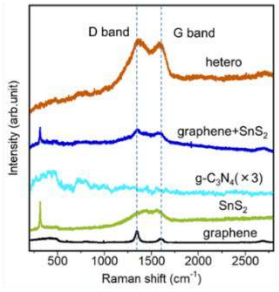

Fig. 2 Raman spectra of each thin film

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A Pseudo-Double Z-Scheme of SnS_2/g-C_3N_4 With Effective Visible-Light Photocatalytic Performance

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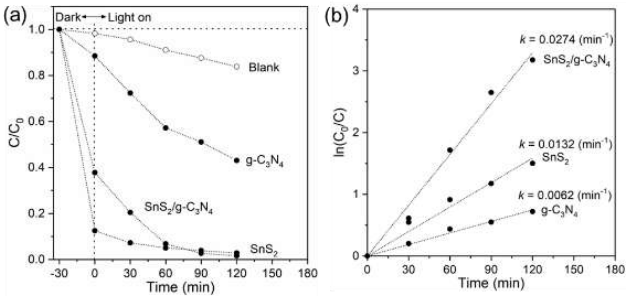
ABSTRACT

Nowadays an ideal approach for solving environmental pollution is the main concern. Constructing a direct Z-scheme between two semiconductors reduces its recombination and enhances its efficiency than using a single component is one of the new approaches. Formation of Z-scheme in SnS_2/g-C_3N_4 composites by attaching SnS_2 nanoparticles on the surface of g-C_3N_4 gives a well-attached junction area between it shows an enhanced photocatalytic performance. Then, SnS_2/ g-C_3N_4 composites are prepared by ultra-sonication and hydrothermal methods while its structural analysis, morphological, optical properties, surface area, and element composition were analyzed using XRD, SEM, TEM, UV-Vis, BET, and XPS respectively. The photocatalytic performance was done by using a very weak power light source (LED Solar lamp with Power - 16.9 W) towards the degradation of methylene blue dye. Under photoexcitation, a charge transfer occurred when the photoexcited electrons in SnS_2 combined with the holes of g-C_3N_4, which enhanced the extraction and utilized the photoinduced electrons in g-C_3N_4. This photoexcited electrons and holes which efficiently degrade the dye into a non-toxic pollutant. Then, SnS_2/g-C_3N_4 (urea-based) shows promising photocatalytic materials for dye degradation.



(a) MB adsorption curve and photocatalytic degradation of MB on g-C_3N_4, SnS_2, and SnS_2/g-C_3N_4 composites in the dark and under visible-light irradiation, (b) linear transform ln(C_0/C) of the kinetic curves of MB degradation.

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Formation of 3-Dimensional Electrodes for High Response and Wide Range Detection of Glucose Sensors

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ABSTRACT

Glucose sensors have been considerably explored due to their wide range of uses, particularly in diabetes diagnosis[1]. Electrochemical enzymatic glucose sensors are currently widely used in daily life for glucose detection and have been commercially successful as glucose meters due to their outstanding selectivity, high reliability, and ability to operate under physiological pH levels. Despite the inherent limitations of enzymes, such as high fabrication cost and poor stability, non-enzymatic glucose sensors have sparked increased research interest in recent years due to their low cost, high stability, rapid response, and low detection limit[2]. Furthermore, the advancement of nanotechnology has provided new potential to create nanostructured electrodes for glucose sensing applications. In this work, the alcohol chemical vapor deposition approach was used to deposit graphene on the three-dimensional nickel foam at 1000 °C. It is anticipated that this technique will enhance the uniform distribution of graphene and function as a layer for charge transmission on nickel foam. The deposition of graphene on the 3D-Ni foam is visible in the scanning electron microscopy image, as depicted in Figure 1. Furthermore, the Raman analysis's detection of the G-band (1581 cm^{-1}) indicates the presence of graphene, as seen in Fig. 2.

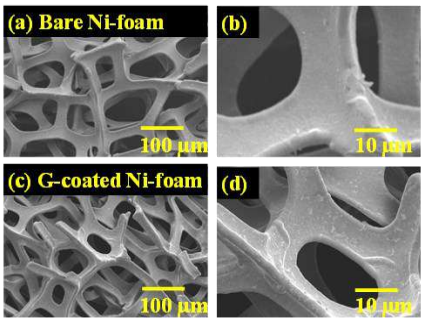

Fig.1 SEM image of Bare & Graphene deposited Ni-foam

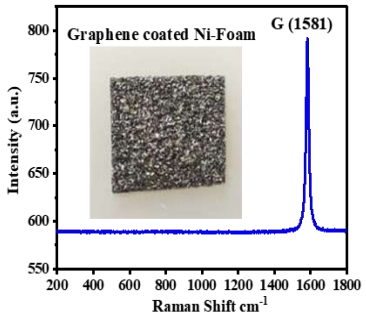

Fig.2 Raman Spectra of Graphene deposited Ni-foam

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AuAg Bimetallic Nanoparticles: A Promising Catalyst for the Reduction of Hexavalent Chromium and Anionic Dyes

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ABSTRACT

Chronic inhalation of Hexavalent Chromium [Cr(VI)] increases the risk of respiratory cancers. It is a heavy metal which is highly toxic and one of the major environmental contaminant. Chemical reduction of Cr(VI) to Cr(III) has attracted a lot of interest in the past few years because, the reduction product [Cr(III)] is one of the essential nutrient for organisms. Various nanoparticle-based systems have been designed for the conversion of Cr(VI) into Cr(III). In this work reduction of Cr(VI) to Cr(III) is effectively done by AuAg bimetallic nanoparticles synthesized by chemical reduction method, using trisodium citrate and ascorbic acid as reducing and stabilizing agents. In presence of formic acid, the catalytic reduction efficiency of AuAg bimetallic nanoparticles against chromium were 98% within 20 minutes. The method is environmentally friendly, since no hazardous chemicals are used. As-synthesized nanoparticles were characterized using X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), Energy dispersive X-ray spectroscopy (EDX), and UV-Visible spectroscopy for analyzing the optical and physicochemical properties. The dye degradation efficiency of the AuAg nanoparticles were tested against the anionic dyes methyl orange and congo red in presence of $NaBH_4$ and it is found that the bimetallic nanoparticles are highly effective in removal of anionic dyes.

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Catalytic Degradation of Organic Dye and Heavy Metal Reduction on Porous Gold Nanostructure

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ABSTRACT

Herein, the kinetically controlled synthesis of porous gold nanostructures is of great importance for their catalytic performance was reported. The formation of porous gold nanostructures using transmetallation reaction (TM reaction) between sacrificial silver nanoparticles and Au(III) ions using an eggshell membrane at room temperature. The optical, morphological, and structural properties of the synthesized nanoparticles were characterized using ultraviolet-visible spectroscopy, field emission scanning electron microscopy (FESEM) with energy-dispersive X-ray (EDX) spectroscopy, and X-ray diffractometry analysis. Further, the Kinetics and mechanism of nanoparticles catalyzed reduction of Hexavalent Chromium Cr(VI) and dye degradation of Methyl orange (MO) and Congo red (CR) using sodium borohydride was monitored using UV-vis spectroscopy. The result revealed that porous gold nanostructures performed as a superior catalyst, which degraded Cr(VI) (82.9%) in 12 min whereas MO (96.86%) and CR (85.71%) degraded within 4 and 6 min respectively. The results demonstrating that nanocatalysts had superlative catalytic activity, which can be applied for environmental-based applications such as dye degradation and removal of heavy metals from aqueous solutions.

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F 188

Insitu Synthesis and Characterization Studies of Nano Titanium Oxide and Its Bio Medical Application

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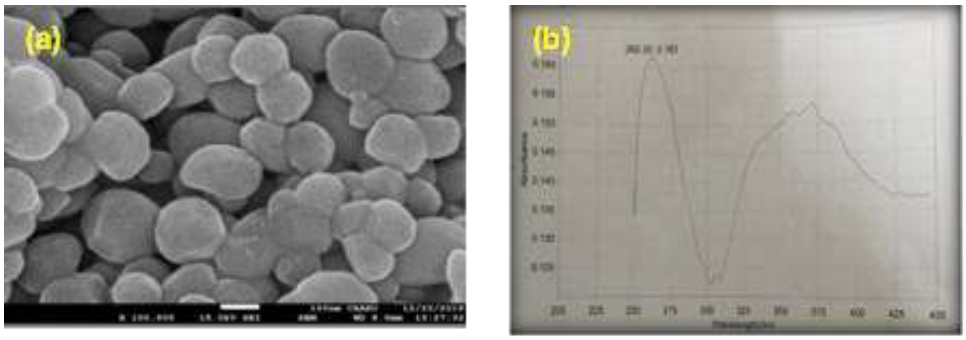
ABSTRACT

Titanium oxide is a white powder extensively used to decontaminate water and food, ensuring environmental and industrial safety, while also serving to protect the skin against harmful radiation. Nano titanium oxide is prepared by using aloe vera gel extract. In the present investigation aloe vera gel was used as reducing agent in the green synthesis of titanium oxide nanoparticles. Nano titanium oxide was synthesized and characterized by using X-ray Diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) and biologically by antimicrobial assays to evaluate their potential use for bio medical applications. The results showed that the size and crystallinity of nano titanium oxide. SEM confirmed the presence of nano spherical morphology of nano titanium oxide

Keywords: Aloe Vera, Green Synthesis, nano titanium oxide , XRD, SEM, Antimicrobial studies



(a)SEM image of nano titanium oxide; (b) UV analysis of nano titanium oxide

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β-Ga_2O_3/Activated Carbon Nanocomposite as Photocatalyst for Dye Degradation Application

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ABSTRACT

Environmental pollution has become a major threat due to development of industrialization. Harmful dyes from textile industries, cosmetics, paints mix into fresh water bodies and are major concern as they are often resistant to biodegradation. Additionally, it has adverse effects on human health such as malfunction of brain, kidneys, liver and central nervous system [1-3]. Many semiconductor metal oxides are used in dye degradation application because they have good physical and chemical properties and their nanocomposite exhibit large surface area, high mobility of charge carrier and catalytic activity. Recently gallium oxide (β-Ga_2O_3) has gained attention of researcher as it is non -toxic and it has excellent thermal and chemical stability [4]. It is a wide band gap semiconductor photocatalyst (4.2 to 4.5eV). Also, strong redox ability of photogenerated electron-hole pairs makes it superior candidate in comparison with commercial TiO_2 [5]. Alternatively, nanocomposite-based photocatalysts were extensively developed for remediation of water pollution [6]. The major strategy for developing a visible light photo-catalyst is a support of metal oxide on activated carbon (AC) due to its larger surface area, high adsorption capacity [7].

In this work β-Ga_2O_3 was synthesized by co-precipitation method followed by calcination at 900°C. X-ray diffraction pattern indicates the formation of monoclinic phase of β-Ga_2O_3. Also, reduction in band gap value was observed for β-Ga_2O_3/AC nanocomposite which attributes to electronic interaction between the nanocomposite. Prepared samples were characterized using FTIR and FE-SEM techniques and degradation of dye has been discussed in detail.

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F 190

Surfactant-Facilitated Surface Functionalized Iron Oxide Nanoparticles with Enhanced Antimicrobial, Antioxidant and Photocatalytic Performance

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ABSTRACT

In the present work, the surface modification of Iron oxide nanoparticles (IONPs) was done using different organic surfactants namely, Sodium dodecyl sulfate (SDS), Cetyltrimethylammonium bromide (CTAB), Ethylenediaminetetraacetic acid (EDTA), and Thioglycolic acid (TGA). X-ray Diffraction (XRD), Field emission scanning electron microscopy (FESEM), Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-ray Spectroscopy (EDS) and UV-Vis spectroscopy characterization techniques etc. confirmed the successful functionalization through alternation in structural, optical and chemical properties of bare IONPs. The antifungal activity was examined against pathogenic fungi *Aspergillus niger* (MZ435863) and *Aspergillus fumigatus* (MZ435922) which unveiled the substantially enhanced antifungal properties of functionalized IONPs. Similarly, the straightened bactericidal effects were exhibited by functionalized IONPs against gram-positive as well as gram negative bacteria. The antioxidant properties were studied by using 2, 2-Diphenyl-1-Picrylhydzayl (DPPH) free radical assay. Furthermore, the photocatalytic dye degradation activity of bare and functionalized IONPs was elucidated toward toxic organic pollutant Malachite green (MG) and Crystal violet (CV) dyes. Hence, the functionalization of IONPs with surfactant is highly efficient approach to achieve potential performance in biomedicine as well sustainable waste water remediation.

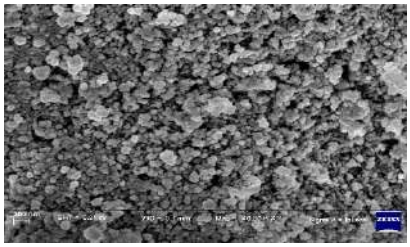

Figure: FESEM image of IONPs at 300 nm resolution

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F 191

Investigation on the Thermoelectric Performance of Ga substituted Bi_2Se_3 for Mid-Temperature Thermoelectric Applications

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ABSTRACT

Thermoelectrics, a promising technology to convert heat into electricity and vice versa. It also gained significant attention due to its peculiar properties of eco-friendly and low maintenance. However, the availability of near room temperature thermoelectric (TE) materials is highly limited, posing a significant challenge in this field. Bi_2Se_3 (Bismuth selenide), a room temperature TE material has attracted much attention owing to its prominent features of n-type to p-type switching and tunable carrier concentration. Here, the series of nanostructured Ga-substituted Bi_2Se_3 ($Bi_{2-x}Ga_xSe_3$; x=0; x=0.05; x=0.1 and x=0.15) samples has prepared through hydrothermal synthesis method followed by cold-pressing densification technique. The as-prepared samples were characterized by XRD, HR-SEM, HR-TEM for structural, morphological and defect analysis. The electrical and thermal transport properties were performed by using Hall effect, thermal conductivity, and Seebeck measurements. The as-prepared samples implies that the negative sign in carrier concentration and Seebeck coefficient confirms the n-type thermoelements. This unique work presents a facile, scalable, cost-effective, and controllable synthesis of nanostructured Bi2Se3 towards high-performance thermoelectric devices.

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Anti-Inflammatory, Antioxidant and Anti-Mycobacterial Effect of Nanocarnosine and Its Anti-TB Drug Composites: A Peptide Based Nanodelivery System for Pulmonary Tuberculosis

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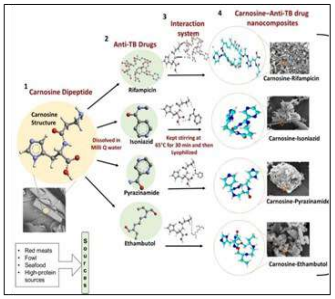
ABSTRACT

The tuberculosis (TB) infection and disease cause altered immune homeostasis and irreversible lung tissue damage leads to functional tissue loss. Host directed therapies with intrinsic anti-inflammatory and antioxidant properties are preferred choice to achieve the immune homeostasis and preserve the functional lung tissue. Carnosine is one such natural dipeptide with intrinsic anti-inflammatory and antioxidant properties and in the present study we have synthesized novel carnosine anti-TB drugs nanocomposites using thermo-hydro-chemical process and characterized their biophysical, biocidal and anti-mycobacterial properties. The spectral analysis using UV measurements established π–π* (214 nm) and n–π* (280 nm) transitions of carnosine along with respective drug during hydrothermal processes. The functional annotation of carnosine-anti- TB drug nanocomposites inhibited protein denaturation in linear ranges (Inhibition % from 65-90% for 1.25–100 µg/mL). Nanocarnosine and carnosine-antiTB drug nanocomposites have comparable cell viability in THP-1 cells with control (>80%). The MIC against the H37Rv Mtb strain were 1 µg/mL, 0.1 µg/mL, >10 µg/mL and >200 µg/mL for carnosine-rifampicin, carnosine-isoniazid, carnosine ethambutol and carnosine-pyrazinamide nanodelivery system respectively. Thus, results reported herein rationalize further investigation on carnosine nanopeptide and carnosine–antiTB drug nanocomposites as a potential drug delivery system for residual lung injury during pulmonary tuberculosis.



Scheme 1: Preparation of Carnosine-Anti-TB drug nanocompositessystem

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Direct Observation of Nanometer Scale Electron Emission Sites in Metal ion implanted/annealed Ultrananocrystalline Diamond Films by Scanning Probe Microscopy

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ABSTRACT

Nowadays miniaturized electron sources based on the principle of electron field emission (EFE) process known as cold-cathodes, are going to substitute the conventional thermionic electron sources. The outstanding EFE properties of diamond, especially ultrananocrystalline diamond (UNCD) makes it an interesting material for cold-cathode applications in vacuum electronic devices. However, the EFE properties of pristine UNCD are poor with higher threshold input bias and lower current density [1]. Metal ions (Pt, Ag) are implanted in UNCD films by ion-implantation techniques followed by post-annealing to enhance the EFE properties. Pt ion implanted/post-annealed UNCD films show low turn-on field (E_0) of 4.17V/μm with high EFE current density (J) of 5.08 mA/cm^2 at an applied field of 7.0 V/μm [2, 3]. Silver (Ag) ion implanted UNCD films have lower E_0 of 8.5 V/μm with J value of 6.2 mA/cm^2 (at an applied field of 20.5 V/μm). Ion implanted films show better EFE properties (lower E_0 values with higher J values) compared to their pristine counterparts. The straight imaging of the electron emitting, grain boundary (Gb, ~1 nm)/non-emitting, grain (G, 2~3 nm) sites in a local scale is directly mapped by the energy dissipation in dynamic scanning tunnelling microscopy (D-STM) mode. Energy dissipation mapping and local I-V measurements illustrate that the Gbs are the conducting/emitting sites. Nanoscale investigation by atomic force microscopy based peak force-controlled tunneling atomic force microscopy (PF-TUNA) and ultra-high vacuum STM based current imaging tunneling spectroscopy (CITS) reveal that the UNCD Gbs are the preferred electron emission sites. However, PF-TUNA measurement is found to be better in explaining the EFE behavior than the STM-based CITS technique.

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F 194

Green Synthesis of Silver Nanoparticles using *Azadirachta Indica* (Neem) Fruit Extract and their Antioxidant, Antibacterial, Anticancer and Catalytic activity

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ABSTRACT

In recent years, inorganic nanoparticles currently being studied extensively because of their several useful applications in science and technology. For the first time, the *Azadirachta indica* (Neem) fruit pulp extract has been used to produce a simple and eco-friendly method of synthesising silver nanoparticles (AgNPs) [9]. The successful formation of silver nanoparticles (NFE-AgNPs) and their characterisation has been done by UV–visible, FT-IR, DLS, XRD, EDX, AFM and HR-TEM techniques. AgNPs production was observed visually as a dark brown colour, which was corroborated by a UV-visible absorbance peak at around 455 nm [2]. FT-IR analysis recognises the functional groups of the phytochemicals that are reason for reduction of Ag^{+} ions to Ag^{0} nanoparticles. That the average hydrodynamic size of the synthesised NFE-AgNPs is 36.8 nm, with a PDI of 2.861 and the Zeta potential is -36.7 mV by DLS. The XRD spectrum represent the face-centred cubic (FCC) of synthesised NFE-AgNPs and the average crystallite size is found to be 20.8 nm [3]. AFM image provides 3D surface topographic imaging, the AFM data revealed that the particles are agglomerated, spherical shape and the average grain size of the sample is below 40 nm. EDX spectrum had high-intensity Ag absorption peaks at 3.2 keV, which may be attributed to the binding energy of silver. The HR-TEM image of NPs indicated nearly spherical mono-scattered with diameters ranging from 5 nm to 50 nm and the average size dispersal was 31.58 nm [4]. The antioxidant ability of AgNPs showed good free radical scavenging activity against DPPH with the percentage of inhibition values at 66.72% with an IC_{50} value of 70.19 µg/mL [5]. The synthesized NPs moderate cytotoxic effect on the A549 cell lines at 100 µg/mL and exhibit 61.07% of cell viability [6]. The antibacterial activity results indicated that these nanoparticles exhibited moderate activity against all four bacteria strains of bacteria and showed the diameter of zone of inhibition 15 mm average at 100 µg/mL [7]. These nanoparticles shown remarkable catalytic activity in the reduction of nitrophenol with sodium borohydride. The NFE-AgNPs formation and their applications will be helpful in developing nanoparticle leads in pharmaceutical fields and nanotechnology.

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Modeling Investigations on Ultra-Fast Capacitive RF MEMS Switch

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ABSTRACT

This paper is focused on designing and modeling of Capacitive RF MEMS Switch with T-shape geometryfor moving beams of varying dimensions (Length: 50µm-500µm, width: 10µm-50µm, thickness: 1µm- 5µm). Selection of materials for moving beam (lightweight SiC), dielectric layer (high dielectric constant Al_2O_3), and fixed electrodes (Gold or copper) are carried out based on the simulation results providing theultrafast response in addition to minimized applied voltage. The proposed switch involves an actuation mechanism depending on the electrostatic principle rather than piezoelectric, electromagnetic, and electromechanical. Furthermore, the moving beam may be provided with a stress-concentrated region (SCR) concept to explore the high response in addition to low power consumption that makes it appropriate for different communication window applications. The aforesaid modeling investigations were carried out using the MEMS Module present in the COMSOL Multiphysics Software tool v 5.2. The modeling investigations exhibited insertion loss is less than 0.35 dB up to 30 GHz, isolation of more than 50 dB, and switching speed which is less than 4µs and found high pull in voltage 23V. From the simulation results, a set of optimized parameters in terms of geometry, materials, and input voltage of the moving beam is finalized. RADAR systems often require fast switching between various RF components,including antennas, transmitters, and receivers. Capacitive RF MEMS switches can assist in achieving rapid switching times and low signal loss, improving RADAR performance by rapid signal routing and offering dynamic adjustments.

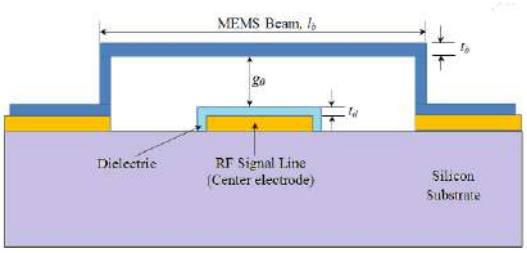

Fig. 1. Proposed schematic diagram of Capacitive RF MEMS Switch.

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F 196

Novel Hybrid Fe_3O_4@Mn-MOF-NH_2 Core-shell MOF as Electrode for Supercapacitors

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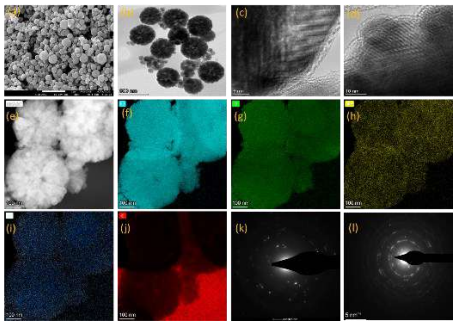
ABSTRACT

Encapsulating an active guest compound into Metal–Organic Frameworks (MOFs) is a very promising technique to achieve properties that are absent in the pristine MOFs and guest molecules. Contrary to the conventional guest encapsulation into the MOF cavities, core–shell composites exhibit better performance in terms of pores accessibility ultimately ensuring an optimal diffusion of the substrate at the same time presenting a unique architecture that prevents the agglomeration and the leaching of the active guests and ensures a tight interaction between core and shell, leading to synergistic effects. Recently, many core–shell MOF hybrids have been reported in various fields, wherein MOFs were hybridized with metal oxides to overcome the intrinsic issues of the parent MOFs. However, the morphological adjustment of MOFs from the parent structure to a core shell morphology still remains unexplained. Herein, a novel flake like MOF was synthesized and further transformed into core-shell hybrid Fe_3O_4@Mn-MOF-NH_2 via sequential growth strategy and an attempt was made to understand the driving force for the change in morphology. This work presents a comprehensive understanding for designing a core shell MOF hybrid with MOF morphology adjustment as a shell on top of metal oxide core. Further, we have used the synthesized Fe_3O_4@Mn-MOF-NH_2 hybrid as an electrode material for supercapacitor and investigated its electrochemical properties. This study provides an insight for the controllable preparation of core shell hybrid MOF architectures which would further broaden the application opportunities of metal-organic framework materials.



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Structural, Optical and Dielectric studies on Hydrothermally synthesised Yttrium Oxide nanoparticles

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ABSTRACT

Nanosized metal oxides have attracted a great deal of attention owing mainly to their physico-chemical properties associated with their technological application. Synthesis of nanosized material is one of the major challenges in the development of advanced functional materials because they exhibit interesting properties conferred by particles of very small dimension in contrast to its corresponding bulk. Yttrium Oxide (Y_2O_3) is a chemically stable rare earth oxide having unique optoelectronic and dielectric properties and are of great interest in various fields due to their potential applications in advanced technologies. The present study focusses on the synthesis and characterization of Yttrium Oxide nanoparticles. The synthesis of nanocrystalline Y_2O_3 samples were achieved by surfactant assisted hydrothermal method with a view to incorporate them in polymer matrices for biosensor applications. The effects of heat-treating on the morphology and crystallinity of nanoparticles were investigated. The synthesized nano materials were characterized by XRD for structure analysis. Field emission scanning electron microscopy (FESEM) with energy-dispersive X-ray (EDX) was performed to elucidate the morphology and elemental composition. The FTIR spectroscopy confirmed the formation of Y_2O_3 from its precursors. Energy band gap and optical constants were evaluated from UV/VIS/NIR absorption spectrum. The dielectric characteristics of the samples were evaluated from impedance spectroscopy. The photoluminescence spectra of the samples were studied. The ferroelectric hysteresis response of the material was also evaluated.

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Exploring *Allium Cepa* as a New Surface Passivating Agent for Synthesis of CdS QD's:From Green synthesis to Highly Fluorescent Molecular Probe

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ABSTRACT

Surface passivation of quantum dots is the inimitable key for eliminating voids, dangling bond and non – stoichiometry present on surface and primarily acting as origin of trap states for electrons, holes or excitons and substantially altering their optical properties. In the present article *Allium Cepa* extract (ACE) first time has been established as a novel surface passivating agent for synthesis of CdS quantum dot's (QD'S) producing significantly high photoluminescence spectra. Highly soluble surface passivated CdS have been developed at 75-80°C temperature in aqueous medium. Fourier transform infrared spectroscopy (FTIR) analysis shows very good interaction of CdS quantum dot with ACE through head groups. X-ray diffraction study confirms predominant formation of cubic CdS. Scanning electron microscopy (SEM) images clearly supports that surface passivation plays important role on size and shape of nanocrystals. UV–visible as well as photoluminescence spectroscopy clearly confirms size and shape-dependent quantum confinement effect of ACE passivated CdS quantum dots. Significant hypsochromic shifting of absorption peak to lower wavelength have been recorded in aqueous solution. Commendable reports have been made on effect of surface functionalization on microstrucral parameters like crystallite size, average strain and dislocation density. Systematic data analysis concludes that ACE passivation results in effective surface passivation resulting in highly fluorescent CdS QD's.

Keywords: *CdS, Allium Cepa extract (ACE), Surface functionalization, XRD, FESEM, UV-VIS analysis*

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Synthesis and Characterization of Ytterbium Oxide nano particles for dielectric applications

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ABSTRACT

Rare earth compounds have been widely used because they possess outstanding optical, electrical, magnetic and catalytic properties. The rare earth compounds in 1-D nanostructures are poised to exhibit extraordinary physical properties as a result of specific size and shape associated with quantum confinement effects. Lanthanide based nanomaterials specifically Yb_2O_3 nanoparticles are considered as potential material for developing highly sensitive biosensors. Their chemical and thermal stability has further supported their application in developing super capacitors and other electrochemical applications. The well controlled optical, luminescence and thermal properties made them useful material in optoelectronics, catalysis and bio imaging applications and paramagnetic devices. In this work Ytterbium oxide nanoparticles were synthesized through wet chemical route using aqueous 0.1 molar solutions of ytterbium nitrate and sodium hydroxide as precursors. The Ytterbium hydroxide nanoparticles thus formed after the reaction turned into Ytterbium oxide nanoparticles on heating to elevated temperatures. After annealing at three different higher temperatures, nanoparticles were structurally characterized by XRD. From Debye Scherer formula, the average particle size is found to be 9.57 nm for 600^{o}C annealed particles and 18.6nm for 900^{o}C annealed nanoparticles. The lattice strain and average grain size were evaluated from W-H plot. The values obtained from W-H plot also agreed very well with the values from Scherer's formula. Formation of the compound from the precursors were confirmed using FTIR. The optical band gap of nanoparticles sintered at three different temperatures were calculated by UV-VIS-NIR spectroscopic analysis. The variation of dielectric constant and loss tangent was studied with varying frequency. Ferroelectric P- E response of the prepared nanoparticles was also investigated.

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Development and characterization of carboxylated copper oxide conjugated polymeric nanocomposites and correlating with computational techniques

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ABSTRACT

The quality and effectiveness of composite-based components are influenced by their mechanical properties. Hence, a structured approach is essential to identify the key factors that contribute to achieving superior mechanical characteristics. This study investigates the utilization of an artificial neural network (ANN) to predict the mechanical characteristics, explicitly density and hardness, of carboxyl copper oxide nanoparticle (CCONP)/Poly Lactic-co-Glycolic Acid (PLGA) nanocomposites fabricated through microwave-assisted sintering. The research explores the effects of various microwave sintering conditions on the microstructure and mechanical properties of the nanocomposites. Physical characterization techniques including FTIR and TEM analysis are employed to confirm physical interactions and nanocomposite size. A back-propagation neural network with a 2–10-2 structural design and Levenberg-Marquardt algorithm is developed to predict density and hardness. The predicted values are compared with experimental results, showing good agreement with correlation coefficients (R) of 0.883 for density and 0.9737 for hardness. This demonstrates the effectiveness of the ANN approach in evaluating the mechanical properties of CCONP/PLGA nanocomposites, providing a reliable tool for decision-making and potentially reducing experimental characterization costs.

Keywords: *Nanocomposites, microwave sintering, artificial neural network*

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Ramification of Li-ion array on Structural, Optical and Dielectric Properties of Vanadium Pentoxide for Energy-efficient Material

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ABSTRACT

A recent area of research environment is focused on energy-efficient devices and finding sustainable solutions for the energy crises. The development of different TMOs is predominantly centered on these issues. Lithium incorporates with V_2O_5 established energy efficiency of the material and the composite roll in lithium-ion batteries and other devices. $Li_xV_2O_5$(XRD) measurement imparts orthorhombic and monoclinic structure. V_2O_5 phase variation surfaces due to the lithium concentration increasing from 0.2 to 0.8. The X-ray density, molar volume, and bulk density also show variation. UV- DRS spectroscopy determined the energy band gap (Eg). The significant change in the optical energy band decreases from 3.37 eV to 2.44 eV for the present specimens. The relation between energy band gap refractive index is derived using different theoretical fitting formulas. This data can be extended to other vanadium oxide phases and similar materials with transition metals. The refractive index, reflectivity, molar refractivity, and molar electronic polarizability show decreased values with lithium dominance increases. The complex impedance spectroscopy analysis was performed to find the effect of lithium on the electrical and dielectric properties of the vanadium pentoxide. Electronic components and equivalent circuits represent the effect on the impedance. Cole-Cole/Nyquist and Bode plots represent an equivalent circuit to analyze the complex parameter of the $Li_xV_2O_5$ (x = 0.2 to 0.8) system. An equivalent circuit has been adopted with the help of a computer program by fitting the experimental data. All the equivalent circuits carried out different fitting parameters.

Keywords: *TMOs, X-ray density, reflectivity, bulk density, cole-cole/Nyquist, bode plot*

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Nanoscale modified monodispersed microporous SiO_2 Microspheres as a stationary phasefor liquid chromatography applications

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ABSTRACT

Nanoscale modified monodisperse SiO_2 microspheres have found wide applications in liquid chromatography techniques. Synthesis of nanoscale modified monodisperse microporous SiO_2 microspheres were developed by hydrolysis of tetraethyl orthosilicate (TEOS) in a water–ethanol mixed solution and using dodecyl amine (DDA) as hydrolysis catalyst and template. The monodisperse SiO_2 microspheres obtained were compared with monodispersed microporous SiO_2 microspheres developed by using cetyltrimethylammonium bromide (CTAB), tetraethyl orthosilicate (TEOS), diethanolamine (DEA).[1-3] The monodisperse SiO_2 microspheres were characterized with differential thermal analysis thermogravimetry, scanning electron microscopy, high-resolution transmission electron microscopy and small angle X-ray diffraction. The effects of experimental conditions on the size dispersion, morphology, and chemical yield of the as-prepared SiO_2 microspheres by both methods of synthesis were investigated and discussed.

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Structural, Morphological and Luminescence Properties of Sm^{3+} ion doped Cadmium Magnesium Phosphate Nano powder for W-LED Applications and Display Devices

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ABSTRACT

Samarium-doped cadmium magnesium phosphate (CMP) nanopowder was prepared by a well-known and frequently used solid-state reaction technique. The prepared sample was analyzed by using a variety of analytical techniques, including Powder X-ray diffraction (P-XRD), FESEM with EDX, Diffuse Reflectance Spectroscopy (DRS), Fourier Transform Infrared Spectroscopy (FTIR) and Photo Luminescence (PL). The P-XRD results reveal that the produced nanopowder has a crystalline size 30 nm and also indicate the CMP nanopowder has a monoclinic structure. The morphological studies of FESEM results suggest that the nanopowder has a flower-like structure with the presence of elements Cd, Mg, Sm, P, and O [1]. The DRS spectrum of Sm3+ ion doped CMP nanopowder exhibits five prominent peaks, with wavelengths of 287 nm, 459 nm, 946 nm, 1086 nm, and 1243 nm which are located in the UV to IR region. The PL spectrum studies examined four sharp peaks attributed to the wavelengths 564 nm, 598 nm, 648 nm, and 707 nm were observed in the emission spectra upon excitation at 403 nm and five sharp peaks attributed to the wavelengths 360nm, 375nm, 403nm, 415 nm,432 nm, and 475nm were observed in the excitation spectra upon emission at 598 nm. The calculated values of color purity, CRI, and CCT confirm that the CMP nanopowder coordinates were found in the orange region. This prepared nanopowder was suitable for the applications of W-LEDs and display devices. The prepared nanopowder's ions associated with the phosphate group were confirmed by FT-IR [2].

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Controlled Synthesis of $BiFeO_3$, $Bi_2Fe_4O_9$ and $BiFeO_3/Bi_2Fe_4O_9$ Nanostructures with Enhanced Photocatalytic Activity on Degradation of Eosin Blue under Visible Light

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ABSTRACT

Multiferroic BiFeO3, Bi2Fe4O9 and BiFeO3/Bi2Fe4O9 nanostructures were synthesized by low temperature hydrothermal method by varying reaction temperature and time without any post heat treatment process. The physicochemical properties of the as prepared samples were investigated via X-ray diffraction (XRD), UV-Visible spectroscopy (UV-Vis), Fourier transform-infrared spectroscopy (FTIR), Scanning electron microscopy (SEM) studies. The XRD analysis confirm the formation of BiFeO3, Bi2Fe4O9 and BiFeO3/Bi2Fe4O9 with average crystallite size in the range of 34- 49 nm [1, 2]. UV analysis reveals that the nanostructures having bandgap in the range of 2.1- 2.19 eV for direct and 1.72-1.85 for indirect bandgaps respectively [3, 4]. The narrow bandgaps indicate that they might have promising applications in photocatalysis due to the prominent absorption in the expanded visible-light region.The photocatalytic activity of the as-prepared samples was evaluated by photocatalytic decolorization of Eosin Blue aqueous solution, at ambient temperature. Compared with bare BiFeO3 and Bi2Fe4O9, the optimized BiFeO3/Bi2Fe4O9 composite displayed higher photocatalytic activity under visible-light irradiation. The promoted photocatalytic activity could be attributed to the increased light absorption and the enhanced charge separation due to the synergistic effect of both (BiFeO3 and Bi2Fe4O9) samples, which could be a suitable candidate in the photocatalytic degradation of organic pollutants [5].

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Cross-dehydrogenative coupling using organic dyes as photoredox catalyst

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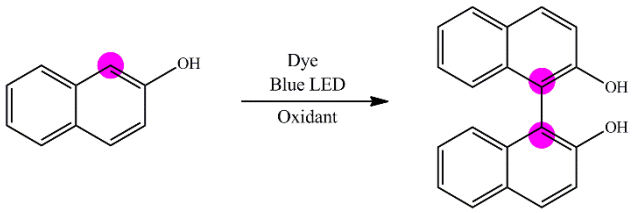
ABSTRACT

Photoredox catalysis is a branch of catalysis that generally uses visible light to carry out chemical reactions via single electron transfer. Biaryl moieties are found in various biologically active natural products, pharmaceuticals, liquid crystals and ligands for transition-metal catalysts. During last few years considerable attention has been received on synthetic methods that enable the formation of biaryl derivatives in an atomic and step economical way. Many important chiral ligands are synthesized from the binaphthyl staffold and ultimately derived from BINOL as a starting material. Due to this properties and their asymmetric synthesis has attracted the scienctific community. Many important chiral ligands are construted from the binaphthyl scaffold and ultimately derived from BINOL as a starting material BINAP being one of the most-well known and important. So far different catalysts has been used to synthesize biaryl moieties such as iridium, ruthenium, Ru(II) salen complex, TiO_2, di-tert-butyl hydroperoxide, acridinium salts. Though the BINOL has been synthesized by a different methodologies. We came up with the photoredox pathway to synthesized a model substrate (**Scheme 1**). It is a simple and cost effective pathway to synthesized a BINOL. Herein, we report the following synthesis of biaryl compounds (**Scheme 1**) using 2-naphthol as starting substrate and using oxidant via visible light mediated photoredox catalysis. This will be the first example of photo-initiated cross-dehydrogenative coupling using dye as photoredox catalyst.



Scheme 1: cross-dehydrogenative coupling using dye as photoredox catalyst

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Application of Nanotechnology in Biological System and Medicine

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ABSTRACT

Functionalization of Nanoscale (<100nm) particles at the cellular level is highly specific and can be employed to develop efficient diagnostic and therapeutics procedures with the minimum side effects. Several nanoparticles have been used in Bio-medicine such as gold, iron oxide, silver, carbon Nanotubes, Grapher, Zinc oxide, alumina, silica, and titanium. Nanoparticles come in direct contact with all components of the blood that is erythrocytes, platelets and leukocytes. Nanoparticles can be channeled in cancer therapy to encapsulate active pharmaceutical ingredients and deliver them to tumor site in more efficient manner by carbon Nano tube, Nano crystal, Nanowire. The advancement of nanotechnology helps in the treatment of Neuro degenerative disorders such as Parkinson's disease and Alzheimer's disease. Even in cardiovascular diseases for delivering therapeutic agents effectively. In this research article the focus is on various applications of nanotechnology in biological system and medicine.

Keywords: *Nanoparticles, Bio-medicine, Gold, Iron oxide , cardiovascular, cancer treatment, Carbon, Grapher, Erythrocytes platelets and leukocytes.*

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Extraction of Nanocellulose using Sugarcane Baggase and Applications of Nanocellulose

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ABSTRACT

In the last decade, nanotechnology has played a key role by occupying various application across industries beneficial to human race. Nanotechnology is the art of science of manipulating matter at the nanoscale. One of the recent application is nanocellulose. Nanocellulose refers to the nano-structured cellulose which can be extracted in a large scale using wastes from agriculture. The use of agro-waste as a precursor not only offers advantages for raw material costs, but also for the climate, low processing costs, availability. In this particular experiment, Nanocellulose is obtained by sugarcane baggase, by acid hydrolysis method. Sugarcane baggase was isolated and it was hydrolyzed by 50% sulfuric acid at 40^0 C for 10 minutes. Various references were taken to analyze the characterization, that is the analysis of Fourier Transform Infrared Spectroscopy [FTIR], X-Ray Diffraction [XRD]. Additionally, Nanocellulose is used in Paper, Packaging, Medicine and Food industries due to its broader applications. Nanocellulose has a potential application with its future scope still being discovered and rediscovered.

Key words – *Cellulose, Nanocellulose, Sugarcane baggage, Acid Hydrolysis.*

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Influence of Sol-Gel Route on Phonon Behavior of Polycrystalline $BaTiO_3$ Nanoparticle

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ABSTRACT

Polycrystalline BaTiO3 (BT) samples have been prepared via conventional solid-state (BT1 & BT2) and sol gel (BT3) routes. A comparative XRD and Raman analysis have been performed on the effects of crystallite size and calcination temperature on the sample crystallization at room temperature. Crystal lattice parameters obtained from Rietveld refinement exhibited tetragonal structure of all samples with higher c/a ratio and average crystallite size at higher calcination temperatures. Also, with higher crystallite size, emergence and shift of tetragonal peak around 45° towards lower 2 theta value has been observed. From Room temperature Raman spectral graph, Overtone phonon mode 2E and 2A1(TO3) wereidentified at ~886 cm^{-1} and ~1059 cm^{-1} respectively in BT3. Change in line width of Deconvoluted tetragonal characteristic Raman bands A1(TO) and B1,E(LO+TO) inferred comparatively increased asymmetric Ti-O..Ti bonds with sol-gel route. Also, comparatively smaller crystallite size measured for BT2 sample may be due to intermediate grinding between two calcination steps.

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Synthesis and Characterization of Selenium Nanoparticles Coated with Folic Acid and Ellagic Acid Against Cancer Cells

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ABSTRACT

There are around 18.1 million cancer cases globally, with over 10 million leading to death [1]. Urgent action, like implementing nanotechnology-based treatments, is necessary to tackle this issue. Nanocancer therapeutics are precise delivery systems smaller than 200 nm that target specific sites. Selenium nanoparticles (SeNPs) exhibit anti-cancer properties and are considered a sophisticated drug delivery system due to their pro-oxidant conversion specifically in acidic microenvironments [2]. Ellagic acid, a recognised anti-cancer compound, was utilised in this research to cover SeNPs as a medication [3]. Furthermore, a folic acid coating was applied to SeNPs to target cancer cells more effectively than normal cells [2]. The SeNPs synthesised with and without folic acid and ellagic acid were individually compared and characterised using SEM, FTIR, and DLS. The particles have a spherical shape and are smaller than 150nm. Various functional groups were also detected on the particles. Moreover, the selenium nanoparticles coated with folic acid and ellagic acid exhibited potent cytotoxic effects when exposed to cancer cells. Therefore, we think that the SeNP coated with folic acid and ellagic acid that was synthesised can be efficiently utilised to target cancer cells.

Keywords: *Selenium nanoparticle, Folic acid, Ellagic acid, cancer, targeted delivery*

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Synthesis and Characterization of Liposome-Mediated Delivery of Selenium Nanoparticles Against Cancer

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ABSTRACT

Our bodies naturally contain the Selenium metal. Selenium nanoparticles have demonstrated encouraging medicinal qualities recently, such as antibacterial and anticancer effects. Selenium nanoparticles (SeNPs), although having intriguing biological properties, have a limited cellular uptake [1]. Liposomes are small, circular molecules that have a high bioavailability and great efficiency of medication loading. Liposomes and cell membranes have comparable biochemical structures. Its shape is round and amphiphilic, having a hydrophilic head and a hydrophobic tail. Since it may be used to transport both hydrophilic and hydrophobic chemicals, it is one of the most often utilised drug carriers in nanotechnology. SeNPs cellular intake can be increased by loading it into a liposome, which indeed raises SeNPs bioavailability and anticancer efficacy. In this work, a chemical synthesis method was used to produce SeNPs, and thin-film hydration was used to incorporate them into liposomes [2,3]. Using SEM, DLS, and FTIR methods, the characterisation of the SeNPs encapsulated in liposome was compared with that of the liposome-free SeNPs. The results of characterization investigations showed that the synthesised SeNPs and Se-Liposome were almost spherical, with respective sizes of around 151.2 nm and 163 nm. The determined values of zeta potential were -15.7 mV and -5.71 mV, respectively. The liposomal Se-release and Se-entrapment efficiency in liposomes on analysis revealed better bioavailability. The synthesized liposome-free SeNPs, liposome-encapsulated with SeNPs, and Free Selenium alone when exposed to cancer cells caused superior cytotoxicity suggesting its anticancer potential.

Keywords: Selenium nanoparticle, liposome, bioavailability, thin film hydration, anticancer

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Remineralization Potential of Egg Shell Derived Nano Hydroxyapatite incorporated with Niobium Pentoxide on Demineralized Dentin

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ABSTRACT

To analyze the remineralization potential of eggshell derived nano hydroxyapatite (ESnHA) with the addition of 25 wt% niobium pentoxide (Nb_2O_5) on demineralized dentin when tested under in vitro pH cyclic conditions at 7th,14th and 28 th days. **Methodology**: ESnHA powder was synthesized by microwave processing method and incorporated with Nb_2O_5. Characterization of synthesized ESnHA and ESnHA-Nb powder was done. 55 human third molars were used to prepare the dentin slabs, their baseline microhardness MH(B) were recorded and were demineralized to mimic an active carious lesion. Based on the therapeutic agents used, dentin samples were grouped as artificial saliva (AS, control), casein phosphopeptide-amorphous calcium phosphate (CPP-ACP), ESnHA and ESnHA-Nb. The surface topography with elemental variation and microhardness was assessed using Vickers microhardness testing (VMT) and SEM-EDX analysis. **Results**: Characterization of synthesized egg shell powder showed its similarity to the stoichiometric ratio of HA. The results of CPP-ACP, ESnHA, and ESnHA-Nb showed a significant increase in MHV, greater mineral deposition, increase in Ca/P levels and higher Ca/P ratio than AS. When compared to CPP-ACP a significant increase in MHV was observed with ESnHA at 28th day and with ESnHA-Nb at all tested time periods. SEM revealed complete masking of demineralized dentin with ESnHA at 28th day and with ESnHA-Nb at 14th and 28th day. Elemental analysis demonstrated rise in Ca/P ratio with significant difference between AS and ESnHA-Nb at all intervals. **Conclusion**: ESnHA and ESnHA-Nb remineralized demineralized dentin better than CPP-ACP and AS. Addition of Nb_2O_5 promoted faster remineralization process to a greater extent in a shorter period of time.

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F 212

Development of Aluminum Nanoplasmonic Structures for Chemical Sensing

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ABSTRACT

Periodic plasmonic metal nanostructures exhibit a significant absorption peak due to the interaction ofelectromagnetic radiation with the conductive sea of electron oscillations viz., Plasma oscillations on its surface. This interaction produces quantized plasma oscillations called plasmons. An Aluminum (Al) film is deposited by DC magnetron sputtering on a 500 nm self-assembled nanospheres with hexagonal close packed structure, present on a glass substrate. The thickness of the aluminum film over nanospheres (AlFON) is varied from 20 nm to 150 nm to study the properties of photonic and plasmonic sensing. The Al films of 20 nm and 125 nm are noticed with an appreciable sensing characteristics. The AlFON of 125 nm is observed as the best bulk sensing and volatile organic molecule sensing in the present study. This is a simple and viable technique for the development of a large-scale optical sensors. All the samples i.e., AlFONs of various thickness and their sensing behavior with volatile organic molecules are characterized by optical and morphological techniques. The FE-SEM image of one of the AlFON is given in Figure 1.

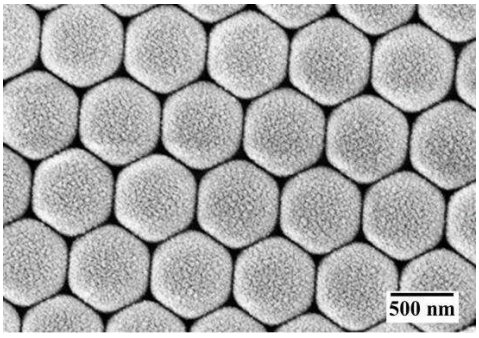

Figure 1: FE-SEM image of 70 nm Aluminum deposited on 500 nm spheres

Keywords: *Optical Sensor, Photonics, Chemical Sensor, Localized Surface Plasmon Resonance,Sputtering*

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F 213

GCMS Analysis and Invitro Antihyperlipidemic Effect of Homoeopathic Medicine Gautteria GaumeriQ,6C, 30C In HepG2 CELLS

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ABSTRACT

Guatteria gaumeri, is a traditional plant medicine synonym G. leiophylla Safford belonging to Anonaceae family has been indigeniously used for the treatment of hyperlipidemia. Hyperlipidemia is one of the life style disorders due to today's detrimental life style and it is a critical risk factor for cardiovascular diseasese which occupies the first place of the world and national mortality. Homoeopathic medicine, Gautteria Gaumeri, has been traditionally used to manage lipid metabolism disorders.(1)(2) However, its mechanism and efficacy at different potencies and the nanoparticles and the chemical composition of Homoeopathic Preparations remain underexplored. This study aims to explore the GC-MS profile of various potencies of Gautteria Gaumeri and potential antihyperlipidemic effect of Gautteria Gaumeri, Q, 6C, and 30C through in vitro experiment using HepG2 cells. Gautteria Gaumeri Q, 6C, and 30C potencies were subjected to Gas Chromatography-Mass Spectrometry (GC-MS) analysis to identify the chemical constituents of nanoparticles present in the ultrahigh dilution of Gautteria Gaumeri. HepG2 cells were treated with different concentrations of Gautteria Gaumeri, and intercellular lipid levels will be assessed using standard biochemical assays. Cell viability and cytotoxicity also were evaluated to determine the safety profile of the treatments.

GC-MS analysis revealed the presence of bioactive compounds in Gautteria Gaumeri(3), including those with potential lipid-lowering properties. In vitro studies demonstrated a significant reduction in lipid accumulation in HepG2 cells treated with Homoeopathic medicine Gautteria GaumeriQ, 6C, and 30C compared to the control group. Moreover, cell viability remained unaffected, suggesting the safety of the tested potencies.

Keywords: *Antihyperlipidemic, Guatteria gaumeri, Hyperlipidemia, HepG2 cells, Homoeopathy*

F 214

Investigation of Inverse Perovskite Oxides for ThermoelectricApplications

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ABSTRACT

Thermoelectric materials are important for converting unused heat into usable electricity, providingan eco-friendly solution for energy generation and cooling needs. In this study, we focus on the thermoelectric properties of inverse-perovskite Oxide Ba_3BO (B = Si and Ge) as a potential environmentally benign material. Through a comprehensive investigation combining experimental measurements and first-principles calculations, we unveil the unique characteristics of Ba_3BO that contribute to its high performance. The negatively charged B ions in Ba_3BO facilitate efficient hole transport with extended carrier lifetime, while the highly dispersive bands with multiple valley degeneracy result in elevated p-type electronic conductivity and Seebeck coefficient, leading to a high-power factor. Additionally, the lattice thermal conductivity of Ba_3BO is remarkably Ultra-low at temperatures between 300 K and 600 K. This low thermal conductivity is attributed to the highly distorted O–Ba octahedral framework with weak ionic bonds, which hinders phonon propagation and enhances phonon scattering within the material. Overall, our results highlight the potential of inverse-perovskite Ba_3BO as a high-ZT thermoelectric material without toxic elements, offering a sustainable alternative for energy conversion applications.

Keywords: Inverse Perovskites Oxide, Ultra-low thermal conductivity, Carrier lifetime, Phononpropagation, Hole Transport

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F 215

Graphene Based Flexible Supercapacitor for Energy Storage Device Using Electrospinning Technique

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ABSTRACT

Graphene-based flexible supercapacitors have emerged as a highly promising device in energy storage technology, due to their unique combination of remarkable properties and versatile applications. This abstract provides a detailed overview of the recent advancements in the fabrication of Graphene based flexible Supercapacitors and material properties for enhancing the conductivity, using advanced nanofabrication technique for the Electrospinning. As graphene, a two-dimensional carbon material, exhibits exceptional electrical conductivity, high specific surface area, and mechanical flexibility, is an ideal candidate for supercapacitor electrodes. There are various fabrication techniques, including chemical vapour deposition, solution-based methods, and electrospinning process. Among these, Electrospinning method is one of the promising process where we can obtain a very thin Nanofibers. This abstract concludes that graphene-based flexible supercapacitors having good conductivity and represent a highly promising energy storage device.

Keywords: *Graphene, Electrospinning Process, Flexible Supercapacitors, Nano fibers.*

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F 216

Enhancement Of Solar Cell Efficiency with Graphene Reinforced Electrospun Nanofibers

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ABSTRACT

The study reports the development of graphene reinforced polyvinylalcohol(PVA) nanofibers through the electrospinning technique for application in dye sensitized solar cells(DSSCs). Graphene, renowed for its exceptional mechanical and electrical properties, is incorporated into PVA nanofibers to enhance mechanical strength and electrical conductivity. Electrospinning method is utilized to fabricate uniform and well-defined nanofibers, ensuring improved surface area between the active materials and electrolyte in the DSSC. The effects of graphene reinforced nanofibers are systematically investigated through comprehensive techniques, including SEM, Raman Spectroscopy. Preliminary results demonstrate promising enhancements in power conversion efficiency, highlighting the potential of graphene-reinfored PVA Nanofibers for next generation DSSCs with improved performance and sustainability.

F 217

Fabrication of Gold Film Over Nanosphere (AuFON) Plasmonic structures for chemical and biomolecules sensing

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ABSTRACT

Plasmonics is the science and engineering of confinement of electric field of free propagating electromagnetic radiation on the surface in low-dimensional systems like zero-dimensional, one-dimensional, and two-dimensional. These low-dimensional systems are very exciting, and are playing a vital role for technical and biological applications. The alcoholic dispersion of poly-styrene nanospheres (PSS) is drop-casted on a glass substrate followed by the evaporation of the solvent produced a layer of self-assembled structure of PSS with 2D hexagonal close packing, which are characterized by optical and morphological techniques. The Gold (Au) films of various thickness viz., 50 to 100 nm are deposited by thermal evaporation technique over the self-assembled layer of PSS. It is observed that the nano cavities are formed with Au deposition on the PSS nanospheres. These cavities with metal produce localized surface plasmons (LSP) with the free electrons on its surface. The electronic resonance formed by LSPs i.e., LSPR with the chemical/biomolecules is recorded by its reflection spectra. The shift in the LSPR due to the interaction of chemical / biomolecules with the metal surface acts as an optical sensor. The 75nm thick Au film over nanospheres (AuFON) showed an optimum LSPR shift for chemical and biomolecule sensing. In the present studies, physical vapor deposition techniques are used to develop a largescale and cost-effective AuFON sensors.

Keywords: *Biosensor, chemical sensor, localized surface plasmon resonance, gold, optical sensor.*

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F 218

Optimization of organic dyes photodegradation and investigation of the anticancer performance by copper oxide/graphene oxide nanocomposite

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ABSTRACT

This study investigates the enhancement of organic dye photodegradation and evaluates the anticancer potential of a copper oxide/graphene oxide nanocomposite, thereby furthering environmental remediation and biomedical applications. This study aims to bridge the divide between environmental remediation and biomedical advances by optimizing the photodegradation of organic dyes using a copper oxide/graphene oxide nanocomposite while investigating its potential anticancer properties. The as-prepared nanocomposites were characterized using several methods, such as HRTEM, FTIR, XRD, and XPS spectroscopy. The GO@CuO nanocomposite was utilized to adsorb and photodegrade Rhodamine-B (RhB) and Malachite green oxalate (MGO) from an aqueous solution. The GO@CuO nanocomposite exhibits considerably enhanced adsorption and photodegradation when exposed to visible light compared to when it is kept in the dark. The GO@CuO compound displayed a remarkable ability to remove 84.77% of RhB and 87.81% of MGO for a duration of 60 minutes. RhB and MGO are resistant to adsorption alone, but photodegradation under visible light is more efficient. The anticancer activity of GO@CuO nanocomposites was shown to be considerable when examined on the ACHN cancer cell line. The results indicate that GO@CuO nanocomposites have the potential to be an innovative cancer treatment. The study concludes that the copper oxide/graphene oxide nanocomposite exhibits remarkable efficacy in both organic dye photodegradation and anticancer activity, offering a promising multifunctional material for diverse applications. The novelty lies in the synergistic combination of environmental and biomedical capabilities within a single nanocomposite, opening new avenues for sustainable and therapeutically relevant materials.

Keywords: *Evolvulus Alsinoides, copper oxide, graphene oxide, photodegradation, anticancer.*

G 001

Review on High Reflective Thin Al/Tialxn Film Coatings for Industrial Application

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ABSTRACT

Aluminum thin films and alloying of ternary TiAlN have outstanding coating qualities that make them appropriate for applications in the fields of optics, physical, telecommunications and structural engineering. The deposition of an Al and alloying of ternary TiAlN thin film is typically carried out using either physical or chemical processes, with variable deposition circumstances, parameters, and substrates. This investigation focuses on the preparation of thin Al and alloying of ternary TiAlN films by means of physical methods rather than chemical ones because previous research has shown that physical methods produce films with superior qualities than those produced by chemical methods. In this paper, the characteristics of thin Al, alloying of ternary TiAlN films and the intricate relationships between those qualities and the process parameters are discussed. In addition to the kind of substrate, the post-deposition treatment of the films affects the properties of thin films. As a result, the importance of finding ways to optimize the deposition procedures is brought to light in this study, as is the need to identify research gaps in previously published studies. This work has the potential to be a key resource for choosing the crucial process variables involved in the physical deposition of aluminum and alloying of ternary titanium-aluminum-nitride films.

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G 002

Microstructural Analysis and Mechanical Properties of Sisal Fiber in High Performance Concrete

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ABSTRACT

To increase the characteristic strength of the concrete, the sisal fiber available naturally is collected and added. The use of sisal fiber in concrete production leads to reduce the environmental problem. Sisal fiber was added with various proportions of 0.5%, 1%, 1.5% and 2% of cement. The fiber added concrete samples were cast and test conducted on the mechanical characteristics, including compressive strength, tensile strength, flexural strength, bond strength and impact strength. Micro-structural analysis like Scanned electron microscopic image (SEM), X-ray diffraction image (XRD), FTIR and Image J were examined to study the surface structure of the concrete. According to the findings, 1% of sisal fiber gives higher compressive strength in the production of concrete.

Keywords: *Environmentally friendly, Mechanical properties, Micro-structural analysis and Sisal fibre.*

G 003

Investigation of Structural, Morphological, Mechanical, Thermal and Electrical properties of PVA, PVP, PEG and Polymer blends

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ABSTRACT

In this work, the PVA, PVA-PEG, and PVA-PVP polymer membranes were prepared by ultrasound-assisted solution casting technique. The prepared polymer membranes- Structural, Morphological, Mechanical and Electrical properties were characterized by XRD, SEM, Young's modulus and National Instruments I-V Source meter. XRD results show the semi-crystalline and amorphous nature of the polymer membrane. SEM image confirmed the porous free and smooth surfaces of the ultrasound-assisted polymer membrane. Young's modulus results show that the mechanical properties of PVA: PEG polymer membrane with the highest elongation break, have high tensile strength among all the other prepared polymer membranes. Electrical studies carried out by National Instruments I-V Source meter.

G 004

Facile Fabrication of g-C_3N_4/ Bi_2S_3 Coated Melamine Foam for Oil -Water Separation

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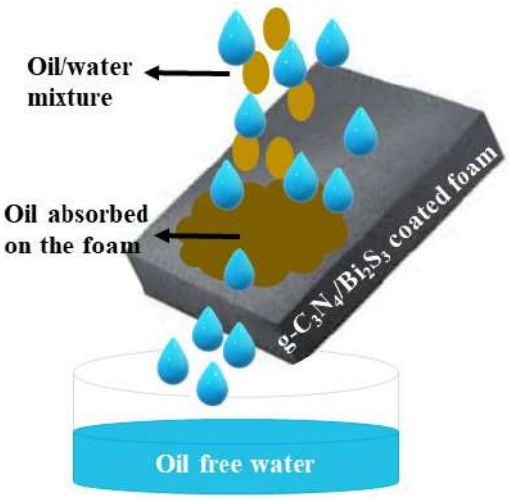
ABSTRACT

Regular occurrences of oil leaks are recognized as a significant contributor to water pollution, resulting in substantial environmental and ecological challenges, as well as posing the potential for fires and explosions[1,2]. Therefore, there is an imperative to create a cost-effective and exceptionally effective absorbent material for separating oil and water. Hydrophobic, foam-like materials have garnered considerable attention as potential absorbers for addressing oil spills and recovering oil from water sources. In this experimental study, simple, low-cost, environmentally friendly, highly hydrophobic and super oleophilic g-C_3N_4/Bi_2S_3 nanocomposite- coated melamine foam was introduced for the first time for oily wastewater treatment. The g-C_3N_4 and Bi_2S_3 were synthesized by thermal decomposition and hydrothermal methods, and the g-C_3N_4/Bi_2S_3 composite coated foam was prepared by simple dip coated method. The g-C_3N_4/Bi_2S_3 composite coated melamine foam showed good absorption capacity, and it can absorb various oils and solvents and separate different oils and solvents from water. Hence, the developed g-C_3N_4/Bi_2S_3 -composite coated melamine foam-absorbent has excellent potential in oil/water separation applications.



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G 005

Evaluation of Photocatalytic Activity of Organic Pollutant by using the CA@GEL@CeO_2 Nanocomposite

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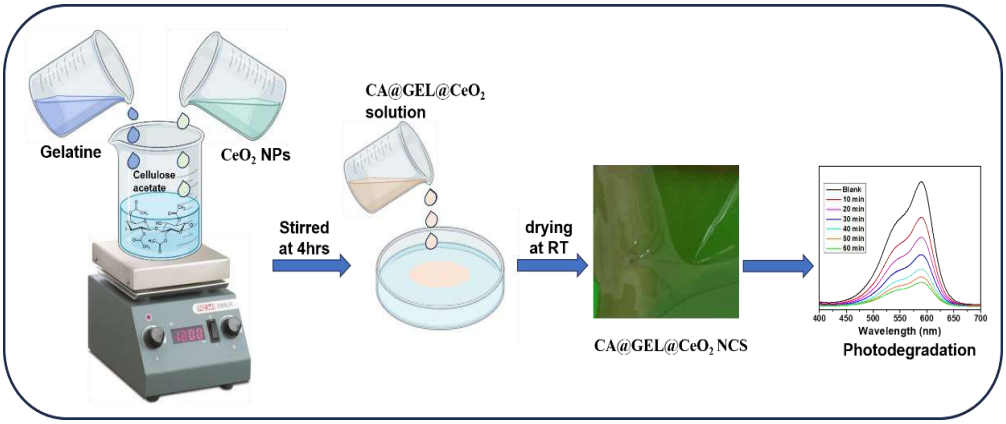
ABSTRACT

In this study, CA@Gel@CeO_2 nanocomposites were successfully made employing an affordable magnetic stirring method. The nanocomposites were characterized using XRD, Photoluminescence, FTIR, and XPS. The developed CA@Gel@CeO_2 nanocomposites size and shape were described using FE-SEM. For the evaluation of CA@Gel@CeO_2 nanocomposites, crystal violet (CV) obtained from the dye industry was photo-catalytically degraded. Additionally, the degradation of crystal violet (CV) in an aqueous solution by photocatalysis was studied. CV degradation in an aqueous solution was decreased by 80 % in just 60 minutes when exposed to UV-visible light. These results open the path for the discovery of visible light responsive photocatalysts that are more efficient in removing organic pollutants from water.



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G 006

Development of Diffusion Barrier in IC Circuits

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ABSTRACT

The reduction in the size of devices in the electronics industry has brought challenges to Moore's law and has also presented difficulties in material diffusion. As devices become smaller, it becomes a challenge to manage the diffusion of materials within them. Al and Cu are commonly employed as metallization materials in semiconductor devices. A brittle layer is formed when Cu and Sn(used as a solder) establish an interface and are aged above 150C. Due to its low electrical resistivity (bulk,1.67μΩcm) and improved resistance to electromigration, Cu exhibits a promising candidate as an interconnect for ultra-large semiconductor integrated circuits. A thin barrier film is required to prevent the production of Cu and Sn intermetallics. In this study, we assess how copper metallization affects the diffusion barrier. A barrier component can be created using materials that can tolerate high temperatures and have good adhesion to Cu. A medium entropy alloy system is one possible contender for diffusion barrier between Cu and Sn. Here, we will use CoFeNi, a MEA with a single-phase FCC structure as a component for the barrier. The alloy element is deposited on Cu using a thermal evaporator device. We next create a diffusion couple containing Sn and the as-deposited material. Barrier performance may be assessed by annealing this diffusing couple at various temperatures and thicknesses. The resistivity of the entire structure at the chosen temperature and thickness is calculated using four probe station. The existence of the deposited material is verified, and the phase of the structures is examined using XRD. SEM is used to ascertain how intermetallics develop inside the material.

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G 007

Unveiling the Influence of Anions on the Dynamics of Redox Reaction-Mediated Wettability Change in Cu-CuO_x Superhydrophobic Surface

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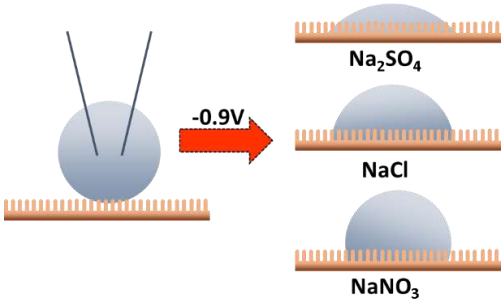
ABSTRACT

The oxidation and reduction of metal and metal-oxide surfaces form an integral part of pseudocapacitive energy storage devices. Among the various metal-metal oxides reported, Cu-CuO_x has been explored extensively for pseudocapacitor devices. Wetting of the Cu-CuO_x surface has been shown to undergo an enhancement in the wetting behavior under the effect of negative electrode potential due to electroreduction[1]. Wettability and electrochemical interaction are intricately related as electrochemical reactions influence surface wettability by changing the composition or roughness features which leads to reconfiguration of the interfacial energy of the electrode-electrolyte interface[2,3]. Considering the wetting change occurs under the negative potentials, the role of cations in the redox reaction and the wettability change is expected. In this work, we show that the anions present in the electrolyte affect the electroreduction process and the resulting change in the wetting behavior of the Cu-CuO_x surface. This work presents a systematic study of the effect of anion on the redox reaction kinetics and the dynamic evolution in wetting behavior. Employing a superhydrophobic Cu-CuOx surface, we examined three electrolytes, namely Na_2SO_4, NaCl, and $NaNO_3$, each with a 0.1M concentration, utilizing a droplet cell to analyze anion dependency. Specifically, in-situ tension-electrochemical investigations were carried out where the droplet shape was quantified along with the electrochemical behavior. The progression of droplet shape under different bias potentials was characterized by tracking contact angle and baseline size changes[1]. Our observation showed that the degree of droplet spreading is different for each electrolyte. The sequence of spreading follows the trend: Na_2SO_4 > NaCl > $NaNO_3$. These results correlate the influence of anions' characteristics upon reaction kinetics and wettability of the electrode-electrolyte interface. The findings provide fundamental insights into the role of anions in surface-mediated redox reactions and could also benefit in advancement of various applications involving tailored surface properties.



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G 008

A Study on the Mechanical and Viscoelastic Characteristics of Compression Molded Acrylonitrile Butadiene Styrene (ABS)/Cocoanut Fiber (CF) Bio - Composites and the Cole – Cole Plots

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ABSTRACT

Despite the fact that plastic and plastic composite materials offer the advantage of being lighter and more cost-effective in comparison to their metallic counterparts, the issue of waste accumulation after use poses a global concern. In this investigation, the utilization of cocoanut fiber as a natural fiber reinforcement in the ABS matrix is implemented, with the objective of enhancing its biodegradability. The ABS/cocoanut fiber composites were prepared through the process of compression molding, incorporating varying ratios of cocoanut fiber (5%, 10%, 15%, and 20%) within the ABS matrix. Subsequently, the prepared composites underwent extensive testing to assess their biodegradability, water absorption, mechanical properties, viscoelastic behavior, and thermal characteristics. Prior to the composite fabrication process, the ramie fibers' surface was subjected to chemical surface modification utilizing sodium hydroxide (NaOH). The results of the biodegradation test indicated a clear association between the concentration of fibers in the pure ABS material and the extent of biodegradation. The incorporation of various ratios of coconut fibers had an impact on several mechanical properties including tensile strength, modulus, elongation at break, storage modulus, loss modulus, biodegradability, and water absorption percentages. Specifically, the tensile strength decreased from 17.7 MPa to 3.7 MPa, while the tensile modulus of the composites increased by 5.33 times compared to the ABS matrix material. The biodegradation test conducted through soil burial revealed a 4.2% degradation after 30 days and an approximate 5% degradation after 45 days of keeping the samples in the prepared soil. Notably, both the hardness and impact strength of the composites decreased as the fiber content in the matrix increased. The viscoelastic characteristics experienced improvement as a result of the fortification of the organic fibers and the percentage of water absorption increased gradually in correlation with the augmentation of the fiber content. The main aim behind the development of ABS/cocoanut fiber composites is to deploy them as a material that is environmentally sustainable in the realm of automotive manufacturing industries.

Keywords: *ABS, Cocoanut Fiber, Mechanical Properties, Storage Modulus, Cole – Cole Plot, Biodegradation, FTIR, SEM*

G 009

Effective Nano-Patterning on Metal by Optical Near-Field Processing using Self-Assembled Polystyrene Monolayer

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ABSTRACT

Nano-patterning on metal surfaces has diverse applications in bio-sensing, display, data storage, solar cells, and security [1]. Nanoscale designs or patterns on metal surfaces can provide a high level of security against fraudulent activities [2]. Herein, we present a technique that utilizes a self-assembled monolayer of polystyrene colloidal microspheres (PS) as a near-field optical confinement structure on 316L stainless steel (SS). Each microsphere, acting as a micro-lens, focuses the incident picosecond laser beam (at 532 nm, 30ps, single shot) leading to material ablation and pit formation underneath, as shown in the schematic in Fig. 1a. Scanning Electron microscope images (SEM) of PS monolayer and laser-induced pits on SS samples are shown in Fig. 1b and 1c, respectively. Various patterns were engraved on the SS sample using a computer-controlled X-Y translational stage, as shown in Fig. 1d. The Comsol multiphysics 5.3 software was used to simulate the near-field nano-patterning process. The electric field distribution through PS particles of size about 2 µm at 150 mW laser power and corresponding energy density underneath of microparticle as a function of their position is shown in Fig. 1e. The characteristics of the nano-pits can be altered in a controllable manner by changing the laser parameters and the dimension of the particles. The technique of contact particle lens array-assisted surface patterning is promising in inscribing security features on metal surfaces.

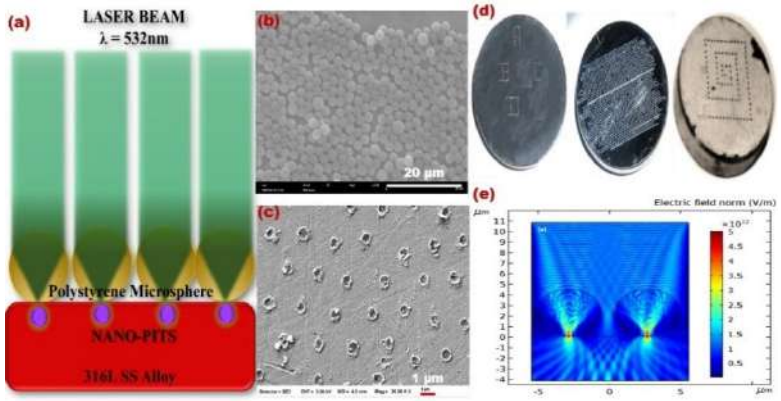

Figure 1: Schematic representation of laser-assisted pitting on SS substrate with PS monolayer; (b) SEM image of PS monolayer (c) Pits generated on SS (d) Various designs on SS sample (e) Electric field distribution through microparticles

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G 010

Synthesis of NiO/ZnO/g-C_3N_4 Heterojunction for the Visible Light Photocatalytic Degradation and Antimicrobial Activity in The Treatment of Wastewater

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ABSTRACT

In this work, NiO/ZnO/g-C_3N_4 (p-n-p) Hetrojunction nanocomposite was prepared by employing the co-precipitation method. The prepared nanocomposite NiO/ZnO/g-C_3N_4 was characterized using (XRD), UV-DRS, RAMAN, FTIR. The powder XRD analysis showed crystal structure, and SEM images shows surface morphology due to their crystalline/amorphous combination. FTIR analysis confirms the nature of the interaction between organic and inorganic counterparts. The PL emission spectrum shows an enhanced emission band, indicating that the presence of organic molecules reduces or controls the size of defects fluorescence spectroscopy, scanning electron microscope (SEM), and X-ray photoelectron spectroscopy (XPS). The morphology or crystal structures of NiO/ZnO/g-C_3N_4 nanocomposite have not undergone any change by the inclusion of carbon nitride. The superiority of our synthesized catalyst is that the better optical band gap matching and the fact that it regulates internal charge transfer of excitons within the hetero junction. However, it was observed that presence of carbon nitride had increased the visible light absorption and recombination rate of photo-excited charges. It was observed that the NiO/ZnO/g-C_3N_4 composite have shown the distinct shift to higher binding energy when compared with that of NiO/ZnO Nano composite. Furthermore, the inclusion of g-C_3N_4 had increased the quantity of hydroxyl groups in photo generated holes. Thus, prepared nanocomposite has been employed for the degradation of dye and antimicrobial activity in the treatment of wastewater.

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G 011

Development of 316L Low Alloy Steel Using Wire Arc Additive Manufacturing (WAAM): Microstructure and Property Correlation

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ABSTRACT

Metal additive manufacturing techniques is an advanced manufacturing technique that revolutionized the production of complex manufacturing structures, which was earlier difficult using conventional routes. Some of the applications of 316L stainless steel include Medical and Surgical Instruments, aerospace, Marine, etc. The main challenges in developing 316L steel using WAAM include controlling its microstructure to obtain the desired mechanical properties. For instance, small and equiaxed grains have superior mechanical properties to large and elongated ones. However, various factors, such as Chemical composition, WAAM parameters, etc, make obtaining the proper mechanical and metallurgical properties difficult. In this work, we have developed 316L low alloy steel using Wire arc additive manufacturing and compared its properties with the conventional 316L low alloy steel. Figure 1(a) shows the developed 316L low alloy steel and (b) shows its corresponding microstructure with the grain size of about 10µm. The mechanical properties show superior hardness, i.e., 30% higher than the traditional 316L low alloy steel. The SEM micrograph shows the presence of FeO particles throughout the structure, which can contribute to increased strength in 316L stainless steel fabricated using WAAM.

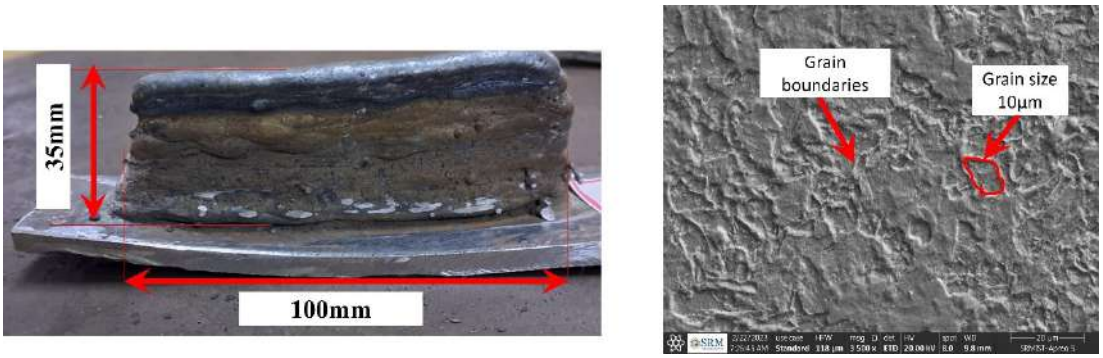

Figure 1(a) As-developed 316L low alloy steel using Wire arc additive manufacturing process (WAAM) and (b) its corresponding HR- SEM microstructure

G 012

Wear Behavior and Nanomechanical Properties of Tungsten-Copper Composites

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ABSTRACT

Tungsten-copper composites represent an interesting class of materials with their applications being explored in electronic packaging, electrical contacts and heat sinks. Thus, it is in scientific interest to assess their tribological and nanomechanical properties. In the present work, a tungsten-copper composite consisting 12 weight % copper and a relative density of 81% has been successfully synthesized using powder metallurgy route, and friction and wear properties of the same have been investigated. The tribological characterization has been carried out in dry conditions at room temperature, which has not been reported in any other previous study, under reciprocative sliding conditions, using a counter body of tungsten carbide (WC ball) at different loads and frequency fixed at 10 Hz. Analysis of the wear mechanism has been carried out via SEM-EDS. Nanomechanical response of the composite has been analyzed via nanoindentation, wherein a Berkovich tip has been employed as the indenter and Oliver and Pharr method is used for calculating the hardness and elastic modulus.

Coefficient of Friction (COF), wear volume and wear volume have been calculated for each of the experiments. A decrease in COF from 0.133 to 0.085 was observed when the load was increased from 5N to 20 N. The specific wear rate also showed a similar trend with the highest value of 0.57×10^{-5} (mm^3 /Nm) recorded at 5N, and a lowest value of 0.57×10^{-5} (mm^3 /Nm) recorded at 20N. Abrasion and tribo-oxidative wear were the predominant mechanism observed on the worn-out W-Cu alloy surface. An average elastic modulus of 450 GPa and an average Nanohardness of 6.4 GPa was calculated.

G 013

A Novel Composite Coating of SiO_2 and PVDF for Daytime Passive Radiative Cooling

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ABSTRACT

Passive radiative cooling (PRC) technology can reflect sunlight and radiate excess heat through the atmospheric window to outer space by utilizing the material's inherent properties without requiring any energy input or generating any pollution[1]. PRC can effectively reduce the use of traditional air conditioning, thereby reducing the energy consumption and greenhouse gas emissions associated with industrialization, effectively palliating energy crises and global warming. Therefore, passive radiative cooling technology has become a novel cooling technology[2].

In this study, we employed the Stöber method[3] to synthesize SiO_2 particles and modulated their surface morphology and particle size by adding cetyltrimethylammonium bromide(CTAB), thereby improving the solar reflection of silica capability and thermal radiation performance. According to the experimental results, it has been confirmed that the addition of CTAB can effectively control the surface morphology and particle size of SiO_2 particles, resulting in higher solar reflectivity and excellent selective emissivity. By blending SiO_2 particles with polyvinylidene difluoride (PVDF), which has high thermal radiation performance, we successfully prepared a passive radiative cooling paint and used a simple blade-coating method to fabricate a radiative cooling coating.

As the result of the outdoor experiment, our radiative cooling coating can achieve a cooling performance lower than the ambient temperature under high solar irradiance and high humidity conditions unfavorable for daytime radiative cooling, proving the radiative cooling coating has an excellent radiative cooling ability.

Keywords: *Passive radiative cooling coating, SiO2 particles, PVDF, CTAB*

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G 014

Investigation of Electrical Transport Properties of rGO-ZnO Based Composites

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ABSTRACT

Over the past few decades, Graphite and graphene-based composites have been the most researched materials due to their novel, extraordinary, remarkable and promising properties. In the present work, Graphene Oxide and Zinc Oxide were synthesized by using modified Hummer's method and Hydrothermal methods respectively [1]. The composites are synthesized and varied weight ratios of Zinc Oxide and Graphene Oxide respectively (50:50, 60:40, 40:60) and labeled as ZNG_1 (50:50), ZNG_2 (60:40), ZNG_3 (40:60) [2]. All the prepared samples were characterized by X-Ray diffraction (XRD), Raman spectra, FTIR, UV- Visible diffusion reflectance spectroscopy, Scanning electron microscopy (SEM) and Impedance spectroscopy. The X-Ray Diffraction pattern of pristine Graphene Oxide, Zinc Oxide and all the composites were studied. The XRD pattern of Graphene Oxide shows only one intense peak at 10.25^0 which corresponds to (001) plane, while pure Zinc Oxide shows all the peaks index as per the JCPDS card no. 36–1451 and in all the XRD pattern of composites a small hump appear which resemble not only the presence but the reduction of graphene Oxide in the sample. In Raman spectra the G (Graphitic) and D (Diamond) bands proves the presence of Graphene Oxide in all the including pure and composite samples. Pure Zinc Oxide shows Raman peak at 437.4 cm^{-1}. From UV-Vis spectra (Kubelka-monk graph), it is seen that the band gap of composites is increasing as compare to pure Zinc Oxide and Graphene Oxide. The introduction of metal oxide onto the surface of the Graphene Oxide sheet leads to enhanced electrical conductivity, electrochemical, charge storing and catalytic properties as compared to the Graphene oxide [3] and zinc oxide.

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G 015

Diffusion of Yttrium in Iron Matrix Studied using Secondary Ion Mass Spectrometry

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ABSTRACT

Oxide dispersion strengthened alloys (ODS) is an advanced class of structural alloy to be used in sodium cooled fast reactors and fusion reactors [1] owing to the combination of two important aspects such as superior mechanical properties and radiation resistance. These alloys are based on nanoscale Y-Ti-O dispersoids in steel matrix. It is important to understand the diffusion of the constituent elements in the matrix as it plays a crucial role in formation and stability of these alloys in radiation environment. Specific interest has been shown in the study of diffusion of yttrium in iron matrix, as yttrium is the least mobile of all hence limiting the kinetics. There are some reported values of yttrium diffusion parameters in iron matrix [2] calculated by different modelling approach, however, there is no experimentally determined values to our knowledge.

We have designed a set of experiment based on a sandwich thin film geometry of Fe/Y/Fe. The layer stack was fabricated by magnetron sputtering by depositing Fe/Y thin films on toα-Fe substrate. These Fe substrates were polished and preannealed at 800 °C. The deposited thin film samples were annealed at temperatures from 200°C to 500°C. Elemental transport parameters such as diffusivity and activation energy for diffusion process were estimated from the broadening of Yttrium elemental profile from SIMS measurement upon annealing.

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G 016

Shear Thickening Coatings for Enhanced Ballistic Protection

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ABSTRACT

Shear thickening fluids (STF) possess a distinctive and advantageous property characterized by an increase in both energy dissipation and elastic modulus. This unique combination of attributes makes STF particularly well-suited for applications where shock absorption is crucial [1,2]. The focus of this study is to comprehensively explore and understand how the rheological properties of STF are affected by the characteristics of colloidal silica, specifically its particle size and concentration. In this investigation, colloidal silica particles within the range of 100 to 750 nanometers are examined. By studying the interplay between these two factors, we aim to gain valuable insights into how STF can be optimized for applications requiring effective shock absorption [3,4]. Moreover, the research goes a step further by considering the application of STF in the context of ballistic performance. Specifically, it delves into the performance of STF when combined with a colloidal silica suspension featuring various particle concentration levels within a medium such as polyethylene glycol (PEG). The objective is to assess how different concentrations of colloidal silica affect the ballistic properties of STF, further enhancing our understanding of its potential uses in high-impact scenarios. The investigation explores the rheological properties of STF, with a particular focus on the influence of colloidal silica characteristics and extends its scope to evaluate the ballistic performance of STF in diverse suspension scenarios.

Keywords: *Bullet Impact; Shear Thickening Fluid; Strain-Thickening; Particle Dispersion; Rheology.*

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G 017

Synthesis and Characterization of Multiferroic composites

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ABSTRACT

Multiferroic composites of $K_{0.5}Na_{0.5}NbO_3$ -$NiFe_2O_4$ has been synthesised successfully through solid state reaction method. XRD has been performed to determine the nature of synthesised sample which confirmed crystalline structure of prepared samples. For additional structural analysis, Rietveld refinement using Full Prof Software was done. The VESTA software was used to create 3-D crystal structures, and the size-strain plot method was used to calculate strain (ε) and crystallite size (D). Dielectric constant (ε′) as well as tangent loss(δ) has showed dispersive behaviour at low frequency region whereas nearly constant behaviour at high frequency region. The high value of dielectric constant at lower frequencies was possibly due the space charge polarization.AC conductivity is found to have increasing trend as the frequency and temperature increases. The Nyquist plot of impedance showed semi-circular arcs having centre lying below the real axis and the radius of the semi-circular arc gets decreased with temperature indicating the semiconducting behaviour of the sample. Dc conductivity study indicated that the samples behaviour was semiconducting.

Keywords: *lead-free ceramic, Perovskite, space charge polarization*.

G 018

Experimental Investigation of GNP-Modified GFRP Composites in Scarf Repair

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ABSTRACT

Composite materials often require repairs due to manufacturing defects or in-service damage. Depending on the type of defects, various repair methods are employed, including bonded, bolted, filled, or injection repairs. Among these, adhesively bonded scarf repairs have shown remarkable efficacy in restoring residual strength. Recent research highlights the potential of incorporating nano-fillers into glass fiber-reinforced plastic (GFRP) to enhance its performance. This study investigates the effects of adding Graphene Nano Platelets (GNP) as a nano-filler to GFRP composites. While existing literature extensively covers quasi-static indentation testing of composite materials and scarf repair techniques, few studies focus on the combination of GFRP incorporated with GNP and scarf repair using patch geometry. This study explores the influence of different weight content percentages (0.25%, 0.5%, 0.75%) of GNP on GFRP material properties. Both modified and unmodified GFRP specimens are subjected to quasi-static indentation tests, followed by scarf repairs with the corresponding weight content percentages. Subsequent tests are conducted on the repaired specimens to assess their performance. Furthermore, nondestructive testing methods, including ultrasonic testing, are employed to evaluate the integrity of the repaired specimens. The findings of this study provide valuable insights into the effectiveness of GNP-enhanced GFRP composites in scarf repair scenarios, offering a new perspective on improving the structural integrity and strength of composite materials.

G 019

Impact of Embedded System-Based Automatic Spin Coating machine in the growth of Pure Zinc Oxide and Magnesium-Doped Zinc Oxide Thin Films for LPG Gas Sensing Application

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ABSTRACT

Embedded system-based spin coating machine is developed for the growth of thin films. Pure zinc oxide (ZnO) and Magnesium doped zinc oxide (ZnO:Mg) thin films with different doped samples have been prepared using the spin coating technique for LPG gas sensing application. The spin coating machine is fully controlled by PIC microcontroller (PIC16f877A), which could be driven by driver circuit to drive a spinning motor and ZnO:Mg thin films are deposited using this machine. XRD results indicated that the films are hexagonal wurtzite structure with preferred orientation and the crystallite size increase with increasing doping concentration of Mg. The surface morphology investigation shows grains are shapes in irregular and doping concentrations are not influence the surface morphology. From TEM image observed particle sizes ranging between 23 nm and 28 nm with an average value of ~25.8 nm. The maximum visible average transmittance was observed to be 96% for optimum Mg doping concentration of 10 wt %. The investigated DC electrical conductivity of Mg doped ZnO thin films shows the enhanced electrical conductivity than pure ZnO and the AC conductivity is decreased with increasing Mg doping concentrations from 5 to 10 wt%. The concept of operation and sensing mechanism of Pure ZnO and ZnO:Mg thin films behind their impressive results has been studied in depth.

Keywords: *Thin film; Zinc oxide; magnesium; embedded systems; spin coating;*

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G 020

Oriented Aggregation of Non-Homogenous 'Ag' Particles in FE-SEM, Spectral and Thermal Analysis of PVACeAgSe: V^{2+} Polymer Composite Films

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ABSTRACT

Polymer films are versatile materials used for the innovation of devices like micro-lenses, optical waveguides, allied items and optical fibres [1]. In our daily life, polymeric materials play an important role in energy storage, film capacitors and power pulsed applications [2]. The present work refers to the development of PVACeAgSe:V^{2+} films synthesized by traditional slow evaporation process. This technique was recognized as a suitable process for the fabrication of polymeric films. The prepared polymer composite films were characterized by FE-SEM with EDX, XRD and FT-IR technical analysis. X-ray patterns confirm that the prepared films are of polycrystalline nature. The grain size derived from FE-SEM images exist in nanometer range for the prepared films. It is also observed that the concentration of Vanadium (V^{2+}) has greatly influenced the morphology as well as the particle size as evidenced in SEM and XRD. The EDX graph confirms the stoichiometry of all starting materials.

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G 021

Fabrication of Lead-free Rudorffite Solar Cell using Solution Process

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ABSTRACT

Organic-inorganic hybrid lead halide perovskite solar cells (PSCs) have achieved significant progress in recent years. However, most of the reported high-efficiency PSCs were made with harmful lead (Pb), which is one of the major obstacles to large-scale adoption. Silver bismuth iodide (Rudorffite) light absorbers have been identified as promising lead-free and low-toxic materials for solar cell applications. Here, we demonstrated a carbon-based Rudorffite ($AgBiI_4$) solar cell without a hole transport layer. To deposit $AgBiI_4$ film, 1:1 M ratio of AgI and BiI_3 precursors was dissolved in DMSO: DMF solvents and the prepared precursor solution was spin coated over the mesoporous layer of TiO_2. All the above process has been done in an ambient condition. X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM) and UV visible absorption studies were used to characterize the $AgBiI_4$ films. The performance of the fabricated device was analyzed using incident photon to current conversion efficiency (IPCE), current density-voltage (J-V) characteristics and electrochemical impedance spectroscopy (EIS). Under standard illumination test conditions, a solar cell made with FTO/c-TiO_2/m-TiO_2/$AgBiI_4$/Carbon architecture showed a power conversion efficiency of 1.04%. The device also has good stability and retained 96% of its initial PCE after 200 hours.

G 022

Strain-Rate Dependent Behaviour of Polyborodimethylsiloxane (PBDMS) Based Polyurethane (PU) Foam Composite

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ABSTRACT

Polyurethane (PU) foam is widely recognized for its exceptional impact absorption behavior, making it a key material in applications requiring cushioning, shock absorption, and protection. Its unique ability to dissipate and absorb energy upon impact has led to its extensive use in diverse industries, including automotive, sports equipment, and personal protective gear [1-3]. One drawback of polyurethane foams in impact absorption applications is their limited durability, as they can degrade over time, reducing their effectiveness. Additionally, polyurethane foams may exhibit a tendency to compress and lose their original shape, impacting their long-term performance in repetitive impact scenarios. Polyborodimethylsiloxane (PBDMS) serves as a promising material for shear thickening gels, exhibiting the capacity to transform from a liquid-like state to a solid-like state under shear stress, enhancing their impact resistance in various applications. PBDMS-PU composite foam is a class of strain sensitive dilatant material that has attracted increasing attention from developers and researchers owing to a whole set of incredible properties.

In this study, PBDMS-PU foam was synthesized using one shot method. Prior to mechanical testing PBDMS-PU foam was studied and compared with PU foam for surface morphology and shape using scanning electron microscope (SEM) and thermal stability using thermogravimetric analysis (TGA). PBDMS-PU foam was then tested for compression under dynamic conditions using a split Hopkinson pressure bar apparatus for strain rates of 1400-2077 s^{-1}. The present investigation has great application in designing trauma mitigation pack required for high velocity impacts.

Keywords: *Shear Thickening Gel. Polyborodimethylsiloxane, High Strain Rate Study, split hopkinson pressure bar test.*

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G 023

Growth, Structural, Morphological, Optical, Electrical, Thermal Properties of Hybrid Inorganic-Organic Single Crystal: $[Li(C_{12}H_{24}O_6)].[Cd(SCN)_3]$ for Photonics applications

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ABSTRACT

Hybrid nonlinear optical single-crystal of lithium 18-crown-6 ether cadmium (II) tris(thiocyanate); $[(C1_2H2_4O_6)Li].[(Cd(SCN)_3)]$, (CLTC) was grown by a facile slow solvent evaporation technique (SSET) with the dimensions of 10 x 5 x 5 mm^3. To estimate the lattice dimensions and get the structural information, a powder x-ray diffraction (PXRD) study was performed, in which we found that the crystal belongs to the orthorhombic crystal system with space group $Cmc2_1$. Moreover, the optical cut-off wavelength of the grown single crystal of CLTC was found to 233 nm in the UV optical spectrum. The optical direct bandgap (E_g) was calculated using the Tauc relation $[(\alpha h\gamma)^2 = 0]$, and it was found to be 3.02 eV. The lower cut-off wavelength (270 nm) is good for nonlinear optical properties. It is noteworthy, the measured second harmonic generation (SHG) of the CLTC crystal is found to be 2.5 times higher than that of the KPD single crystal. The presence of various functional groups and the corresponding vibrational mode (C= N) present at 2100 were confirmed using the FT-IR spectrum. Additionally, the thermal stability of the title compound is found to be 171°C. The thermal stability, SHG efficiency are greater than that of other thiocyanate family crystals.

Fig.1 As grown single crystals of CLTC by SSET.

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G 024

Effect of Temperature on Manganese Mercury Tetra-Thiocyanate ($MnHg(SCN)_4$) Single Crystal Grown by Simple and Modified Solution Growth Technique for SHG Applications

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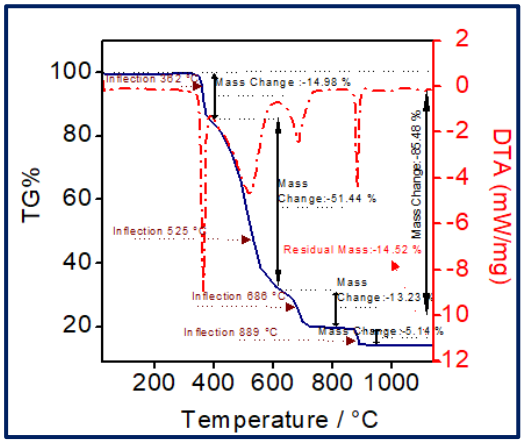
ABSTRACT

The second-order nonlinear optical material (SONLO) of manganese (II)-mercury (II)-tetra-thiocyanate $MnHg(SCN)_4$ (MMTC) bulk single crystals ($10\times7\times5$ mm^3, $24\times5\times5$ mm^3, and $30\times11\times10$ mm^3) were grown by slow evaporation solvent technique and constant temperature method using aqueous solution. The solubility is an essential factor of grown a good quality bulk size single crystal of MMTC. The solubility of the synthesized material as systematically analyzed. X-ray diffraction analysis confirmed the grown single crystal of MMTC tetragonal crystallographic system with the non-centrosymmetric space group I4. The various functional groups are involved in the present compounds of MMTC to verify by FT-IR, FT-Raman. The UV-Vis-NIR spectrum shows the cut-off wavelength of MMTC is 380 nm and they have a full transmittance range from ultraviolet to infrared radiation (380 nm to 2200nm). The TG and DTG analyzer is used to investigate the thermal decomposition and thermal stability (362 °C) at the different temperature. The synthesized chemical compound confirmed by CHNS analyzer. From the Vickers hardness measurements shows the MMTC is excellent mechanical stability compared with other organometallic materials like (TMTM, ZMTC, and MCCTC).



Keywords: *Bulk single-crystals, XRD, Vicker's hardness, thermal stability, linear and nonlinear optical studies.*

G 025

Comparative Analysis of the Vibration Energy Harvester Using Laminated Composite Beam

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ABSTRACT

Energy harvesters (EH) are apparatuses designed to transform electrical energy from environmental energy sources, including thermal, electromagnetic, and vibrational energy. In the present study, a laminated composite beam substrate with a PZT patch is considered. The mechanical, dynamic, and electrical performance of the harvester are evaluated using finite element analysis (FEA). Different composite materials and their combinations determine the harvester's performance. The obtained FEA results are validated using analytical calculations. A multi-objective optimization is carried out to find the optimal harvester design using ANSYS. The lamina thickness and the ply angle orientation are considered as the design variables, and frequency and voltage are considered as objectives. The proposed model can be used to develop high power output in low-frequency environments.

Key words: *Energy harvester, Piezoelectric patch, FEA, Laminated composite, Optimization.*

G 026

Optimization of Additive Manufacturing Parameters of the Magnetic Shield for EV Wireless Charging: A Materials Informatics Approach

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ABSTRACT

Metal additive laser powder bed fusion (LPBF) processes play a pivotal role in advanced manufacturing, offering intricate designs and lightweight components. This research focuses on optimizing the LPBF machine parameters, viz. laser power, scan speed, layer thickness, baseplate temperature, hatch spacing and laser beam diameter, for manufacturing aluminium magnetic shield for wireless charging of electric vehicles with improved build quality, lesser defects, and good mechanical properties. To achieve good quality component, it is important to minimize the residual stress and distortion of the component during the manufacturing process. AlSi10Mg alloy is used for the finite element analyses of LPBF process with varying parameters, and the simulated database is used for developing artificial neural network surrogate models for the residual stress and the distortion of the component. These metamodels are used as the objective functions for minimizing the residual stress and the distortion simultaneously using multi-objective genetic algorithm. The results indicate that the optimized process parameters lead to improved part quality, reduced defects, and enhanced mechanical properties.

Keywords: *Additive manufacturing, laser powder bed fusion, finite element analyses, artificial neural network, metamodel, genetic algorithm, multi-objective optimization*.

G 027

Effect of Fiber Properties in Frontal Crash of Polymer Composite Car Bumper: A Finite Element Analyses

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ABSTRACT

A car bumper is a safety structure that is used to protect passengers during low-speed collisions. Moreover, it protects the vehicle's structure from serious damage by absorbing the energy produced during collisions. Due to its energy-absorbing property, the car bumper becomes a vital structure during collisions. Among many materials fiber reinforced polymers are emerging as the leading candidate for bumper material, due to its good specific strength and toughness. As the properties of the composites are chiefly controlled by the property of the fiber, in this work bumpers of Glass Mat Thermoplastic, Epoxy carbon UD, Epoxy carbon woven, and Epoxy S-Glass UD are used for the frontal crash analyses. A Mercedes-Benz S-class car bumper is designed using Autodesk Fusion 360 and analyzed (frontal impact) using the full frontal fixed rigid barrier test, the offset frontal fixed rigid barrier test, the oblique frontal fixed rigid barrier test and the frontal overlap crash test (Federal Motor Vehicle Safety Standard (FMVSS) No. 208). The analyses are done using the explicit dynamic analysis module of ANSYS. Also, the bumper is optimized based on the results such that adequate deformation, von-mises stress and the energy absorbed could be achieved.

Keywords: *Car bumper, fiber-reinforced plastic, frontal crash analysis, finite element method, explicit dynamic analysis.*

G 028

A Continuum Damage Mechanics (CDM) Model for Composite Structures under High-velocity Impact with Unilateral Effect

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ABSTRACT

The mechanical response of carbon fiber reinforced composite laminate under impact load is simulated to predict the anisotropic damage evolution. This paper develops a continuum damage mechanics (CDM) considering the asymmetric tension-compression behavior. A projection tensor is developed to split the strain tensor into positive/negative strain tensors to avoid crack interpenetration in the compression. The symmetric fourth-order damage effect tensor is applied to the positive projection of the strain tensor to calculate the progressive damage in the material. The 3D Hashin failure criterion considering the through-thickness direction of compression failure, tension failure, and in-plane shear failure are incorporated in this constitutive model to predict the failure mode in the composite laminate. The cohesive elements are placed in between the lamina to simulate the inter-laminar delamination governed by the bilinear traction separation relationship. The user-defined subroutine VUMAT involving the modified constitutive modelis coded and implemented in the ABAQUS/Explicit to predict the behavior of the carbon fiber-reinforced laminates. A detailed comparison of the present strain degraded continuum damage (CDM) model to the other CDM model is provided.

G 029

Atmospheric Pressure Plasma Deposition of Interstellar Dust Analogues Based on Amorphous Hydrogenated Carbon and Evolution After Proton Irradiation

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ABSTRACT

Natural or artificial carbonaceous particulate matter is of great current interest for e.g. atmospheric and environmental sciences, human health, engineering, and astrophysics. We present here our latest results on the synthesis and characterisation of hydrogenated amorphous carbon (a-C:H) products, deposited using low temperature plasma, at atmospheric pressure [1-2]. Dielectric Barrier Discharge (DBD) is a relatively new method for amorphous hydrogenated carbon (a-C:H) synthesis, and even more so for producing diffuse interstellar medium (DISM) dust analogues. The dust analogues were thoroughly characterized using a combination of analytical techniques such as Fourier-transform infrared spectroscopy (FTIR), micro-Raman spectroscopy, X-Ray photoelectron spectrometry (XPS), optical microscopy, scanning and transmission electron microscopy (SEM, TEM), or mass spectrometry. In order to study the effect of cosmic rays on the disappearance of the carriers of 3.4 μm band in astrophysical environments, the dust analogues were irradiated with 3 MeV H^+. We observe morphological and chemical changes and evidence of the evolution of H/C, CH_2/CH_3, and sp^2/sp^3 ratios with increasing proton fluence. Using the observed 3.4 μm band decay with proton fluence we calculated the CH destruction cross sections and it was found that direct effects of cosmic rays are very likely responsible for the disappearance of the 3.4 μm band.

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G 030

Tribological study of Nano Graphene oxide Coating by Electrophoretic Deposition on Textured and Untextured Surface

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ABSTRACT

Electrophoretic deposition (EPD) is a versatile and widely employed technique in the field of materials science and engineering. EPD has been utilized in coating diverse substrates for various applications, as well asenhancing tribological characteristics. Texturing the substrates with different patterns has been shown to enhancethe retention of lubricants within the surface features which resulted in reduced tribological characteristics. Theprimary objective of this study is to utilize the EPD method for depositing graphene oxide (GO) onto a laser- textured AISI 52100 alloy steel surface. The subsequent analysis aims to explore the tribological impact of bothtextured and untextured coated substrates. Results reveal that laser-textured substrate (Peano pattern) has the lowest coefficient of friction (0.25) compared to that of uncoated substrate (0.59), GO coated substrate (0.29) asshown in Figure 1. The reduced coefficient of friction indicates that texturing provides better adhesion of GO tothe substrate. The findings highlight the potential of utilizing GO coatings in conjunction with laser techniquesto enhance the tribological properties of various materials, with implications for reducing friction and wear in automotive, aerospace, and other industries where solid lubricants can provide critical advantages.

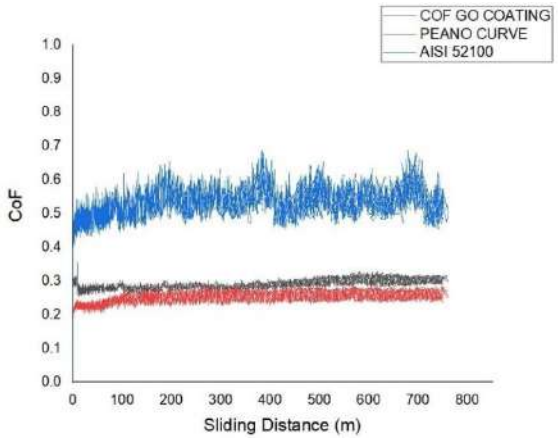

Fig. 1. COF Vs Sliding distance

G 031

Application of Nanoindentation Testing to Study the Nano Alumina-Reinforced Metakaolin Phosphate Geopolymer

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ABSTRACT

Enhanced functional properties are achieved by introducing a small quantity of the nano sized source material, into the geopolymer cement since it affects mechanical strength and microstructure. To investigate these properties in metakaolin phospho alumino geopolymer paste, (M) nano-Al_2O_3 was added to metakaolin at dosages of 0.5-3.0% by weight (MA_x) and hardened by 10 M of phosphoric acid at a constant liquid to binder ratio of 0.80. The samples were matured for 28 days by adopting hot curing at 80 C temperature for overnight and then air annealed. Nanoparticle integration with the gel resulted in superior mechanical properties and the optimum content of nano-Al_2O_3 for improving the mechanical compressive strength was 1% which significantly improved the strength from 46.2 MPa (0wt%) to 65.2 MPa (1wt%). The microstructural investigation was carried out by employing micro-RAMAN spectroscopy, AFM, optical microscopy, SEM, EDAX, and quasi-static nanoindentation. The indentation modulus of the silico phosphate and alumino phosphate network in geopolymers measures 44 GPa and increases to 48 GPa with the addition of n-Al_2O_3. Similarly, the hardness increases from 1.5 to 1.85 GPa. According to Raman spectral lines at 600-630 cm^{-1} at M and MA_1 to Si-OH and an octahedral Al-O-P in MA_1 are attributed and related to the observed enhancement of crystalline aluminium phosphate and silico alumino phosphate gels. The microstructure-mechanical property correlation was understood and discussed. Our study provides new insight into the design of metakaolin phosphate nanocomposites.

Keywords: *Geopolymer, statistical nanoindentation, microstructure, nanoparticle, metakaolin, phosphoric acid*

G 032

Bio-mass Assisted Magnetite Bimetallic Nanocomposite: A Giant Probe for Energy Storage and Eradication of Noxious Drugs

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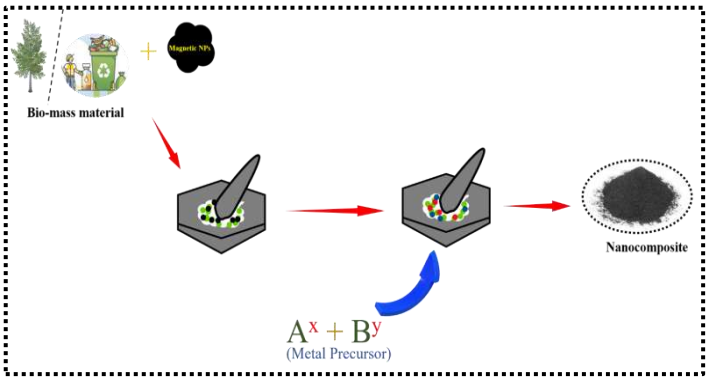
ABSTRACT

Bio-mass Assisted Magnetite Bimetallic Nanocomposite (NC) were synthesized through an eco-friendly in-situ green synthesis method. This process involves employing bio-mass derived supporting agent (BA) which plays a twin work such as reducing and capping agent for nanoparticles during the preparation of the NC. This NC was synthesized via a solid-state energy efficient hand-made grinding method. This is one of the simplest low-cost techniques in which the nanoparticles are incorporated to a bio-supported magnetic core matrix. The hand-crafted material was characterized via several analytical techniques. This NC was tuned in a way to employ it on energy storage applications like supercapacitors. Additionally, the as-same NC was also utilized in the eradication of carcinogenic drugs present in the water sample. This material foots a remarkable place for energy storage via the modulation of electronic band structure and it is one of the promising tool for the degradation of drugs from the waste water. Furthermore, it has good reproducibility, recyclability even after several cycles. Thus, the bimetallic NC flagged a better way for drug eradication and for the supercapacitor applications due to its low cost, highly efficient, and stability holds good for many cycles.



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G 033

PVA/rGO Composites for Advanced Electronic Devices - A Comprehensive Analysis of Structural, Electrical, Mechanical, Thermal Properties and Concentrations

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ABSTRACT

This research focuses on the synthesis of reduced graphene oxide (rGO) with polyvinyl alcohol (PVA) using a modified Hummers method and a casting method for the synthesis of PVA/rGO composites (85-10) has been characteristic. Concentrations of PVA/rGO (85%-15%, 90-10% and 95-05%) were systematically investigated to clarify their structural, electrical, mechanical and thermal properties, The structural analysis included X-ray diffraction (XRD) characterization of the crystalline structure, where the crystalline size was determined using the Scherrer's equation. Electrical behavior was studied extensively through impedance and current-voltage (I-V) characteristics, with Nyquist plots providing insight into impedance dielectric loss spectra, and conductance plots for resistance, modulus spectra, and dielectric loss tangent spectra at the expense of the dielectric properties were thoroughly tested. The transient hot wire method was used for thermal conductivity. Thermal conductivity was determined by calculating tensile strength, load, modulus, and elongation for different PVA/rGO concentrations. The multidimensional analysis in this study provides insight complete with rGO/PVA composites, opening the way for their integration into flexible and high-performance electronic devices.

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G 034

Forecasting Material Degradation: A Machine Learning Approach to Corrosion Prediction

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ABSTRACT

Corrosion causes widespread damage and financial loss in many sectors by weakening structures and causing equipment to fail. To combat this, the study focuses on using modern machine learning methods to predict where and how badly corrosion will strike, which helps in planning timely repairs and protective actions. The research looks into factors like temperature and how fast corrosion happens. It teaches computer models, such as Linear Regression, Random Forests, Support Vector Machines (SVM), and Artificial Neural Networks (ANN), to foresee corrosion by using real data on how materials corrode under certain environmental conditions. The models are trained with actual corrosion measurements and the conditions under which they were taken. The models' accuracy was tested in a simulated seawater environment with a high salt content, at temperatures ranging from 30°C to 50°C. Tests at 33°C and 55°C showed that the Random Forest model was the most accurate, judging by the lowest error scores and an R2 value close to one, indicating a strong match between predicted and actual data. This model outperforms others and shows that machine learning can effectively predict corrosion in a variety of settings, with the ultimate aim of developing a machine learning-based tool that can accurately detect and gauge corrosion's impact in real-world situations.

Keywords: *Artificial Neural Networks Algorithm, Machine Learning, Linear Regression, Corrosion Rate Prediction Model, Support Vector Machines (SVM), Random Forests.*

G 035

Analytical Investigation of Co-precipitated SnO_2-CuO Nanocomposite: Synthesis, Characterization, and Performance Assessment

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ABSTRACT

This work focuses on the synthesis of SnO_2/CuO Nanocomposite using the co-precipitation method and material calcination at different temperatures from 300°C to 600°C was performed. For this prepared material SEM, XRD, UV-Spectroscopy, FTIR, and IV characteristics were carried out. SEM analysis of the single metal oxides and nanocomposite shows an excellent morphology of the material with slight agglomeration, Structural study shows a highly polycrystalline structure using Scherer's formula, Material confirmation prepared with crystallinepeaks and its corresponding plane. UV analysis shows a Band gap in the range of semiconductor state, Finally IV characterization was measured, the measurement of IV characteristics for nanocomposite materials is essential for analyzing their structural arrangement, confirming chemical composition, showing different phases, ensuring quality control, confirming the presence of functional groups, and assessing performance in various applications. This study reveals the current conductivity of the nanocomposite which has good electrical conductivity. This can be used for high-performing electrical devices in the future.

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G 036

Effect of Post-Weld Heat Treatments on Microstructure and Mechanical Properties of High Entropy Alloy Reinforced Aluminum Matrix Composites Using Friction Stir Processing

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ABSTRACT

High entropy alloys (HEAs) have a new potential reinforcement for Aluminum metal matrix composites. Friction stir processing (FSP) is employed to produce a composite material by embedding dual Phase AlCoFeNiMn (HEA) with 10µm-sized particles reinforced within an Al-6061-T6 matrix. The FSP-engineered Al composite shows the microstructure with BM, SZ and TMAZ region which shows a refinement grain size of d = 5 □m in the stir zone. The strong and consistent interface zone between the Aluminum alloy matrix and the HEA particles indicates good metallurgical bonding. The severe chemical reactions were avoided, and no intermetallic compounds were formed at the interface. Following the T6 heat treatment, the composite hardness increased to 115 Hv, representing a remarkable 119% improvement over the base material hardness and offered an ultimate yield strength of 315 MPa, exhibiting a significant 69% improvement over FSPed AMC. The substantial improvement in the strength and hardness of composites can be attributed significantly due to Hall-Petch strengthening, thermal mismatch strengthening resulting from differences in the coefficients of thermal expansion between the particles and matrix, and Orowan strengthening. These results could promote Aluminum metal matrix composites to be extensively utilized in the aerospace, marine, and automotive sectors.

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G 037

Strategic Age Hardening in AlFeCoNiCr High Entropy Alloy: Precision Control of Sigma Phase for Enhanced Strength and Ductility

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ABSTRACT

Recent observations reveal the emergence of the σ phase in several high-entropy alloys (HEAs). While significantly boosting alloy hardness, this phase diminishes ductility. Consequently, effective control over σ phase formation is imperative for HEAs. In this investigation, an AlFeCoNiCr HEA was fabricated via vacuum induction melting. The as-cast HEA exhibited a singular B2 phase structure. Subsequent aging at 800 °C and 1000 °C for 10 hours aimed to explore phase transformations and associated mechanical behaviour, emphasizing solid solution strengthening. The study delves into the intricate relationship between σ phase formation in high-entropy alloys and factors such as atomic radius difference (δ), valence electron concentration (VEC), and paired sigma-forming element content. Notably, alloying composition plays a pivotal role in shaping sigma phase formation in the AlFeCoNiCr high-entropy alloy, offering valuable insights for customized alloy design and improved performance.

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G 038

Synthesis, Characterization and Aqueous Stabilization of Iron Oxide Nanoparticles (IONPs)

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ABSTRACT

The Iron oxide nanoparticles (IONPs) finds numerous application in water treatment, magnetic resonance imaging (MRI) and drug delivery etc. The literature shows the influence of temperature, pH and reactant conditions (type and concentration of salt used) on the size, shape and magnetic behaviour of the synthesized product. Our aim is to synthesize aqueous stabilized IONPs and study the effect of annealing temperature on particle size. Further study includes the influence of cationic and anionic surfactant (Sodium dodecyl sufate (SDS) and Cetrimonium bromide (CTAB) respectively) on its stability. The Zeta sizer and Dynamic Light Scattering (DLS) analysis provided the surface charge and particle size respectively. Further the stability analysis is done using Turbiscan, where the Turbiscan Stability Index value (TSI=0.1) indicates the stabilized suspension. The crystalline size, shape and phase is obtained via X-ray Diffraction (XRD) analysis. Transmission Electron Microscopy (TEM) showed the presence of nanoparticles and micro-platelets obtained under different annealing conditions. Scanning Electron Microscopy (SEM) along with Energy Dispersive X-ray (EDX) spectroscopy showed the morphology and elemental composition of the sample respectively, where the EDX data gives an idea of the phase of iron oxide. Determination of these physical and chemical parameters of the synthesized particles could help us to prepare the product of desired shape, size and phase.

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G 039

Combining Carbo-Gel Nanospheres Extraction Material and Microextraction Device for Detection of Potentially Toxic Metal Ions

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ABSTRACT

Sensing and identifying of toxic materials within a complex matrix requires development of sensitive and selective devices that can enrich the targeted chemicals for analysis. A simple and easy approach to enrich and detect various potentially toxic metal ions from different sample matrices using a microextraction platform device was developed. We fabricated a well-defined carbo-gel nanospheres extractant by combining carboxymethylcellulose as a core template with lysozyme, a structural directing compact globular protein, using hydrothermal carbonization. This was packed into a three dimensional printed miniaturized microextraction device, which could be repacked and reused multiple times. The surface chemistry and structural significance of the fabricated extractant was studied using electron microscopy and spectroscopy, as well as infrared spectroscopy technologies. The resultant extractant had a well- defined structure and the surface was rich in carbon and oxygen moieties. The analytical performance showed good precision, appropriated detection limits and linear dynamic ranges with acceptable correlation coefficients. The developed approach can sustain more than six regeneration cycles without deteriorating the analytical performance, proving its applicability and sustainability in the real and spiked biological samples. Compared to other solid-phase extraction approaches, our device by significantly reduced the amount of sample and sorbents needed for each analysis and the improved extraction kinetics significantly reduced needed extraction times. The multiplex approach of both extractant and device development can significantly improve selective analytical sensing of toxic or emerging contaminants of concern in complex solutions.

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G 040

$BaFe_{12}O_{19}$ Composite for Shielding Intra-Oral Energy X-rays

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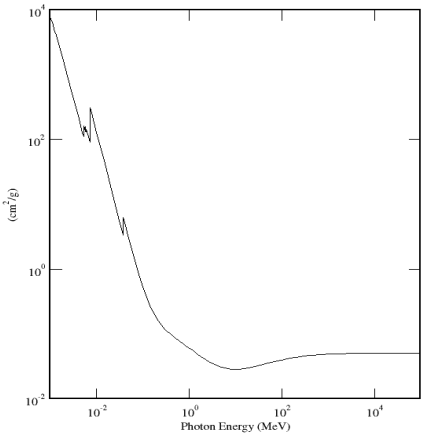
ABSTRACT

Increased use of X-rays particularly in the field of medical and dental diagnostic has necessitated a significant demand for flexible shielding materials. A non-toxic material with high attenuating nature, significant flexibility, exceptional stability, high atomic number and density are preferred for shield X-rays. Since material having high density exhibits higher attenuation, $BaFe_{12}O_{19}$ (ρ = 5.3 g/cm^3) was selected for the composite development in the present study. Primarily phase purity and morphology of the as-prepared sample was characterized respectively using X-ray diffraction and electron microscope. The obtained XRD pattern was analyzed by Rietveld refinement method using Fullprof software using respective JCPDS card. Shielding capability of composites was tested using a real-time intra-oral diagnostic X-ray machine. The observed behaviour explores the possibility of utilizing $BaFe_{12}O_{19}$ – rubber composite for X-ray shields development.



Energy dependent total attenuation of $BaFe_{12}O_{19}$

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G 041

Surface Oxidation of Grown REMs-Doped CuO:CdTe Thin Films Heterostructure Based Photocatalyst and PECs Materials for Solar-Driven Water Splitting

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ABSTRACT

Recent years, REMs doped CuO:CdTe thin films materials have been investigated extensively as catalyst materials in energy and the environment due to easy manipulation, easy scale up production, low-cost, abundant, etc. Present work, REMs doped CuO:CdTe thin films were successfully prepared via chemical vapour deposition at 450 °C for solar-driven H_2 production by water splitting. It can be useful for various characterization techniques such as XRD, FT-IR, SEM-EDX, TEM, UV-Visible and PL. All diffraction peaks indexed as single cubic phase, which is in strong agreement with standard data of JCPDS No. 4532-5432.The absorption spectra of REMs doped CuO:CdTe thin films indexed red shift in the visible region, which moves from shorter wavelength to longer wavelength due to increasing particle size.In PECs properties, REMs doped CuO:CdTe thin films have better photocurrent response compared to CuO and CdTe thin films due to charge transfer at the electrode-electrolyte interface.In addition, the degradation efficiency of H_2 production can be enhanced by using efficient photocatalyst and it shows REMs doped CuO:CdTe thin films catalyst enhanced at 94, 85, 80 and 71 %, respectively. It clearly indicates that REMs doped CuO:CdTe thin films materials have configurations of highly efficient photocatalyst and photo-electrode and it is useful for used in water splitting.

Keywords: *REMs; CuO:CdTe; Optical; PECs; Photocatalytic; Water splitting*

G 042

Multidirectional FRP for Structural Resilience

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ABSTRACT

This research focuses on enhancing the flexural strength of concrete structures by employing multidirectional Fiber-Reinforced Polymer (FRP). The study investigates the impact of multidirectional FRP, which involves strategically oriented fibers within a polymer matrix, on flexural performance. The research delves into the intricate relationships among fiber orientations in multidirectional FRP and their effects on structural materials, composites, and layers. Through a series of comprehensive experiments, the study reveals that concrete beams reinforced with multidirectional Carbon (CFRP) and Glass (GFRP) fibers exhibit superior flexural strength compared to conventional materials. The insights gained from this research contribute to the advancement of innovative composite materials and sustainable construction practices in the field of structural engineering.

Keywords: *CFRP, Fibre orientations, Flexural strength, GFRP, Multidirectional, Polymer matrix*

G 043

Structural Integrity Assessment of Resin-injection Repaired GFRP Composites

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ABSTRACT

Glass Fiber Reinforced Polymer (GFRP) composites have gained widespread acceptance in various engineering applications due to their excellent strength-to-weight ratio and corrosion resistance. However, like any structural material, GFRP composites may experience damage or degradation over time, necessitating repair to restore their structural integrity. Resin injected repairs are a commonly employed technique to address localized damage in GFRP structures. This research project aims to comprehensively analyze the effectiveness and long-term performance of resin injected repairs in GFRP composites. The study will encompass experimental investigations, numerical simulations, and material characterization to provide insights into the behavior of resin injected-repaired GFRP structures under different loading conditions and environmental exposures. Key aspects of the research will include the development of repair guidelines, and placement, and the assessment of repair techniques' impact on the mechanical properties of the composite. Non-destructive testing methods will also be explored to monitor the quality and durability of resin injected repairs over time. The findings of this research will not only contribute to the fundamental understanding of resin injected repair in GFRP composites but will also have practical implications for engineers and practitioners involved in the maintenance and rehabilitation of GFRP structures. Ultimately, the goal is to enhance the reliability and safety of GFRP composite structures while prolonging their service life through effective resin injected repair strategies.

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G 044

In vitro study of Sc_2O_3-PPI Dendrimer Nanocomposite as Antimicrobial Implant Coating for Orthopedic Titanium Implants

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ABSTRACT

Polypropylene imine (PPI) dendrimer is used for improving its antimicrobial efficiency, bioactivity and improved biocompatibility while applying coatings onto Ti substrate. Scandium oxide (Sc_2O_3) has been employed to significantly increase the coatings cell viability, cell growth, proliferation and biostability. *In-vitro* bioactivity was evaluated by immersing the Sc_2O_3-PPI dendrimer nanocomposite coated Ti substrate in Kokubo's 1.5 simulated body fluid for 21 days at 36.5°C (pH: 7.4). XRD revealed a high level of crystallinity and FTIR identify the functional groups present in Sc_2O_3 and PPI dendrimer. The electrochemical behavior of the coating was investigated by electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) analyses in 0.9% NaCl solution. The results showed that the Sc_2O_3-PPI dendrimer nanocomposite coating exhibited a superior resistance to delamination and biostability to Ti substrate. SEM-EDS have demonstrated a homogeneous distribution within the coating, surface revealed some nucleation without any detachment. AFM analyses show high surface roughness and the thickness of the coating was also predicted. The formation of a bone like-apatite layer confirms that simulates on the top surface of the coatings which was produced by the interaction of the Sc_2O_3-PPI dendrimer nanocomposite coating on Ti substrate and simulated body fluid. *In vitro* antibacterial and cytotoxicity tests were used to evaluate antibacterial properties and toxic effect of the Sc_2O_3-PPI dendrimer nanocomposite coating respectively. The Sc_2O_3-PPI dendrimer nanocomposite coating excellently inhibited bacterial activity and the highest zone of inhibition was obtained for *Staphylococcus aureus* (gram positive bacteria) and *Pseudomonas aeruginosa* (gram-negative bacteria). According to the findings, preferential doping of PPI dendrimer into Sc_2O_3 proved high bioactivity, effective antibacterial properties, great mechanical stability of the coating, and no evidence of cytotoxic effect suggests that the Sc_2O_3-PPI dendrimer nanocomposite coating is expected to be a promising bioactive long-term orthopedic implant.

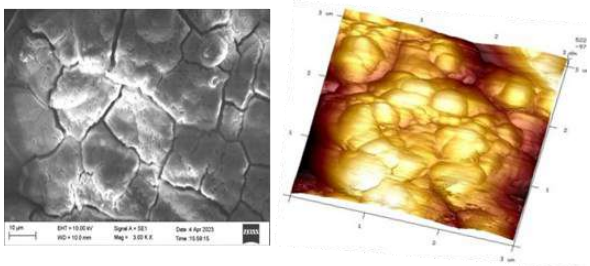

Figure: SEM and AFM image of Sc_2O_3-PPI dendrimer nanocomposite coating on Ti after immersion in SBF for 21 days at 36.5°C (pH: 7.4)

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G 045

3D Printed Cell and Fiber Guiding Scaffold Mimicking Periodontal Architecture

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ABSTRACT

Periodontal disease, a common non-communicable disease, pose a big threat to oral health in mankind. This disease affects the tissues that both support and surround the tooth. The prevailing surgical treatments control the damage, but do not regenerate tissues. To get to the original functional periodontium, regeneration of lost tissues in same quantity, nature and position is essential. Complying with the mechanical and biological architecture of the host tissue, multilayered scaffolds are currently required for effective tissue regeneration. Our suggested scaffold is a customizable three-layered structure that is intended to mimic the natural periodontium and be used in future regenerative applications as shown in figure 1. The innovative movable three-layered polylactic acid (PLA) scaffold that replicates the cementum, periodontal ligament, and alveolar bone layers found in vivo is created using the fused deposition modeling platform. Multiple angulated PLA fibers are also added to the scaffold, which helps to facilitate the anchoring dependent on cell adherence and provides directional guidance. Furthermore, coatings such as collagen and varying amounts of Gelatin Methacryloyl were added to the PLA scaffold's surface in order to enhance cell adherence and proliferation. We used micro-computed tomography, contact angle measurement, scanning electron microscopy, and atomic force microscopy to characterize the surface of our developed scaffolds. Furthermore, attenuated total reflectance-Fourier transformed infrared spectroscopy was used to study the material characteristics of this scaffold. Furthermore, compression testing proved the scaffold's mechanical characteristics, including strength and modulus of compression. Using flow cytometry, MTT assay, and fluorescence dye with fluorescence microscopy, the scaffold's enhanced biocompatibility was assessed. To sum up; our research has shown how to create a movable scaffold with several layers that are extremely biocompatible and ideal for a variety of downstream uses, including periodontium and in situ tissue regeneration of intricate, multilayered tissues.

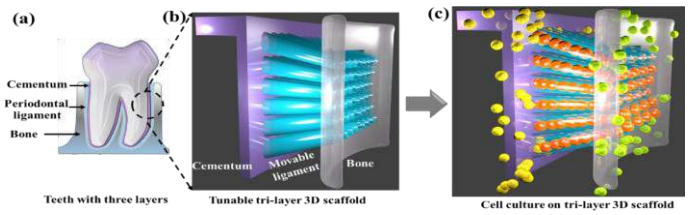

Figure 1: Schematic of direction-oriented fiber guiding with tunable tri-layer-3D scaffold (a) teeth with three layers (b) fabricated direction-oriented fiber guiding with tunable tri layer -3D scaffold (c) cell culture on direction-oriented fiber guiding tri layer 3D scaffold.

G 046

Performance of Recycled Aggregate in Concrete

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ABSTRACT

Construction and Demolition (C&D) materials encompass waste generated during the demolition of buildings, roads, and bridges, resulting in substantial amounts of debris. Disposing of C&D debris/waste directly impacts natural resources, limiting excavation and contributing to landfill accumulation. Recycled waste serves as a potential alternative source for aggregate production, with dry recycled aggregate exhibiting higher water absorption than natural aggregate. In this research work, accumulated debris/waste from C&D was utilized as an alternative aggregate. In this research, (C&D) debris/waste was gathered from a nearby demolition site in Puducherry. The collected material underwent segregation and treatment processes. The treatment methods, namely thermal treatment, cement treatment, fly ash treatment, and acid treatment, were applied to the collected aggregate. Samples were prepared for structural components, including conventional concrete with natural aggregate, acid-treated recycled aggregate, untreated recycled aggregate, thermal-treated recycled aggregate, cement-treated recycled aggregate, and fly ash-treated recycled aggregate. These samples were combined with different percentages of normal coarse aggregate to achieve appropriate concrete mixes, adhering to Indian Standard recommendations for various replacement proportions. The resulting concrete mixes were tested for their strength properties. In this study, natural coarse aggregate was partially replaced with treated recycled aggregate up to 100%, with different combinations (0, 30, 60 and 90%), without compromising the strength of the concrete. Concrete cubes, and beams were cast, and various mechanical properties such as compressive, split tensile, flexural, and impact strength were assessed. The results indicated that the use of treated recycled aggregate led to improvements in mechanical properties. Fly ash-treated recycled aggregate at a 30% replacement rate demonstrated better structural stability compared to other treated recycled aggregates. In conclusion, this work presents a comprehensive approach to analyzing various treated recycled aggregates as alternatives to conventional natural aggregates.

Keywords: *Compressive strength, recycled coarse aggregate, replacement percentage.*

G 047

Rehabilitation of Concrete Structures Using FRP Composites

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ABSTRACT

Fibre Reinforced Polymer (FRP) is used to reinforce a range of structural elements, slabs, beams, and columns. By attaching FRP strips along the axis of bending at the soffit portion of beams can be reinforced. Wrapping around the cross-section of beams in a U-shape can strengthen beams under flexure and shear. The ultimate stress and strains of FRP composites are far higher than most of the alternatives available for structural strengthening. The density of FRP composites is low, thus adding less additional dead weight to the structure. Recent years have seen a substantial increase in the adoption of seismic retrofit using FRP materials among the civil engineering community. The current state of using FRP materials as a retrofitting strategy for structures not built to withstand seismic activity is presented in this study in a representative overview. It provides an overview of the applications and range of FRP materials in seismic retrofitting plans for RC structures. The study also discusses the benefits, design principles, and restrictions of FRP applications for seismic retrofit. Beams are cast and tested till the ultimate and the tested beams are fixed on the soffit of the beam with FRP. The affixed FRP are tested once again and the improvement of the strength are discussed in this paper. By performing this methodology paves way for the FRP strengthening method which improved the performance of the existing structure. Aesthetic appearance of the building maintained and also improved the strength aspects. After rehabilitation the structure requires less maintenance due to adherence of FRP laminates.

Keywords: *Concrete, Ductility, Fibre reinforced polymer, Rehabilitation, Retrofitting, Strengthening.*

G 048

Investigating the Impact of h-BN and Graphite Reinforcement on the Mechanical Properties of Al7075 Alloy

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ABSTRACT

This research focuses on exploring the enhancement of mechanical properties in Aluminum alloy (Al7075) composites through the incorporation of hexagonal Boron Nitride (h-BN) and Graphite (Gr). The fabrication of hybrid composites with varying compositions of h-BN and Gr, adhering to ASTM standards for specimen preparation. A comprehensive examination of mechanical characteristics such as Hardness, Impact Toughness, and Tensile Strength is conducted to assess the efficacy of these reinforcements. The study employs stir casting as the fabrication method, ensuring uniform distribution of h-BN and Gr within the Al7075 matrix. Key insights into the surface characteristics and the interfacial bonding between the matrix and the reinforcements are gleaned through Scanning Electron Microscope (SEM) analysis. The research systematically evaluates the impact of differing h-BN and constant Gr compositions on the mechanical properties of the composites. Comparative analysis highlights the role of these reinforcements in optimizing the material properties, potentially leading to novel applications in engineering and industrial domains.

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G 049

Development and Characterization of Single Walled Carbon Nanotubes (SWCNTs) Dispersed Water Borne Epoxy (WBEP) Coatings with Enhanced Adhesion and Corrosion Resistance Using EIS Techniques

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ABSTRACT

The effect of uniformly dispersed single walled carbon nano tubes (SWCNTs) into water borne epoxy resin (WBEP) towards anti-corrosion performance on mild steel was evaluated. Dispersed (SWCNTs) act as corrosion inhibitor, increasing the adhesive strength of WBEP coatings to a greater extent. Consequently, the WBEP coatings displayed outstanding barrier properties against H_2O molecule compared to the neat WBEP coatings. The corrosion resistance of 0.5% SWCNTs-WBEP determined after 60h of immersion in 3.5 % NaCl solution, showed superior performance than 0.3%, 0.1% SWCNTs loaded WBEP and neat WBEP coatings as well. Furthermore, the data resulted from physico-mechanical properties supported and confirmed the enhanced adhesion imparted by 0.5%SWCNTs-WBEP than that of neat WBEP coatings on mild steel. In a similar fashion, the corrosion resistant performance of 0.5%SWCNTs-WBEPmild steel coated specimens was better than 0.3% SWCNTs-WBEP, 0.1% SWCNTs-WBEP and neat WBEP. The SEM images ascertained proper dispersion of SWCNTs in WBEP resins. The WBEP-SWCNTs coating maintained a high $|Z|_{0.01Hz}$ (10^9 Ω.cm^2) when the SWCNTs is 0.5% in 3.5 M NaCl solution when studied after immersed in 25 days. Potentiodynamic polarization studies demonstrated that E_{corr} lies in -0.572 V and J_{corr} is in the order of (10^{-7} A.cm^2) which identifies excellent corrosion resistance. Ultimately, the results from our study demonstrated the positive effects of the incorporation of SWCNTs towards anticorrosive ability of WBEP coatings for better performance and longevity.

G 050

Machine Learning based Accurate Crack Localization Methodology using Reduced Number of Sensors for Real-Time Structural Health Monitoring

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ABSTRACT

Crack detection and localization are significant in real-time structural health monitoring. Acoustic emission (AE) is the most prominent non-destructive technique. In AE, different methods rely on AE signal properties like AE velocity and frequency and provide good results by increasing the number ofsensors, thus increasing the installation costs. Hence, the motivation lies in defining a method independent of the AE signal properties and implemented with a reduced number of sensors. This research proposes a customized machine learning (ML) model implemented with Random Forest Regression. The experimentation setup includes DMR 249 A ship steel material with Fatigue 25KN machine as CT sample with two different loading ratios for fatigue crack propagation and another test with polarization setup to observe corrosion with two wideband AE sensors. The experimental datasets detect and localize cracks considering the time stamps from two sensors. The difference of the time stamps is calculated and tabulated as delta t(Δt), which is the input for the model, and the distance of the crack from sensor1 (d) is the output parameter used for training. Out of the complete dataset, 90% is used for training and the remaining 10% for testing. The testing dataset is untrained data. Fig. (a) shows the summary of the proposed methodology. The model performance is evaluated and observed to achieve 99.97% accuracy with a mean predictionerror of 0.00467mm. The novelty of this research lies in its ability to perform precise co-planar crack localization for real-time structural health monitoring, which is also independent of the AE signal properties and implemented with a reduced number of sensors.

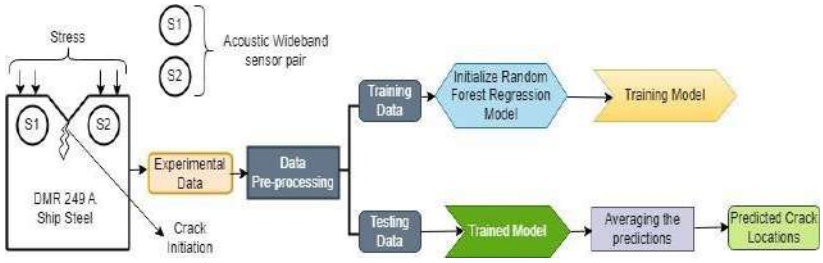

Fig. (a) Proposed Methodology

G 051

Field Emission Performance of Graphene Incorporated Metal Matrix Composite for Possible Application as Cathode

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ABSTRACT

In order to create aluminum-graphene (AlGr) composite materials and assess their field emission performance for possible cathode applications, a simple yet modern methodology has been processed using powder metallurgy. The 'close proximity' configuration has been performed for field emission analysis, where AlGr composites can be served as cathode. From the current density due to field emission (J)-electric field (E) measurements, the turn-on field has been recorded for different samples of metal matrix composites (graphene incorporated aluminium) and has been compared with aluminium (Al) in order to extract the current density due to emission. Further measurement has been done for different composite samples and also for aluminium with respect to the detection of emission current with regard to the increment in potential and the current density due to emission at given electric field. The turn-on value has been visually perceived for different aluminium-graphene (AlGr) composites and has been compared with Al. It also can be studied if any composite has any stable emission current and can be compared with Al. The morphologies and the micro-structures of the samples have been examined extensively with the aid of FE-SEM, TEM, XRD and Raman spectroscopy. The qualitative and quantitative analysis of the samples have been carried via EDAX and electron mapping. Moreover, the assessments of the density have been exhibited for the AlGr composites and the comparison has been done with the density of the pure aluminium following the sintering process. The micro-CT has been characterized for the structural wholeness and the nonexistence porous quality of the sintered composite specimens. These evaluations will help in order recommend the AlGr composites for possible application as cathode.

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G 052

Mechanical Characterization of PMMA Denture Material using Nanoindentation

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ABSTRACT

This research focuses on the comprehensive mechanical study of Poly(methyl methacrylate) (PMMA), a widely utilized material in denture fabrication. The investigation employs nanoindentation as a powerful technique to assess the mechanical properties of PMMA, aiming to elucidate the impact of varying temperature, pressure, and curing time on its mechanical performance. The experimental design involves systematically altering temperature conditions during the preparation process, applying diverse pressure regimes, and manipulating curing times to observe their collective influence on the mechanical characteristics of the PMMA denture material. Nanoindentation, a cutting-edge technique capable of probing material properties at the nanoscale, serves as the primary tool for quantifying hardness, modulus,and other critical mechanical parameters. The outcomes of this study are expected to provide valuable insights into the optimal conditions for enhancing the mechanical abilities of PMMA dentures. Understanding the interplay between temperature, pressure, and curing time will contribute to the optimization of denture fabrication processes, potentially leading to improvements in durability, wear resistance, and overall performance. The findings may have significant implications for the field of prosthodontics, offering practitioners and researchers a basis for refining denture materials and advancing the quality of patient care. This research contributes to the broader domain of dental materials science by offering a nuanced exploration of the mechanical behavior of PMMA under varying processing conditions.The acquired knowledge is pivotal for developing guidelines that can be applied in the manufacturing of dental prosthetics, ultimately benefitting both the dental community and the patients who rely on these materials for improved oral health and comfort.

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G 053

Advancements in Methacrylate-Based Polymer Nanocomposites: Synthesis, Characterization, and Superior Corrosion Resistance

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ABSTRACT

In recent years, methacrylate polymeric nanocomposite coatings have emerged as prominent materials for corrosion resistance. An attempt has been taken to study the Anti-corrosion properties of poly(furfurylmethacrylate-co-ethylmethacryalte)/TiO_2 nanocomposite prepared by in-situ solution polymerization method. To which the oleic acid (OA) modified titanium oxide nanoparticles (OA-TiO_2) were incorporated during the solution polymerization of furfuryl methacrylate and Ethylmethacrylate with using chlorobenzene as solvent, AIBN as initiator. The nuclear resonance spectroscopy (^{1}H&^{13}C-NMR) Fourier Transform Infrared Spectroscopy (FTIR) and X-ray diffraction (XRD) studies confirmed the formation of poly(FMA-co-EMA) and its TiO_2 composites. Additionally, poly(FMA-co-EMA)/SiO_2 and poly(FMA-co-EMA)/ZnO composites were synthesized and confirmed by above characterization techniques. The thermal stability of various feed ratios of poly(FMA-co-EMA) and its corresponding TiO_2, ZnO, and SiO_2 composites was assessed through thermogravimetric analysis and differential scanning calorimetric studies. The comprehensive examination includes corrosion investigations on mild steel specimens coated with these composites, alongside poly(FMA-co-EMA) coated and bare specimens. These evaluations were conducted in a 3.5% NaCl solution using Tafel and electrochemical impedance spectroscopic (EIS) methods. The morphology and embedded nanoparticles were confirmed by scanning electron microscopy (SEM) and energy dispersive x-ray based elemental mapping. The EIS studies shows that the poly(FMA-co-EMA)/TiO_2 coated on mild steel provides tremendous protection against corrosion in 3.5% NaCl than bare specimens or copolymer coated specimens.

Keywords: *Furfuryl methacrylate, ethylmethacrylate, in-situ polymerization, impedance spectroscopic, Tafel plot*

G 054

Tantalum Pentoxide-Poly(Amidoamine) Dendrimer Self-Healing Antibacterial Nanocomposite Coating for Orthopedic Implants

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ABSTRACT

Implantable biomaterials are crucial surgical tools that extend and enhance millions of peoples' quality of life on a global scale. Post-operative infection and immunological reactions however, continue to be major obstacles that hinder the ability of biomaterials and host healing processes. Coating antibacterial material onto Ti surfaces is an effective approach to enhance their intrinsic antibacterial ability. The goal of the current study is to develop a Ta_2O_5-PAMAM dendrimer nanocomposite coating with bioactivity, no toxicity and antibacterial properties on Ti substrate using electrodeposition method. *In-vitro* bioactivity was evaluated by immersing the Ta_2O_5-PAMAM dendrimer nanocomposite coating on Ti in Kokubo's 1.5 simulated body fluid for 14 days at 36.5°C. These coatings physio-chemical, electrochemical, surface morphological and surface roughness characterizations were done. The results proved the formation of a bone like-apatite layer that simulates on the top surface of the coatings is produced by the interaction of the Ta_2O_5-PAMAM dendrimer nanocomposite coating on Ti substrate and simulated body fluid. To verify the susceptibility of implant material surface to bacterial adhesion, *Staphylococcus aureus*, *Escherichia coli*, *Bacillus subtilis*, *Pseudomonas aeruginosa*, four types of major pathogen were chosen for in vitro antibacterial activity. The results showed that Ta_2O_5-PAMAM dendrimer coating has excellent antibacterial property. The *in vitro* cytotoxicity study provides the evidence that the prepared Ta_2O_5-PAMAM nanocomposite coating is compatible and toxic free with L929 cells at lower doses and shows only 0.664% cytotoxicity at higher doses compared to the control.

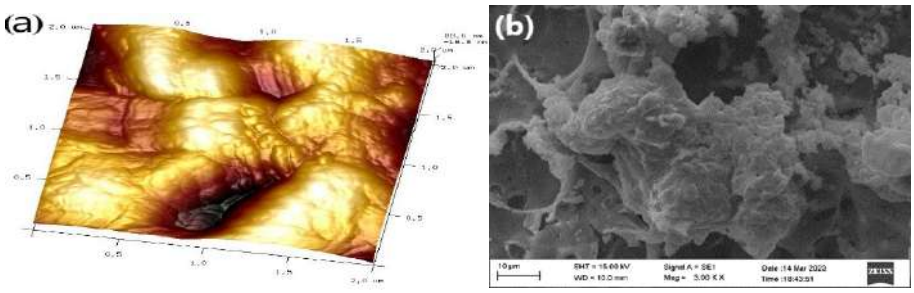

Figure.:(a) AFM and (b) SEM images of Ta_2O_5-PAMAM dendrimer coating

G 055

Thermo-Physical Properties and NDE Studies on BFRC Using Long Pulse Thermography

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ABSTRACT

Thermography is widely used in non-destructive evaluation since they offer rapid and long-range inspection of large structures.Long pulse thermography is a suitable and cost effective technique for defect characterization in composite materials. Basalt composites are new age materials widely used in civil, transport, automobile and windmill structures.In this study, epoxy reinforced basalt composites were fabricated by vaccum bagging method and their thermo-physical properties of basalt composites upto 300°C were observed. For the Non-Destructive studies, basalt composites with artificial defects and low velocity impacted composites specimens were characterized by long pulse thermography. The Depth of the defects were characterized by peak contrast derivative method and the area of impacts were observed for impacted specimens. The results are compared with ultrasonic c-scan.

Keywords: *long pulse thermography, basalt composites, impact studies and ultrasonic c-scan*

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G 056

Love-Type Wave Transference in Piezoelectric (PZT-7) Layered Structure Over a Heterogeneous Elastic Substrate with Imperfect Interface

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ABSTRACT

A systematic study of a Love-type wave being transferred in a piezoelectric (PZT-7) layered structure placed over an elastic heterogeneous substrate with imperfect interface is presented in the paper. The framework of the media appears to be in the form of a direct Sturm-Liouville problem. Electrically open as well as short cases are considered for finding dispersion relations. Substrate heterogeneity, interface imperfections, and thickness of the layer are the factors influencing the velocity profile of Love-type waves and their effect has been described using graphs. It can be clearly seen that phase velocity is directly proportional to any changes in these parameters of the Love-type wave. Substrate heterogeneity has a greater effect on wave velocity as compared to layer thickness. Furthermore, variations in the imperfect parameters have been shown in comparison to the cases mentioned before. The open case is observed to have a higher velocity than the short case. Development of SAW (Surface Acoustic Wave) devices and imperfections measurement can be presented with better information through these obtained results.

Keywords - *Elastic Substrate, Imperfect Interface, Love-type wave, Piezoelectric, Sturm-Liouville*

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G 057

Epitaxial Growth of Copper Oxide Thin Film on MgO (001) Substrate by Dynamic Aurora PLD Method

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ABSTRACT

The epitaxial Cu_2O (011) films are grown on MgO (001) substrate by the dynamic aurora pulsed laser deposition (PLD) method. The structure and epitaxial growth of the as-prepared thin films at 600 °C was investigated. The thin films deposited at 600 °C show single-phase cubic Cu_2O with good crystallinity. The highly oriented epitaxial Cu_2O thin films on the MgO substrate are achieved by applying an induced electromagnetic field during thin film growth. The Cu_2O thin films grown on MgO substrate at 600 °C has high quality and crystallinity. The as-prepared Cu_2O films exhibited an out-of-plane epitaxial relationship of Cu_2O (011) ‖ MgO (001) and two different kinds of domain structure with corresponding in-plane epitaxial relationship of Cu_2O [100] ‖ MgO [110] and Cu_2O [100] ‖ MgO [$1\bar{1}0$]. This report reveals, for the first time, the feasibility of epitaxial growth of cubic Cu_2O at 600 °C by the dynamic aurora PLD method.

Keywords: *Dynamic aurora PLD, Cu_2O thin films, RHEED, surface roughness, epitaxial*

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G 058

Micro Mechanical Properties of Hybrid Gel Phase in FA/GGBS Geopolymer by Depth Sensing Nano Indentation: A Correlation of Physico Chemical and Microstructure Properties

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ABSTRACT

Micro mechanical properties of cementitious materials are useful for predicting the bulk properties. This can be derived from Nano indentation testing applied over different phases present in the complex matrix of binders. Concerning the above, the micromechanical coupled with micro structural characterisation aimed to get an insight of different binding gels in hybrid geopolymer. Firstly, ambient cured geopolymer derived from the fly ash (FA), ground granulated blast furnace slag (GGBS) in the binding ratio of 1:1(FG) under alkali activation. The mineralogical informatics from XRD, structural investigation through MAS-Nuclear Magnetic Resonance, and morphological phases from TEM micrograph obtained and analysed Powder XRD pattern of FG geopolymer revealed the existence of amorphous gel phases of NASH type in the range of 2θ value from 23.4^0 to 32.6^0 and the crystalline gel phase of CSH from 31.62^0. Complex gel was conformed in TEM and SAD pattern. The excitation of fly ash and GGBS in alkali changed the Si, AL nuclei environment and the chemical shift's in which Al sites (IV) at 63.18ppm and VI at 3.61ppm are coordinated and Si is present mainly as Si(Q^4(4Al)) in the chemical shift of -88.32ppm of those conformed the short range network. The Nano indentation test applied to distinguish the types of gels and crystals. From the value of Elasticity 19-24 GPa for low and 25-30 GPa for high density gels characteristics along with CH crystals. This study endorses the findings of micro structure and the bulk mechanical behaviour of the geopolymer. This research contributes for tailoring the formulation of geopolymers with enhanced performance for diverse applications.

Key words: *Geopolymer, Nano indentation, Fly ash, GGBS, micro structure*

G 059

Formulations of Chitosan/TiO_2/ZnO Ternary Nanocomposites-Based Alkyd Nanopaint for Marine Anti-Biofouling Application

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ABSTRACT

The development of microbes, vegetation, algae, and animals on submerged surfaces such as ship hulls, offshore constructions, and undersea equipment is referred to as biofouling. Fouling organism development on ship hulls causes hydrodynamic drag, which lowers fuel economy and raises operating expenses for marine transportation[1]. In addition, fouling issues spreads invasive species, and increasing corrosion problems. Effective anti-fouling paints with various pigments such as Tributyltin, Organotin and copper-based materials are banned or restricted for use due to their toxicity[2]. In this study, chitosan was extracted from shrimp shells by subjecting them for demineralization, deproteination, and deacetylation and used to prepare sustainable anti-fouling paint by incorporating with synthesized ZnO and anatase TiO_2 (CZT). These materials were characterized and confirmed by using UV-vis, FTIR, XRD, micro-Raman, XPS, FESEM with EDAX mapping, and HRTEM[3]. The alkyd resin and xylene were used as binder and thinner in the nano-paint formulations, respectively[4]. Prepared anti-fouling paint was coated on mild steel (MS) coupons. These coated coupons were subjected to the mesocosm study in laboratory conditions in presence of microalgae and real field immersion study for 45 days at Muttukadu boat house, Chennai. The mesocosm study revealed that, pure compounds ZnO and TiO_2 were ineffective with more adherence of micro-fouling organisms. Compared to the pure nanomaterials, binary composites materials such as ZnO/TiO_2, Chitosan/ZnO, and Chitosan/TiO_2 were showing a significant inhibition activity with minimal algal settlement. The CZT Ternary nano-composites materials suppressed the algal settlement. These findings were strongly supported by the field studies and slight microfouling organisms along with few macrofoulers were started to settle over the coated specimens after 45 days of immersion period with minimal peel off effects. This ternary nano-composites materials can be used to prepare antifouling paint with further tuning of formulation process.

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G 060

Mechanical Properties of Polyacetal/Ethylene Octene Copolymer/ Graphene Nanocomposites

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ABSTRACT

Thermoplastics elastomers are an important class of engineering materials with a wide range of applications. However, its mechanical properties limit its applications. The development of polymer nanocomposites that possess a unique balance of properties is of interest and simultaneous addition of stiff and elastomeric particles to the host polymer may provide improvement of the stiffness and toughness. This work focuses on enhancing overall properties by blending polyoxymethylene/ethylene octene elastomer/graphene nanoplatelets in varying ratios. The use of ethylene-octene copolymers (EOCs) in nanocomposites has been a subject of extensive research due to their unique molecular characteristics and physical properties. EOCs have been employed as compatibilizers in various nanocomposite systems to enhance the dispersion of nanoparticles and improve the mechanical properties of the resulting materials. Blends of polyoxymethylene /EOC/graphene nanoplatelets were prepared through melt mixing in a twin-screw extruder. The study encompassed mechanical, dynamic mechanical, thermal and morphological properties. Mechanical properties, including tensile strength, modulus, % elongation and impact strength were analyzed in accordance with ASTM standards. Impact strength exhibited an increase up to an optimum level of compatibilizer. Thermal characteristics indicated enhanced interaction between the plastic and elastomer phases in the compatibilized system. Thermograms suggested a significant shift in Tm values within the compatibilized system. The study also examined changes in crystal size and phase morphology of the blends in relation to blend composition. Scanning electron microscopy observations of impact-fractured surfaces indicated a reduction in the particle size of the elastomer phase and its high dispersion within the polymer matrix. The process of compatibilization notably contributed to the enhancement of mechanical properties in the blends, catering to a wide range of market requirements.

Keywords: *Polyacetal blends; ethylene-octene grafted maleic anhydride; compatibilization; toughening; Mechanical properties.*

G 061

Wear and Fricition Behaviour of TiAl MMC with SiC Reinforcement

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ABSTRACT

This research paper aims to comprehensively investigate the wear and friction characteristics of Titanium Aluminum (Ti-Al) Metal Matrix Composite (MMC) reinforced with Silicon Carbide (SiC) under diverse operational conditions. The study specifically focuses on evaluating the performance of the composite material with varying SiC reinforcement levels, namely 5%, 7%, and 9%, as achieved through meticulousadherence to stoichiometric ratios in the Ti-Al base metal. The Pin on Disk test, conducted in accordance with ASTM standards G99, serves as the primary methodology to assess the wear and friction behavior of the composite. The investigative focus is directed towards scrutinizing the wear resistance and frictional behavior of the Ti-Al MMC with SiC reinforcement using a Pin on Disk tribometer. Through systematic experimentation and analysis, this research aims to contribute valuable insights into the mechanical properties and performance of the composite material, thereby advancing our understanding of its potential applications in real-world scenarios

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G 062

Emergent Material and Conventional Materials: A Comparison of the Electro-Thermal Characteristics of Relay Electrical Contact Surface Interfaces

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ABSTRACT

The utility of emerging Nanomaterial as an electrical contact material for implementing a micro-relay is inspected. A micro-relay has been taken into consideration, and electro-thermal analysis is performed using the COMSOL Multiphysics simulation tool based on Finite Element Modeling (FEM). Electrical contact resistance is one of the significant factors for automotive switches. The flow of current through the electrical contacts may affect the surface of the contacts correspondingly leading to an increase in the electrical contact resistance value. The electrical contact whose surfaces are made up of Silver (Ag), Copper (Cu), and Graphene (Gr) have been examined. A 3D model of the relay was created. The parameters such as Electrical Contact Resistance (ECR), temperature, and current density are obtained over the contact interfaces and the values are verified using theoretical calculations

Keywords: *Electrical contact, FEM, contact surface, electrical resistance.*

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H 001

Therapeutic Effect of Tumor-Targeted Nanovaccine for Photothermal Immunotherapy

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ABSTRACT

The ultimate goal is to meet successful cancer therapy, which is not only treating the primary tumor but also preventing metastatic tumors, therefore the concept of combining photothermal therapy (PTT) with immunotherapy is of great interest.[1] Presently, the treatment of TNBC is more challenging due to the lack of clinical markers for molecularly targeted therapies. Therefore, developing a new nanotherapeutic vaccine approach of targeted combinational therapy could be an effective alternative nano-strategy.[2] Hence, we designed a combination of NIR-responsive renal clearable ultrasmall copper sulfide (CuS) particles conjugated TAT peptides decorated hyaluronan (HA) and co-encapsulated with ICG/R848 denoted as CuS-TAT-ICG/R848-HA nanovaccine composite (NC) that exhibited an adequate photothermal conversion efficiency (PCE) that is highly beneficial for selective CD44-mediated photothermal ablation of TNBC tumors. Furthermore, co-encapsulation of ICG/R848 (immune adjuvant) molecules also triggers an improving photothermal response against the tumor and activation of TLR7/8a agonist R848 for antitumor immune response. The formed CD44-targeted NC selectivity incinerates the CuS-TAT mediated nuclear-targeted tumor cells. With a 1064 nm laser leads to effective photothermal ablation towards specific tumor cells. Concurrently, NIR-II responsive photothermal effects further elicit effective antitumor immunity by inducing ICD at tumor tissues, wherein dying tumor cells release distress signals of damage-associated molecular patterns (DAMPs). The co-presence of R848 and CuS causes dendritic cells maturation (DCs) to stimulate cytotoxic T cell activations, which promote an immune response. Thus, the NIR-II activated photothermal ablation combined with anti-programmed death-ligand 1 (aPD-L1) immunotherapy is a promising therapeutic platform for effective targeted immunotherapy and had great potential for cancer therapy.

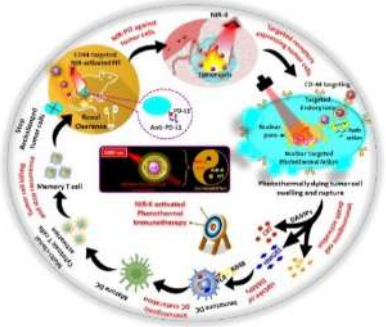

Figure: Schematic depiction of the Nanovaccine for photothermal ablation and cancer immunotherapy

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H 002

Anticancer Efficacy of Green Synthesized Zinc Oxide Nanoparticles mediated by *Calophyllum* species

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ABSTRACT

Cancer treatment remains a pressing challenge, often involving toxic therapies with harmful side effects. Researchers are focused on developing safer drugs that specifically target cancer cells while sparing healthy ones (American Cancer Society, 2016). Therefore, natural products together with other approaches may expand the molecular armamentarium for therapeutic choices, and give way for the finding of new undiscovered routes in drug discovery (Zhang and Demain, 2005). Nanotechnology, dealing with materials at the nanoscale, has gained prominence in this quest. Over the last few decades, the field of nanotechnology has grown profoundly as metal oxide nanoparticles are vastly used in many industrial applications (Ali et al., 2018). Integrating natural compounds with nanoparticles enhances their bioavailability and controlled release, overcoming the limitations like poor solubility in the bloodstream (Wang et al., 2017). Zinc oxide nanoparticles (ZnO NPs) stand out as promising candidates for targeted drug delivery due to their biocompatibility, ease of synthesis, and various nanostructures (Duncan and Richardson, 2012). Green synthesis methods, particularly involving plant extracts, offer eco-friendly and cost-effective approaches to produce ZnO NPs, with demonstrated cytotoxic effects on cancer cells (Selvakumari et al., 2015). *Calophyllum* species, known for their medicinal properties, have provided compounds with potential anticancer activity. Hence, this study aims to synthesize ZnO NPs mediated by the aqueous extract of the stem bark of *Calophyllum teysmannii*, characterizing their properties and evaluating their cytotoxicity and impact on colon and breast cancer cells. This research may contribute to the development of green-based nano-medicines for cancer treatment, addressing the critical need for safer and more effective therapies.

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H 003

Development and Characterization of a Nanoemulsion Based Vehicle for the Delivery of Antioxidant Rich Biopolymer Derived from Ganoderma Gibbosum

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ABSTRACT

The synthetic antioxidants have been long associated with adverse health effects due to which there is a high demand from the consumers for naturally derived alternatives. Mushrooms particularly the genus Ganoderma has been widely studied in the past few decades for its antioxidant properties. This genus is reported to contain approximately 400 different bioactive compounds such as phenolics, sterols, terpenoids etc. out of which exopolysaccharide is considered as a major group. The antioxidant potential of mushroom polysaccharides is a well-accepted fact. However, the major problem in using these polysaccharides as antioxidants is their low solubility and easy degradation. In order to overcome this problem nanoemulsion formulations are sought which have a potential in resolving this solubility and stability problem. In the present study, the development and characterization of a nanoemulsion based vehicle for the delivery of these bioactive polysaccharides was carried out. The nanoemulsion was formulated employing ultrasonication which resulted into a formulation with a droplet size of 101.5 nm, PDI of 0.189, zeta potential value of -8.2mV, 91.8 % transmittance and an encapsulation efficiency of 71.7 %. In terms of the stability testing the nanoemulsion was found to be pH stable, there were no signs of phase separation, creaming or cracking and no apparent changes in the turbidity were observed even after 28 days of storage signifying a stable formulation. Further the in-vivo antioxidant activity of the formulation was evaluated. The mice were subjected to paracetamol induced oxidative stress and were then administered with the different doses of nanoemulsion for 21 consecutive days. Increased activity of serum superoxide dismutase (SOD), catalase and decreased serum level of TBARS were observed suggesting the ability of the nanoemulsion to ameliorate the effect of ROS in biological system.

H 004

Investigating Bacterial Adhesion and Biofilm Formation on Patterned Polymeric Surfaces

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ABSTRACT

Biofilm formation is one of the leading causes of the failure of medical implants. Implanted biomaterials provide a conducive environment for bacteria to attach, colonize, and subsequently form complex, multicellular communities called biofilms. Thus, there exists a pressing need for strategies to inhibit biofilm formation. Surface patterning, or physical alteration of surface roughness of polymeric films with sub-micron or nanoscale features, has emerged as one of the most promising ways of controlling bacterial colonization on surfaces without imparting any chemical toxicity. Parameters such as the 1D or 2D nature of the patterns, pattern height, pattern periodicity, aspect ratio, polymer stiffness, and long-term durability, will have a combined effect on the antimicrobial activity of the surface. In this work, bacterial attachment and biofilm formation were investigated on PDMS surfaces with 1D and 2D patterns with different periodicity and pattern height. The patterned PDMS surfaces were fabricated using the replica molding technique against masters. Bacterial attachment on the flat and patterned surfaces was observed under an optical microscope and SEM after incubation of the surfaces with Staphylococcus aureus (S. aureus) suspension for 24-48 h at 37°C. S. aureus attachment on the patterned surface was lower than that on flat PDMS. Initial results show a greater extent of colony formation on flat PDMS, indicating the initiation of biofilm formation, which was not the case for all patterned surfaces. The results from this study show that patterned PDMS surfaces are promising for controlling bacterial attachment and surface colonization.

Keywords: *Surface topography, replica molding, antibiofilm, S. aureus*

H 005

Role of FeO Substitution on Bioactivity of Strontium Containing Silicate Glasses

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ABSTRACT

Synthesis and characterization of bioactive glasses have gathered significant attention due to their crucial role in promoting tissue regeneration and healing processes. This study is focused on the synthesis and characterization of strontium silicate bioactive glasses dopped with FeO to understand the effect on bioactivity. The compositional framework of the bioactive glasses under investigation comprises SiO_2, CaO, Na_2O, P_2O_5, FeO, K_2O, MgO and SrO synthesised by melt quenching method.

A single broad hump at around 30º and absence of sharp peak in all the XRD plots confirms the amorphous nature of the glasses. Different vibrational modes of Si-O bonds observed in IR absorption spectroscopy in the range of 1080 to 860 cm^{-1}. IR absorption band in range 1530 – 1390 cm^{-1} belonging to carbonates becomes more prominent with increase in SrO content. The band gap was found to decrease with increase in Strontium content of glass as studied by tauc-plots. The interactive effect of other trace elements, such as potassium (K) and magnesium (Mg), is investigated to comprehend their influence on the overall performance of the bioactive glasses. The freshly prepared Simulated body fluid (SBF) was infused in the pallets and kept at room temperature. The surface morphology and microstructure of bioactive glass tablets after immersing in SBF have been studied using SEM, XRD, and IR. The findings of this research bear significant implications for the development of advanced functional materials in the fields of orthopaedics and tissue engineering.

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H 006

Near-infrared Biowindow Assisted Photonic Cancer Nanomedicine for Theranostic Photo-thermal Immunotherapy

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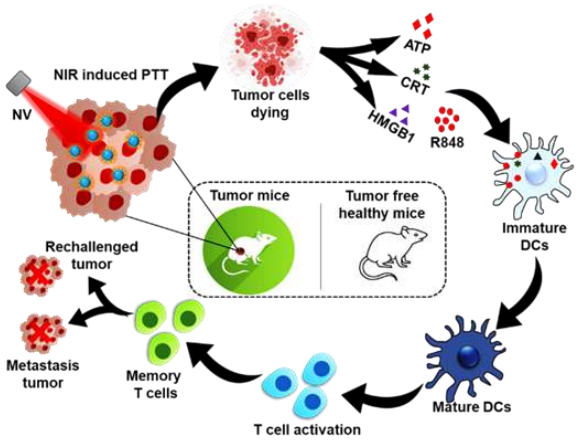
ABSTRACT

Recently, the rapid progress in research on photoactive nanomaterials has led to successful applications of photonic nanomedicines in a variety of healthcare fields including cancer. The photonic nanomedicine (PNM) refers to a specific niche of nanomedicine, which combines photonics principles with nanomedicine. Photothermal therapy (PTT), which uses the hyperthermia produced by NIR-responsive photothermal agents (PTAs) that convert light irradiation to ablate tumors, has received a lot of attention due to its low systemic toxicity, controllability, and noninvasiveness. Herein, developed PNM containing copper sulfide (CuS) as the primary component. PEI was used to assure the material stability, the surface was decorated with hyaluronic acid (HA) for active targeting CD44 receptor overexpressed tumor and loaded the drug resiquimod (R848) a synthetic Toll-like receptor 7 and 8 agonist enhanced immune response in the immune-suppressive tumor microenvironment (iTME). Furthermore, a combination with PTT and immunotherapeutic Nanovaccine (NV) CuS-PEI-HA- R848 to improve the immunological memory effect provided by this strategy helps to prevent the recurrence of tumor.

Key Words: *Near-infrared, Photothermal treatment, Resiquimod, Immunotherapy, Cancer.*



H 007

Release Profile of curcumin when loaded in bare form and in the form of an inclusion complex *via* gelatinpoly(acrylic acid) hydrogel

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ABSTRACT

Poor aqueous solubility of many known drugs is considered as one of the major challenges in drug development owing to low bioavailability and reduced therapeutic efficiency. One of the ways to deal with the solubility issue of a drug is formation of its inclusion complex. Curcumin (CUR) is one of the hydrophobic drugs having anti-inflammatory, anticancer and antioxidant properties which has wide applications in the biomedical field. However,the application of curcumin is restricted due low aqueous solubility, low bioavailability and short half-life period. Also, it can be degraded by the enzymes present in the digestive system. Considering these difficulties of CUR, the present work aims to form an inclusion complex of CUR using β-cyclodextrin to improve the solubility of CUR by developing its inclusion complex. Also, CUR was loaded in a hydrogel nanocomposite system which would protect CUR from the enzymes and aid in its controlled release. Gelatin crosslinked poly(acrylic acid) incorporated with nanofiller was synthesized using a free radical polymerization method. The synthesized CURInc and hydrogel nanocomposite were characterized using various characterization techniques such as FTIR, XRD and FESEM. The in vitro drug release profile of CUR and CURInc was studied under different physiological pH conditions. CURInc loaded hydrogel nanocomposite exhibited more controlled release of CUR over CUR loaded hydrogel system.

Key words: *Bioavailability, Curcumin, hydrogel nanocomposite, inclusion complex, controlled release.*

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H 008

Biocompatible Lipid Patches for Healing Peptic Ulcer Induced Perforations in Stomach Wall

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ABSTRACT

Peptic ulcer disease is a condition in which perforations develop in the lining of the stomach or the duodenum. About 10% of the entire population worldwide suffers peptic ulcer at some point of their lifetime. The most common sites of peptic ulcer are: stomach, particularly in the lesser curvature, gastric ulcer and first part of duodenum, duodenal ulcer. The most common causes of peptic ulcer are infection with the bacterium Helicobacter pylori (*H. pylori*) and long-term use of nonsteroidal anti-inflammatory drugs (NSAIDs). Peptic ulcer generally causes defect in the mucosal layer of the stomach that extends to muscularis mucosa. This leads to exposure of epithelial cells and Helicobacter pylori invades the epithelial cells of stomach. The biocompatible lipid patches are made for biomimicking the feet of gecko lizards. The spatulae of the bottom of geckos' feet interact with the surface through van der Waals forces. This provides high adhesive power. Similarly, these biocompatible patches can easily target the sites of ulcer and stick to the surface through van der Waals forces of attraction. The polymer- lipid nanohybrid fibers were created using a modified coaxial electrospinning process, with the electrospinnable drug- core solution. These patches are made into Ag nanomaterial capsules and will be orally administered. An essential step in the colonization by *H. pylori* and its ability is its selective tissue tropism leading to the establishment of intimate interactions with the epithelial surface. These interactions are mediated *via* outer membrane proteins (OMPs) that serve as adhesins. These proteins are isolated and prepared as the core solution in the lipid nanofibers and helps in targeting the site for adhesion of the patch. These patches, after mucosal regeneration, is degraded and excreted out of the body.

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H 009

Senna Auriculata Flower Extract Incorporated PCL/PCL-Cellulose Acetate Bilayer Electrospun Nanofiber for Wound Dressing Application

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ABSTRACT

This study aimed to prepare Senna auriculata flower extract and encapsulate it into polycaprolactone (PCL)/ PCL and cellulose acetate (CA) blend bilayer nanofibrous mat for potential wound dressing application. The minimum inhibitory concentration of the Senna auriculata flower extract was evaluated against gram-positive and gram-negative bacteria by broth dilution method. The extract was further characterized for its antioxidant and wound closure properties by the DPPH test and wound scratch assay. These results revealed the ability of Senna auriculata flower extract in free radical scavenging and wound closure. Later, the extract was incorporated into PCL/PCL-CA bilayer nanofibrous mat fabricated by the electrospinning technique. FESEM images of the fibrous mat confirmed the morphology of the bilayer. The physiochemical properties of the dressing were characterized, such as FTIR, swelling, extract delivery kinetics, porosity, degradation, and wettability, which are mainly required for effective wound dressing. The biological activity of the dressing was carried out by Invitro studies and confirmed the effectiveness of the wound dressing.

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H 010

Enhancing the efficiency of Olmesartan medoxomil drug through Metal Complexation

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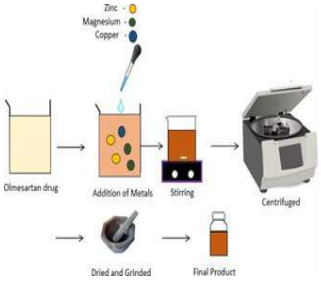
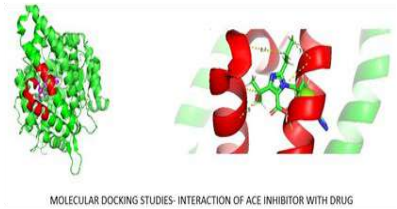
ABSTRACT

Olmesartan medoxomil is an angiotensin II receptor blocker, commonly prescribed for hypertension. It is a medication that helps lower blood pressure by its action on the Angiotension converting enzyme (ACE) and renin- angiotensin-aldosterone system (RAAS). The low dissolution of Olmesartan medoxomil hinders its binding efficacy to (ACE) and (RAAS) inhibitor. This study involves optimizing the dissolution of Olmesartan medoxomildrug through metal complexation, and to enhance the binding efficacy of the drug through novel approach of metal complexation of Olmesartan medoxomil with zinc (Zn), Magnesium (Mg) and copper (Cu) metals. Molecular Docking were performed to assess the binding affinity of the metals with the drug. Angiotension converting enzymes were also docked with apoform of the drug and complexed drug. The synthesized drug-metal complexes are systematically characterized using analytical techniques, such as UV-Vis Spectroscopy, FT-IR spectroscopy, Powder X-ray diffraction (XRD). NMR spectroscopy was employed to investigate the structural changes in drug binding to metals. Furthermore, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) unveil crucial insights into structural and morphological alterations. Comparative analysis of the binding capacity between the metal-complexed Olmesartan medoxomil and the unmodified drug provides insights into the potential advantages of these novel formulations.





MOLECULAR DOCKING STUDIES- INTERACTION OF ACE INHIBITOR WITH DRUG

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H 011

Conversion of microbial metabolites into nanoform for the expansion of their antimicrobial properties

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ABSTRACT

The escalating issue of antibiotic resistane among a growing spectrum of pathogens has given rise to a substantial global health crisis. One potential avenue to combat this crisis involves the investigation of therapeutic secondary metabolites produced by Actinobacteria. Actinobacteria are well-recognized for their production of bioactive secondary metabolites comprising of diverse therapeutic properties, including antibacterial, antifungal, antidiabetic, anticancer, and antioxidant capabilities. Leveraging these metabolites could offer significant prospects for the healthcare and pharmaceutical industries. However, their practical application has been impeded by certain limitations, such as limited solubility, high cytotoxicity, and low bioavailability. In this study, nanotechnology was employed to transform these metabolites into nanostructured forms, aimed at augmenting their therapeutic potential by increasing the surface area-to-volume ratio of the particles and addressing the aforementioned limitations. The resulting nanoparticles were characterized through various bioanalytical techniques including Transmission Electron Microscopy (TEM), UV-Visible spectrophotometry, Fourier-Transform Infrared Spectroscopy (FTIR), and Dynamic Light Scattering (DLS). Their antimicrobial susceptibility and potency was assessed against critical pathogens listed by the World Health Organization (WHO), including Gram-positive bacteria, utilizing the agar-well diffusion assay and determination of minimum inhibitory concentrations. Furthermore, the antibiofilm activity was evaluated and confirmed through Electron Microscopy, revealing biofilm inhibition by the nanoparticles containing therapeutic metabolites as compared to the bulk materials. This highlights their potential for further development as novel pharmaceutical agents. The findings of this study underscore the significance of exploring the extensive reservoir of bioactive secondary metabolites derived from Actinobacteria and revolutionizing the landscape of drug discovery through the integration of nanotechnology to enhance their therapeutic effectiveness. This, in turn, opens up promising avenues for drug development.

Key words: *Actinobacteria, Antimicrobial, Nanotechnology, Drug-Development.*

H 012

In *Silico* Molecular Docking on Bioactive Compounds from *Sphaeranthus indicus*Leaves Extract against the Anticancer Target Protein - Caspase 3

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ABSTRACT

Sphaeranthus indicus is an important medicinal plant used for the treatment of styptic gastric disorders, skin diseases, anthelmintic, glandular swelling, nervous depression, analgesic, antibiotics, antifungal, laxative, and diuretic properties. *Sphaeranthus indicus* possessmanypharmacological activities and possess high antioxidant activity, hence it is suggested to study the molecular docking studiesagainst the target protein caspase 3. Computers and computational methods are nowadays widely used in Biological Researches. *In silico* molecular docking in one of the most powerful techniques to discover novel ligand for proteins of known structure and thus play key role in structure-based drug. Caspase-3 plays a leading role in apoptosis and on activation, it cleaves many protein substrates in cells and causes cell death. Since many chemotherapeutics are known to induce apoptosis in cancer cells, promotion or activation of apoptosis via targeting apoptosis regulators has been suggested as a promising strategy for anticancer drug discovery. Hence in this present work carried out *in silico* molecules docking to analyze the binding properties of 9-Octadecene, 9,12,15-Octadecatrienoic acid, methyl ester, Phytol, 9,12-Octadecadienoic acid and 9-Octadecenoic acid fromthe GC-MS analysis of*Sphaeranthus indicus*to target protein 1CP3 (Caspase 3). This study suggested that 9-Octadecene, 9,12,15-Octadecatrienoic acid, methyl ester, Phytol, 9,12-Octadecadienoic acid and 9-Octadecenoic acid might be able to inhibition of caspase-3. Among the various compounds, 9,12,15-Octadecatrienoic acid has potential binding interactions than other compounds. So, the present study might act as supportive evidence for *in vivo* anticancer activity which surely help these molecules in reaching the market as commercial drug.

Keywords: *Molecular docking, Caspase 3, Sphaeranthus indicus, Apoptosis, Autodock, Anticancer.*

H 013

Measurement of Natural Radioactivity Levels of Rice in Imphal Valley, Manipur, Indiausing HpGe detector

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ABSTRACT

Natural radioactivity is present in all foods, including rice, in detectable amounts that gradually enter the body through eating. The level of naturally occurring radioactivity in rice is a significant factor in determining the population's exposure to radionuclides during daily food consumption. Rice is the most cultivated crops in Manipur, India especially in the Imphal valley areas and also the most staple food of Manipuri's. This study investigated the levels of natural radioactivity in rice samples grown from various locations in Imphal Valley, Manipur, India. A high purity germanium detector (HpGe detector) was used to measure the activity concentrations of Ra^{226}, Th^{232} and K^{40} in the soil samples. The activity concentrationsof these radionuclides were used to calculate the radiation hazard parameters, such as radium equivalent activity (Raeq), annual effective dose for the respective radionuclides caused by the rice consumption were calculated. The results were compared with the global radioactivity measurements and did not show any significant radiological risk for the general public of Manipur due to the daily consumption of the rice samples under study.

Keywords: *Rice, Natural radioactivity, Gamma ray Spectrometry, HpGe detector, Hazard parameter, radiological risk*

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H 014

Functionally Modified Amino Acid Infused into Green-mediated Hydroxyapatite with Cisplatin Integration for Oncological Bone Tissue Engineering

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ABSTRACT

Osteosarcoma is a form of bone cancer that often requires extensive surgical interventions and regenerative approaches for bone reconstruction. Hydroxyapatite is indeed considered a significant biomaterial with various bone and teeth-related medical applications. The wet chemical precipitation technique was employed to synthesize hydroxyapatite nanoparticles as well as green-mediated (*Moringa oleifera* extract) hydroxyapatite nanoparticles and D-Phenylalanine-modified hydroxyapatite nanoparticles. Characterization analyses were conducted to assess their structural, morphological, and thermal properties. Nanoparticles reveal their remarkable resistance to microbial activity against two bacterial pathogens namely *E. coli* and *streptococcus*. The investigation of drug delivery involved the incorporation of cisplatin drug into hydroxyapatite nanoparticles modified with D-Phenylalanine leading to the establishment of a consistent drug release pattern lasting for 48 hours. An in-vitro cytotoxicity study was conducted on MG-63 cells revealing a significant cell mortality rate when exposed to a 2mg concentration of nanoparticles. Similarly, fluorescence staining results indicated an 89% incidence of cell apoptosis. In summary, the nanocomposite loaded with the drug exhibits remarkable biocompatibility and antimicrobial properties and the ability to trigger apoptosis in osteosarcoma cells rendering it a versatile material for various medical applications.

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H 015

Development of Novel Zn-Xmg-Based Alloys for the Potential Biodegradable Implant Application

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ABSTRACT

In recent years, Zn-based alloys have gained increasing interest as biodegradable materials because of their excellent biocompatibility and moderate degradation rates. Nevertheless, the limited strength and ductility of the pure Zn severely restrict their potential application. This study proposes Zn–xMg (x=0, 0.1 and 0.5) alloys as candidates for biodegradable application. The microstructure, mechanical and tribological properties, and degradation behavior of the alloys are systematically evaluated. The microstructure of the Zn–xMg alloys is composed of the Zn matrix and Mg_2Zn_{11} phase, while the amount of Mg_2Zn_{11} phase increases with the addition of Mg. The mechanical strength of the alloys improves due to the formation of the hard Mg_2Zn_{11} phase. The Zn-0.5Mg alloy exhibits the best combination of mechanical properties with yield strength (YS), ultimate tensile strength (UTS), and elongation of 221 MPa, 267 MPa, and 42%, respectively. Magnesium (Mg) addition also improves the tribological behavior of the alloys in dry sliding conditions. Also, the bending strength of the alloys increases with the addition of Mg, and the highest bending strength is 232 MPa for Zn-0.5Mg alloy. The *in vitro* degradation rate of the alloys in Hanks' solution greatly increases due to the micro-galvanic cell formation between the Zn matrix and Mg_2Zn_{11} phase, where Mg_2Zn_{11} acts as a cathode. The potentiodynamic polarization and immersion study follow the sequence of degradation rate as Zn < Zn-0.1Mg < Zn0.5Mg. The unique combination of mechanical properties and *in vitro* degradation behavior establishes the Zn – Mg alloys as a potential candidate for biodegradable implant application.

H 016

Biomedical Applications of Polyherbal extract and Silver Nanoparticles Incorporated in Sodium Alginate Hydrogels

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ABSTRACT

In tissue engineering, biopolymeric hydrogels are gaining prominence for their inherent advantages, marked by exceptional biocompatibility, biodegradability, and biosafety derived from their biological origin. The augmentation of these hydrogels with active compounds and nanoparticles further enhances their foundational characteristics. This study centers on the development of sodium alginate hydrogels incorporating polyherbal extracts and nanoparticles, with a specific focus on their suitability for wound healing. Silver nanoparticles are synthesized in an eco-friendly manner using polyherbal extracts. The formation of sodium alginate hydrogels involves crosslinking with ZnCl2 salt, and the incorporation of polyherbal extracts and nanoparticles prompts a thorough characterization. Comprehensive analyses, including SEM, FTIR, and XRD, are conducted to assess nanoparticle size and hydrogel porosity. Additional evaluations encompass in vitro cytocompatibility, hemocompatibility, and a scratch assay for wound healing assessment. SEM analysis discloses nanoparticles with an average diameter of 32nm and a highly porous hydrogel structure. FTIR results highlight significant vibrations in C-C and OH bonds. The MTT assay affirms cytocompatibility, showcasing a notable 95% cell survival rate after 72 hours. The scratch assay indicates enhanced fibroblast migration compared to the control, while hemolysis assessment reveals minimal hemolytic potential well within the acceptable limit of 1%. To conclude, the integration of polyherbal extracts and nanoparticles into sodium alginate-based hydrogels holds significant promise as wound dressings, promoting both cell proliferation and migration, thereby positioning them as compelling candidates for applications in tissue engineering.

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H 017

Chitosan Hydrogels Infused with Polyherbal Extracts for Tissue Engineering

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ABSTRACT

In recent years, biopolymers have garnered substantial interest in tissue engineering owing to their commendable biocompatibility and biodegradability. Chitosan, with its attributes of easy administration, low toxicity, and excellent water retention, aligns with the requisites of an ideal medication delivery system. Given the susceptibility of medicinal plants to degradation, an efficient delivery system becomes imperative to preserve their antioxidant and anti-microbial properties. Consequently, the incorporation of polyherbal extracts into chitosan not only ensures the retention of medicinal properties but also facilitates sustained delivery. This study focuses on the development of cross-linking chitosan hydrogel loaded with polyherbal extracts, evaluating its physicochemical characteristics, drug loading, and drug release properties. The efficacy of polyherbal extract-infused chitosan hydrogels for drug delivery is further examined in vitro through cytocompatibility and hemocompatibility testing. Scanning electron microscopy (SEM) analysis unveils a highly porous hydrogel structure. The MTT assay demonstrates a remarkable fibroblast cell survival rate exceeding 90% at 72 hours. Additionally, the hydrogels exhibit no blood cell aggregation and less than 1% hemolysis. The combined attributes of sustained drug release and biocompatibility position chitosan hydrogels as promising candidates in the realm of tissue engineering.

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H 018

Fabrication and Characterization of Anthocyanin Rich Flower Extract Incorporated Nanofibrous Membrane for Ph-Responsive Wound Dressing

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ABSTRACT

This study is intended to fabricate anthocyanin-rich extract incorporated into cellulose acetate (CA) and polycaprolactone (PCL) nanofibrous mat for wound healing and pH-responsive wound dressing. The prepared membrane was characterized for its surface morphology and functional groups using scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). The structural analysis of the membrane was carried out using X-ray diffraction (XRD). The wound healing property of anthocyanin extract was studied for its antioxidant properties using a DPPH assay, and an in vitro wound scratch test was carried out to identify the percentage of wound closure within 24 hours. The membrane was also analysed for its antibacterial and anti-inflammatory properties. Further, the light pink-coloured dried nanofibrous membrane was analysed for a pH sensor by immersing it in phosphate buffered solution (PBS) with a pH ranging from 4 to 6. It displayed a pink colour, representing the wound milieu that promotes wound healing; when exposed to pH 7–10, it displayed a green–blue colour, indicating the wound milieu that impedes wound healing.

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H 019

Fabrication of Nanofibrous PVA/HA/Mgo Mats for Bone Tissue Regeneration

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ABSTRACT

Electrospun nanofibrous polyvinyl alcohol (PVA) structures, found to have numerous biomedical applications. They show excellent biocompatibility, flexibility and biodegradability. Highly porous biocompatible structures with adequate strength are required for tissue regeneration applications.Hydroxyapatite (HA) is the main natural inorganic mineral present in human bone as well as teeth. It has high calcium mineralization and collagen deposition capabilities. Reports show that the presence ofMgO improves the osteogenic properties of HA. This paper reports the incorporation of HA/MgO nanocomposites in PVA matrix by the method of electrospinning. An auto-ignited combustion technique was used to synthesise nanostructured HA and MgO. X-ray diffraction technique was used to confirm crystalline phases present in the samples. The crystalline phases obtained from the ICDD file for HA was hexagonal and for MgO was cubic. The crystallite size estimated using XRD was 26 nm for HA and 18 nm for MgO. HA and MgO were mixed in definite proportions to form HA/MgO nanocomposites and dispersed well in 10% (w/v) PVA solution. The spinning parameters were optimized to fabricate highly porous nanofibrous PVA/HA/MgO mats. XRD of the electrospun fibres revealed the presence of HA and MgO in PVA. Morphology of the electrospun fibres was studied usingScanning Electron Microscopy. The composite loading limit was optimized as 1g after which the uniformity of the fibre gets reduced. The incorporation of HA/MgO in PVA matrix is expected to improve the mechanical and biological properties of the nanofibrous structures, and can be used for bone tissue regeneration applications.

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H 020

Biosynthesis of Cuprous oxide Nanoparticle Hydrogel for Bone Regeneration

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ABSTRACT

The endeavour to address the intricate clinical dilemma of bone regeneration, characterized by the scarcity of suitable bone substitutes, necessitates the exploration of innovative and efficacious alternative approaches. Copper ions can stimulate the differentiation of bone marrow-derived mesenchymal stem cells (BMSCs) towards an osteogenic lineage. Cuprous oxide (Cu_2O) nanoparticles exhibit significant antibacterial effectiveness across a wide range of microorganisms. Recognizing the beneficial impact of cuprous oxide on bone regeneration, a hydrogel composed of polymer and cuprous oxide nanoparticles (source of Orange peel) was meticulously fabricated through solvent casting method. Comprehensive *in-vitro* assessments, including analyses of surface morphology, FTIR, XRD, swelling behaviour, gel content, hemocompatibility, and biocompatibility were conducted to evaluate the hydrogel's physicochemical and biological attributes. The outcomes of these extensive analyses unveiled that the fabricated hydrogel exhibited favourable characteristics, notably including their propensity for substantial swelling and adequate gel content, thus providing an environment conducive for cellular proliferation. Hemocompatibility tests showed a commendable performance with a lysis rate below 5%. Moreover, the *in-vitro* assessments of cytocompatibility with Osteoblast-like cell lines revealed a significant enhancement in cellular viability, thus underscoring the hydrogel's potential for fostering cell growth and bone tissue regeneration. The outcome of this study indicate that the developed hydrogel hold considerable promise in the field of bone regeneration.

Keywords: *Cuprous oxide, orange peel, Hydrogel, Cytocompatibility, Bone regeneration.*

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H 021

Nanostructured of Pectin Mediated Cerium Oxide with HAP-Chitosan Scaffold for Tissue regeneration

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ABSTRACT

Biocompatible materials are essential in tissue regeneration, fostering successful therapeutic outcomes. This abstract explores various biocompatible materials, such as hydrogels, ceramics, and polymers, highlighting their crucial roles in providing scaffolds, growth factors, and mechanical support for regenerating damaged or lost tissues. Hydroxyapatite is commonly used in tissue regeneration because it can support the growth of new bone tissue, its porous structure allows for the gradual replacement of hydroxyapatite with natural bone over time, promoting successful tissue regeneration. Chitosan supports cell adhesion, proliferation, and tissue growth, making it valuable for skin regeneration. Pectin-mediated cerium oxide nanoparticles ($pCeO_2$) hold promise in tissue engineering applications. Pectin, a biocompatible polymer, can stabilize and control the release of cerium oxide nanoparticles. These nanoparticles have antioxidant and regenerative properties, making them potentially valuable for protecting cells and promoting tissue regeneration. Polymers and Metal oxide nanoparticles, and their combinations as composite materials possess the necessary properties and hold promise for bio stimulation in tissue regeneration. In this study, Hydroxyapatite/ chitosan/ pectin mediated cerium oxide nanocomposite Scaffolds were created using different concentrations of cerium oxide nanoparticles. The Scaffold was analyzed through techniques such as XRD, FTIR, SEM, UV-DRS, DLS, Zeta potential and TGA. Further, its Antioxidant, swelling behavior, Porosity, degradation and solubility tested to develop a biocompatible Scaffolds. The developed Scaffolds has shown excellent hemolysis and antibacterial activity, the scaffold with the highest cerium oxide nanoparticles content exhibited the highest cell adhesion. The composite Scaffold demonstrated favorable cell adhesion and low cytotoxicity, indicating their potential as biomaterials for tissue engineering.

Key words: *Hydroxyapatite, Metal oxide nanoparticles, Biocompatible scaffolds, Tissue engineering*

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H 022

Biofunctionalized Nanohydroxyapatite Spheres with Mesopores: Synthesis, Characterization, Biocompatibility, and Antimicrobial Activity

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ABSTRACT

Nanohydroxyapatite (nHAp), is an exceptional biomaterial in the healthcare Industry[1]. To enhance its applicability, researchers are currently involved in engineering the morphology using macro-molecules and improving the bio functionality like antimicrobial activity either by loading the antibiotics directly [2] or by doping the ions like Silver, Zinc oxide, Strontium and Cerium, to nHAp[3,4]. Green synthesis is considered an alternative to improve the bioactivity[5]. The present work, reports that the above-mentioned biofunctionalities and fine-morphology control could be achieved by coprecipitation method using the Sodium dodecyl sulphate macromolecules (SDS) based on its critical micelle concentration (CMC) calculation. The parameters to synthesize nHAp of uniform spherical morphology have been explored here. The XRD data shows that, pure HAp phase of the sample is in good agreement with JCPDS#09-0432 data. FTIR spectrum also confirms the same. BET analysis confirms the high surface area and mesoporous nature. MTT assay shows good biocompatibility. Antimicrobial activity is demonstrated against Salmonella typhi, E.coli, V. cholerae, K.pneumonia, S.epidermidis, and V. cholerae. The TA/DGA tests verify thermal stability. The results are discussed in detail.

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H 023

Development of Injectable *in situ* Hydrogel scaffold for tissue engineering

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ABSTRACT

Injectable hydrogels have tremendous potential for tissue engineering due to their versatility for minimally invasive *in situ* delivery and customizable mechanical and biological properties. The perfect design of 3D biomaterials, such as injectable hydrogel scaffolds, is required, taking into account all aspects of physical characteristics and chemical make-up. Hydrogel scaffolds play a significant role in several areas, such as nerve, heart, and bone tissues. In the current study, d an injectable hydrogel scaffold consisting of collagen, aldehyde-modified Nano crystalline cellulose, and chitosan that has been loaded with Phyto mediated gold nanoparticles [1]. The hydrogel scaffold's structure and mechanical characteristics were all strongly impacted by the presence of Chitosan -AuNps - Collagen/NCC in different molar ratios [2]. The results of *in vitro* hemolysis assay, antimicrobial, antioxidant and anti-inflammatory potential showed that the developed hydrogel scaffold framework had a lot of potential for tissue engineering in applications.

Keywords: *Injectable Hydrogel scaffold, Chitosan, Nano crystalline Cellulose, Tissue Engineering.*

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H 024

Anthocyanin-rich bio-composite mat as pH receptive in wound healing

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ABSTRACT

Misdiagnosis of wound infection hazards include improper antibiotic prescription, antibiotic resistance, and unneeded side effects from therapy. The pH level within the wound milieu, directly and indirectly, influences all the metabolic responses occurring during this healing process. The proposed work aims to fabricate a novel bio-composite mat using polyvinylalcohol (PVA) and sodium alginate (SA) with an anthocyanin-rich flower extract by electrospinning for therapeutic and pH monitoring during wound healing. The flower extract of Clitoria ternatea assists with comfy and fast healing as it possesses antioxidant, antimicrobial, and anti-inflammatory properties. The GCMS analysis of flower extract reveals its anthocyanin content. Spectroscopic techniques such as Ultraviolet-visible spectroscopy (UV- Vis), Fourier-transform infrared spectroscopy (FT-IR), Scanning Electron Microscopy (SEM), and X-ray diffraction (XRD) disclose the mat's functional group and surface characteristics. The DPPH assay uses free radicals to measure the mat's antioxidant activity. The phytocomponents in the flower extract provide the mat's antibacterial and anti-inflammatory properties and boost the rate of cell migration within 24 hours, as determined by the scratch experiment. Moreover, the fabricated mat is analyzed for pH sensing potential by immersing it in PBS, which has a pH range of 4 to 6. Effective wound healing is shown by the blue mat of pH less than 7; delayed wound healing is indicated by the green mat of pH greater than 7.5.

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H 025

Antibacterial Effect of Triphala-Mediated SilverNanoparticles Sonicated at Different Amplitudes

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ABSTRACT

The aim of this study is the green synthesis of silver nanoparticles using Triphala extract and to evaluatethe antibacterial effect. Nanoparticles of noble metals such as silver exhibit a wide variety of physical,chemical, and biological properties compared to their bulk which can be applied for antibacterial, antifungal, antimicrobial, anti-cancer and drug delivery. Triphala is an ayurvedic formulation of three fruits namely:- *Emblica officinalis, Terminalia chebula,* and *Terminalia belerica* and shows excellent antioxidant, anti-inflammatory, anti-bacterial, anti- diabetic, anti- cancer, cardio protective, anti obesitic, antidiarrhoea and antiaging properties due to presence of various secondary metabolites. In this work, the reformulating Triphala extract using silver nano-colloids is sonicated at two different amplitudes in DMSO to understand its effect on the distribution of the size of nanoparticles, which canassist in curing the infections caused by bacteria. Biophysical characterization of Triphala derived silver nanoparticles was performed using UV- Vis absorbance spectroscopy (UV-Vis), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR)and photoluminescence. In this study, the antibacterial assay proved that the silver nanoparticles sonicated at different amplitudes have different bactericidal activityagainst two different bacteria such as *E.coli* and *staphylococcus aureus*.

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H 026

Tailoring the rheological properties of biosynthesized Copper oxide nanoparticles decorated Carboxymethyl cellulose hydrogels for biomedical applications

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ABSTRACT

Nanoparticle-decorated hydrogels have seized substantial momentum in recent years, exclusively in biomedical research. In this investigation, Copper oxide nanoparticles decorated carboxymethyl cellulose hydrogels were prepared in an eco-friendly approach without using toxic cross-linkers. Initially, Copper oxide nanoparticles were prepared by biosynthesis approach to diminish the harmful effects of chemicals and to improve the biological activities using the leaves extract of Justicia adhatoda. The prepared nanoparticles are incorporated into the Carboxymethyl solution and carbopol to form a hydrogel by non-covalent interactions. X-ray diffraction analysis of CuO nanoparticles monoclinic crystalline structure without impurity. Rheological investigation of pure hydrogel and CuO-decorated hydrogels revealed that CuO contributed to the progress of hydrogel's mechanical performance. All the hydrogels demonstrated shear thinning behavior and better flow behavior index by adding CuO nanoparticles. The yield stress of the hydrogels was improved and found in the range of 61 to 79 Pa, which matches the ideal yield stress values of transdermal drug delivery. Storage moduli of hydrogels as a function of frequency was increased by double (14 Pa to 47.5 Pa), endorsing the involvement of CuO nanoparticles in crosslinking the polymeric matrix. Temperature and time sweep measurements revealed that the stability of the hydrogels also improved with the CuO nanoparticles. The antibacterial activity of the hydrogels was evaluated using biofilm inhibition and showed better inhibition of 70±0.5 %, 75±0.9 %, 86±0.8 %, and 83±0.8 % against Escherichia coli, Klebsiella pneumonia, Staphylococcus aureus, and Enterococcus faecalis with the increased concentration of CuO nanoparticles. The cell viability of the CuO-decorated hydrogels against MCF-7 and A431 was found to be 39% and 42%. Therefore, the eco-friendly biosynthesized CuO nanoparticles decorated hydrogels and improved mechanical properties can be employed in injectable and transdermal drug delivery systems.

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H 027

Linker size dependent Mechanical Properties of Di-imine based Molecular Crystals

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ABSTRACT

The recent emergence of mechanically flexible molecular crystals is of great importance due to their potential application in various fields, including flexible electronics, mechanical actuators, sensors, tunable dynamic components, etc [1]. There is a recent trend to gainfully incorporate other properties such as electronic, optical, and magnetic properties with flexibility to achieve desired applications [2]. Mechanically flexible molecular crystals have emerged as a fascinating class of materials with the ability to undergo substantial deformation without compromising their structural integrity [3]. We report here four 3,5-di-tert-butyl salicylaldehyde based di-imine crystals. Crystals **1, 2** were plastic while crystals **3, 4** were brittle and elastic, respectively [4,5]. With changing the length of intervening linker molecule, structure and packing factors were influenced greatly resulting in the final outcome of mechanical properties. It is possible to fine-tune mechanical properties by changing the length of the linker moiety while keeping peripheral shape synthons the same. These findings open up new avenues for tailoring the mechanical flexibility of molecular crystals, opening up opportunities for their application in various fields [2].

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H 028

Designing Photoresponsive Cyanostilbene Molecular Crystals with Mechanical Elasticity

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ABSTRACT

Innovative photomechanical dynamic molecular crystals provide platform for harnessing light energy and efficient conversion into mechanical motions. Mechano-responsive materials, exhibiting mechanical responses under the external stimulus of heat, light, solvent, or external force, are essential for smart actuation devices, biomimetics, actuation and soft microfluidics [1]. In this study, the mechanical properties and photomechanical motions of molecular crystals based on a bromo-substituted cyanostilbene (BCS) derivative are investigated. These crystals exhibit excellent mechanical flexibility and photoinduced mechanical behaviours due to topochemical [2 + 2] photocycloaddition inside the lattice. Mechanical flexibility is attributed to absence of slip planes along with corrugated packing features while photoresponsive behaviour is ascribed to [2 + 2] photocycloaddition owing to topochemical alignment of olefinic bond within Schimdt's criteria. Strain generated due to formation of cyclobutane derivatives gets channelized to manifest photoresponsive bending akin to bimetallic strip. It further demonstrates thermal reversible responses with gradual heating. Incorporation of dual mechanical responses in same molecular crystals are essential for fabricating actuation-based devices [2-4]. Our work broadens the insight for developing the flexible photoresponsive molecular crystals.

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H 029

Glaucoma Detecting system based on the Optic Disc and Optic Cup Segmentation from Fundus Images

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ABSTRACT

Fundus imaging is an advanced imaging technique used in healthcare that captures detailed images of the rear of the eye, including the optic disc (OD), optic cup (OD), and blood vessels. This is very useful in ophthalmology for identifying glaucoma, which is a leading cause of irreversible blindness globally. Glaucoma is caused by damage to the optic disc, where the optic nerve enters the eye. The Cup-to-Disc Ratio (CDR) is an important factor in determining the severity of glaucoma and its development. This method involves three stages: preprocessing, segmentation, and classification. The input retinal image is subjected to data augmentation, channel separation, and contrast enhancement to improve the image quality, reduce noise, and enhance the visibility of relevant features. This pre-processed image is segmented using the modified U-Net architecture to delineate the optic disc and cup regions. The architecture is designed to extract intricate features and spatial information from retinal images, enabling precise and accurate segmentation. The CDR value is calculated using the segmented optic disc and cup images. The retinal images are then classified as normal or glaucoma using a machine learning classifier based on the calculated CDR value. To evaluate the performance, metrics such as the Dice coefficient, Jaccard index, and accuracy are computed to quantify the accuracy and reliability of the results. The proposed system's effectiveness is validated using a DRISHTI-GS dataset, and the results show that our method outperforms existing techniques in terms of accuracy and computational efficiency. This can significantly aid ophthalmologists in early glaucoma diagnosis, thereby improving the quality of patient care and reducing the risk of vision loss.

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H 030

Synthesis, Properties and Application of Titanium dioxide (TiO_2)

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ABSTRACT

Titanium dioxide (TiO_2) is widely used because of its good biocompatibility and stability. TiO_2-based nanomaterials are attracting much attention in many areas, such as photocatalysis, photoelectricity, probing, electrochromism, photochromism, etc. They are widely used in paints, polymers, sunscreens, and toothpaste. There are various ways of synthesis that affect the size, shape, and crystallinity of TiO_2 nanoparticles. The main methods of obtaining titanium dioxide (with the structure of anatase, rutile or brookite) in the form of spheres, rods, fibers, and tubes include: sol-gel technology, hydrothermal and solvothermal methods, microwave method involving high-frequency electromagnetic waves, template method, electrodeposition, a sonochemical method using ultrasound, chemical and physical vapor deposition, "green" methods, etc. This literature review presents modern scientific results on the production of TiO_2 nanoparticles by various methods. Titanium dioxide (TiO_2) is a promising material for many emerging applications. Even more promising are the benefits offered by the material when its length scale is reduced to the nanometer range. Nanomaterials usually exhibit unique properties resulting from either the extremely large surface area-to-volume ratio or the quantum confinement effect of energy carriers. In this article we present an overview of recent progress in the synthesis of TiO_2 nanomaterials. The synthesis of nanomaterials, nanotubes, nanorods, nanocomposites by the sol- gel method and thermodynamic, optical, electronic and photon-induced electron-hole properties of TiO_2 is explained here.

Keywords: *TiO_2 nanocomposites; stability; sol-gel method; properties; vapor deposition method;*

H 031

Classification of Various Stages of Diabetic Retinopathy from Optical Fundus Images by Enhanced Morphological filter with Dark channel prior Enhancement Techniques

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ABSTRACT

Diabetic Retinopathy (DR) is a diabetic complication caused by the huge amount of insulin in the blood, damaging the tiny blood vessel that nourishes the retina. Ophthalmologists primarily detect retinal diseases by using optical fundus images. However, the images acquired by the digital non-mydriatic fundus camera are not feasible for the ophthalmologist to appropriately diagnose the disease. Preprocessing techniques are necessary to improve the quality of images before classification. The proposed approach employs an enhanced morphological filter followed by a dark channel prior dehazing as a preprocessing strategy. This research uses a Resnet-based architecture for automatic classification through a transfer learning approach. The weights in the last few layers are frozen and replaced by new layers, and the weights are trained using new hyperparameters. The images obtained from SRM Medical College Hospital and Research Centre are used as the proprietary database for image classification experimentation. The overall validation set accuracy of the proposed method was 99.01% for binary classification and 96.32 percent in the 3-stage classification model. The overall system model is shown in the Figure 1.

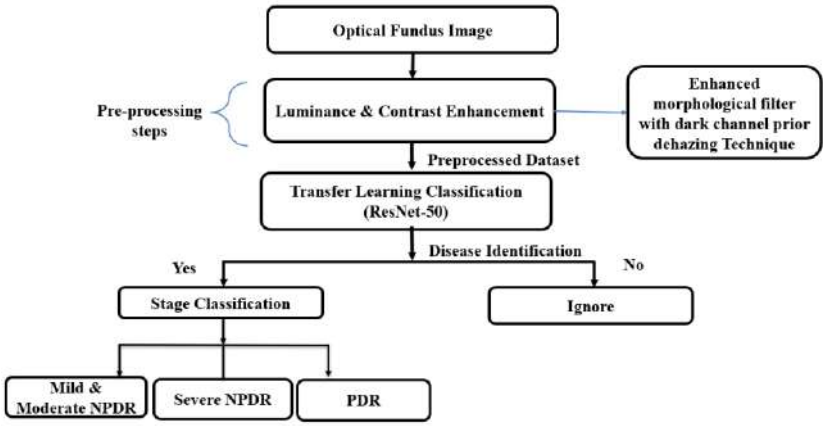

Figure 1 Illustration of the proposed classification model of DR using pre-processed fundus images

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H 032

An Efficient Image Enhancing Approach: Denoising of T1-weighted Magnetic Resonance Imaging for Neurological Disorder Diagnosis

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ABSTRACT

Technological developments in medical imaging, such as Magnetic Resonance Imaging (MRI), are crucial in providing an early diagnosis and a better understanding of brain issues. For children with neurological disorders, denoising MRI data can improve diagnosis accuracy and track the patient's progress. Denoising is a crucial process that eliminates noise from images without affecting any of their structural or diagnostic value. The noises found in MRI scans are mostly Gaussian, Rayleigh, and Rician noises. Therefore, this study aims to remove such noises from T1-weighted brain MRI using a combination of advanced state-of-the-art techniques and basic filtering methods. The proposed denoising method is a combination of deep learning-based denoising and wavelet denoising to efficiently remove the noises from the MRI of children. The results include a comparison of each denoising technique evaluated based on the peak-to-signal noise ratio, mean square error, and structural similarity index. In conclusion, the proposed denoising technique efficiently removes noise compared to existing methods. The denoised images can be taken for the accurate identification or classification of neurological disorders in children.

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H 033

The evolution and recent research trends of Shape Memory Polymers: A Citation Network Analysis.

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ABSTRACT

The development of Shape Memory Polymers (SMPs)-Polymers with the brain- has undergone a captivating journey since its inception. This systematic review offers a comprehensive exploration of the multifaceted realm of SMPs. The historical origins of SMPs can be traced back to their early associations with polymer gels and Shape Memory Alloys (SMAs). This analysis reveals how these distinct roots have given rise to two parallel research trajectories, resulting in diverse developments and applications within the field. The trajectory of global evolution and emerging research trends are systematically examined, along with Mapping the significant milestones, breakthroughs, and interactions with various scientific disciplines using citation network analysis. Diverse classifications and milestones that have evolved based on various parameters, including the stimuli employed, functionalities, and programming methods, are also discussed systematically. The review offers a profound insight into the evolution of manifold applications and adaptabilities within the SMP domain and delves into the cutting-edge advancements driving SMP technology forward. The growth curve indicates that research activities are in the growing stage. We obtained the global main path of the ongoing research and examined each node to identify major milestones and emerging research fronts. The cluster analysis of the available Web of Science (WoS) data was also done.

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H 034

In Vitro Antioxidant Activity of *Enhalus acoroides* Against Hydrogen Peroxide Induced Oxidative Damage in Human Erythrocytes.

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ABSTRACT

Enhalus acoroides, a seagrass contained high amounts of phytochemicals like alkaloids, flavonoids, polyphenols etc., and their crude extract exhibit cytotoxicity activity against cancer cell lines. Hence it was planned to investigate further on the various phytochemicals present in them and to find the *In vitro* antioxidant activity in hydrogen peroxide induced oxidative damage in human erythrocytes to assess its anticancer activity. The present study was aimed to examine the protective effect of ethanolic extract of *Enhalus acoroides* against hydrogen peroxide induced oxidative damage in human erythrocytes in vitro conditions. The experiments are performed in groups (Control, H_2O_2 induced and H_2O_2 + 25µg/ml, 50 µg/ml, 100 µg/ml, 200 µg/ml and 400 µg/ml). The enzymic antioxidants like MDA, CAT, SOD, GPx, and non-enzymic antioxidants like vitamin C, vitamin E and GSH levels evaluated to determine the antioxidant activity of *Enhalus acoroides*. The alkaloids prevent the decline of antioxidant status which in turn decreases LPO levels by preventing MDA formation in erythrocytes. The results confirm the protective effect of ethanolic extract of *Enhalus acoroides* against free radical induced oxidative damage in human erythrocytes. In conclusion, it can be said that ethanol extract of *Enhalus acoroides* exhibit potential antioxidant effect against Hydrogen peroxide induced oxidative stress and possess antioxidant activities. This indicates that the lipid peroxidation and oxidative stress elicited by H_2O_2 intoxication had been nullified due to the effect of *Enhalus acoroides*.

Keywords: *Enhalus acoroides,* Antioxidant, Hydrogen Peroxide, Oxidative stress.

H 035

Exploring the molecular mechanism of Reactive Oxygen Species imparted by Fullerene (C_{60}) nanosystems over lung cancer cell lines: A Review

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ABSTRACT

Lung cancer remains the top cause of cancer-related death worldwide, underscoring the crucial need for novel therapeutic approaches. Fullerene (C_{60}) nanosystems have attracted interest for their achievable application in cancer therapy, owing to their unique and outstanding physicochemical features and innate capacity to either create or quench cell damaging Reactive Oxygen Species (ROS). This study elevates the molecular processes driving ROS-mediated cytotoxicity in lung cancer cell lines produced by Fullerene C_{60} [1]. Implementation of various lung cancer cell lines in in-vitro tests to determine the Fullerene C_{60}'s effect of on cell viability and ROS generation. Many other researches projected that; C_{60} Fullerene are potent to increase ROS levels when treated on a dose-dependent mode. There are more and impactful pathways that is associated with ROS-mediated cell death including oxidative stress, DNA damage, mitochondrial malfunction, and apoptosis. This contribution of signaling pathways and independent genes in ROS generation or quenching was investigated, offering adequate guidance on attainable and feasible therapeutic targets [2]. The effect of Fullerene nanosystems changes from cancer cells to normal lung cells, this paved a way considering uncomplicated access to their potential for targeted cancer therapy. Here, this study sheds light and valuable insights on the molecular pathways by which Fullerene (C_{60}) nanosystems induce ROS-mediated cytotoxicity in lung cancer cell lines [3]. Understanding these pathways is crucial for the development of robust nanoscale-based cancer therapeutics, which could pave the way for targeted and effective lung cancer treatments.

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H 036

Photo Physical Study of an Organic-inorganic Hybrid layer-by-layer Electrostatic Self-Assembled Film of Cationic Small molecule dye Methyl Violet and a clay mineral Laponite

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ABSTRACT

In recent times small molecular weight water soluble fluorescent organic dye materials have attracted significant attraction because of their application in biomedicine and drug delivery applications [1]. On the other hand, numerous scientific research has confirmed usefulness of natural clay minerals as potential Nano drug carrier [2].In our present work, detailed investigation has been carried out to understand the nature of interaction between an inorganicclay called Laponite and anorganic small moleculecationic dye called Methyl Violet(MV) in aqueous solution as well as in organic-inorganic hybrid layer by layer(LbL)self-assembled film. UV-vis absorption spectroscopy confirms formation of H-type aggregates with increasing clay Laponite concentration in Laponite dispersed aqueous solution of MV. On the other hand, the degree of dye aggregation in LbL films is found to be dependent on concentration of clay particles as well as concentration of MV which is evident from UV-vis absorption spectroscopy and steady state fluorescence spectroscopy method. It is really interesting to observe that the organization and assembling behavior of MV molecules on host Laponite matrix in LbL films is significantly depends on external stimuli like pH of dye solution and ionic strength. Fourier Transform Infrared (in ATR mode) spectroscopy method is employed to comprehend the electrostatic attraction between cationic MV and anionic Laponite in LbL film. The surface morphology and roughness profile of organic-inorganic MV/Laponite LbL film onto a solid substrate has been explored using Atomic Force Microscopy (AFM) technique.

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H 037

Purification, Characterization and Molecular Weight Determination of fungal Chitin obtained from *Aspergillus niger*

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ABSTRACT

The present study primarily focuses on the extraction, refinement, and in-depth analysis of chitin derived from the fungal biomass of *Aspergillus niger*. To identify the fungal strain with the highest chitin production capacity, we utilized 18S rRNA sequencing. Following the extraction process, we determined the molecular weight of the chitin polymer using the conventional Pullulan method. Our findings revealed a significantly high molecular weight, approximately 344,000 Daltons, indicating the substantial size of the chitin molecules. For purification purposes, we employed gel permeation chromatography, resulting in a refined chitin product. This purified chitin displayed several notable characteristics, including a remarkably high degree of acetylation, measuring approximately 63.4%. Further analysis highlighted the presence of various functional groups, a smooth surface texture, a well-defined crystalline structure, and importantly, demonstrated its non-toxic nature. These comprehensive characterizations, encompassing structural, molecular, and toxicological assessments, collectively underscore the exceptional quality and potential utility of the obtained chitin.

H 038

Exploring $NiFe_2O_4$-$BaTiO_3$ Nanocomposites: Potential in Drug Delivery Applications

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ABSTRACT

Scientific community is looking for promising and non-hazardous healing therapies in drug delivery. Recently, magnetoelectric (ME) nanoparticles, composite of ferromagnetic and ferroelectric materials is gaining much attention because of their tunable properties and multiple applications in this field. In this study, we explored the potential of $NiFe_2O_4$ (NFO)-$BaTiO_3$ (BTO) magnetoelectric nanoparticles for drug delivery applications. NiFe2O4 nanoparticles were synthesized by hydrothermal method, while $BaTiO_3$ was prepared using sonication. The nanocomposite of these materials is synthesized by varying ferromagnetic and ferroelectric phases in required ratio. The coating of these composites by biocompatible polymer (ethyl cellulose) is done by solgel process. The phase formation and surface morphology of individual phases is confirmed by X ray diffraction and scanning electron micrography study. Drug loading and unloading is confirmed by Fourier transformation infrared spectroscopy. The average crystallite size of NFO is found to be 32 nm and BTO as 26 nm. The nano size of these materials made them suitable for drug delivery application.

H 039

Incorporation of Cholesterol on Oleogel Containing Wheat Germ Oil & Rose Floral Wax and Studying Their Oral Delivery of Curcumin

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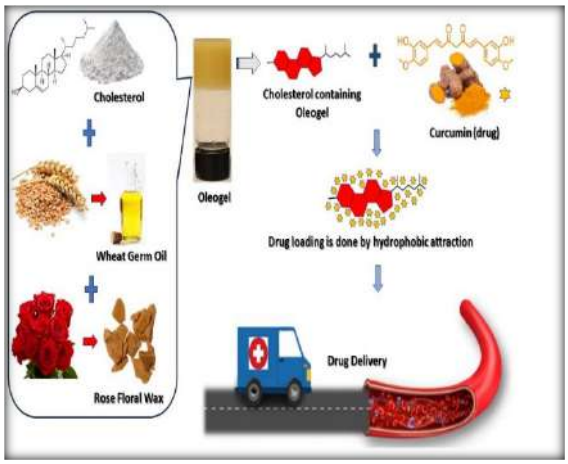
ABSTRACT

In recent times our regular diet contains lots of trans fat which exceeds the limit of regular intake. However, adding extra trans or saturated fat to a diet can lead to serious health issues like high blood pressure, lupus, and coronary artery disease.[1] Therefore replacement of trans fat is necessary without having the side effect. In this regard, the most used strategy is known as oleogelation in which liquid oil is converted into a gel-like structure named oleogel (OG).[2] And an additional solid component is used, which is known as an oleogelator.[3]

In current investigation, we use rose floral wax (RFW) as an oleogelator. It contains high levels of hydrocarbons, sterols, unsaturated fatty acids and their esters which makes it a carrier in drug delivery systems. Wheat germ oil (WGO) is used as liquid oil. Additionally, we incorporated cholesterol in the system. There is another type of cholesterol present, which is known as high-density lipoprotein or "good" cholesterol. It helps to reduce the risk of heart attack and stroke.[4] Curcumin used as a drug for our synthesized OGs and observed that the introduction of cholesterol increases the drug-delivering capacity which we studied by Korsmeyer–Peppas and Peppas–Sahlin models. The synthesized OGs were analysed for their physiochemical, thermal, structural, and rheological properties.



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H 040

Zn-Doped Anisotropic Iron Oxide Nanoparticles as a Hyperthermic Therapeutic Agent

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ABSTRACT

Superparamagnetic magnetite (Fe_3O_4) nanoparticles were successfully synthesized by reducing the stoichiometric ratio of aqueous solutions of Fe^{2+} and Fe^{3+} with NaOH solution via a simple co- precipitation method. The prepared nanoparticles were doped with Zinc ions by reducing aqueous solution of Zn^{2+} along with Fe^{2+} and Fe^{3+} in the presence of NaOH. X-ray Diffraction measurement confirmed the single phase and uniform size distribution formation of as prepared and doped Fe_3O_4, which shows the average crystallite size of 15 nm to 22 nm for increasing doping concentration (0% to 11% of Zn). Fourier Transform Infrared spectroscopy and Energy dispersive X-ray analysis evidence the presence of Fe, O, and Zn atoms in Zn-doped Fe_3O_4. High-resolution Scanning Electron Microscopy and High-resolution Transmission electron microscopy confirmed the spherical shape of the nanoparticles. The superparamagnetic nature and the saturation magnetization behaviour were analyzed using Vibrating sample magnetometry which shows high saturation magnetization of 59.6 emu/g for 11% of Zinc. The correlation among saturation magnetization (Ms), crystallite size (D), particle size (d), and microstrain (ε) was described. The heating efficiency of the Zn-doped Fe_3O_4 nanoparticles was probed using induction heating studies, and the effect of dopant concentration on the hyperthermic efficiency was analyzed. The antibacterial activity of the as-synthesized and Zn-doped Fe_3O_4 nanoparticles was confirmed by investigating the inhibition zones against Gram-negative Escherichia coli and Gram-positive bacteria Staphylococcus aureus. Hence, the zinc-doped Fe_3O_4 nanoparticles could be employed as therapeutic agents.

Keywords: *Fe_3O_4, Zinc ferrite, Antibacterial, Superparamagnetic, Hyperthermia*

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H 041

Metal-Based Hydroxyapatite Nanoparticles as Adjuvants for Cancer Immunotherapy

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ABSTRACT

Modern vaccines usually require accompanying adjuvants to increase the immune response to antigens. Hydroxyapatite (HAP) has been formulated as adjuvants in vaccines for human use as it is composed of calcium phosphate that work itself as adjuvant. Nevertheless, a comprehensive understanding of the ideal characteristics of HAP nanoparticles (HAP-NPs) for inducing adjuvanticity and the underlying mechanisms of immunopotentiation remains incomplete. A major challenge in the development of more effective cancer vaccines is in the development of strong adjuvants that can substantially, easily and safely enhance vaccine immunogenicity. The incorporation of metalloimmunology principles into cancer vaccine development has the potential to enhance their clinical efficacy. This is due to the significant involvement of essential nutritional metal ions, including iron (Fe2+/3+), zinc (Zn2+), and manganese (Mn2+) in several critical immunological processes. These metals can be effectively integrated into the compositions of nano- vaccines to serve as beneficial adjuvants, hence augmenting the immune response. Therefore, in this study, more detailed systematic exploration on structural influence of metal impregnated HAP and its behavior on physiological environment was studied. Rod-shaped HAP was impregnated with different percentages of metals. The physiochemical and structural properties of metal impregnated HAP were comprehensively investigated. Their immuno-stimulating potentials and possible mechanisms will be evaluated and its potential as immunoadjuvant will be accessed. The physiochemical and structural properties of metal impregnated HAP were comprehensively investigated. The influence of metal doping on protein adsorption and cytotoxicity effects will also be discussed.

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H 042

Detection of Diabetic Retinopathy from Fundus Images with Convolutional Neural Network

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ABSTRACT

Vision loss is a severe threat for those with diabetes, as this disease can trigger diabetic retinopathy (DR), damaging the eyes. A critical warning sign is the development of microaneurysms (MAs) in the retina. Detecting MAs early allows timely medical intervention to prevent blindness. This research presents a new automated three-step technique to spot MAs in retinal scans. First it preprocesses the images. Then it identifies potential MAs. Finally, a pioneering convolutional neural network architecture distinguishes actual MAs from other regions. This neural network outperforms previous methods, despite minimal pixel data, showcasing its potential to enhance DR screening. By pooling the judgments of this network across patches of the image, the locations of MAs are pinpointed. Tested on a key dataset, this approach achieved outstanding accuracy of 92% in detecting MAs. Overall, this automated technique shows promise to catch the first signs of DR through improved identification of MAs in retinal images. This can aid doctors in early intervention to thwart vision loss in diabetic patients. With further development, this approach could be integrated into routine eye exams, helping preserve sight for multitudes with diabetes worldwide.

Keywords: *Retina • Microaneurysm • Blood vessels • Optic disc • Deep learning • Convolutional neural network*

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H 043

Fish Collagen-Based Nanocomposite Polymeric Films: A Design Approach for Antibacterial and Hemostatic Activity in Tissue Regeneration

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ABSTRACT

A novel class of wound dressing material was developed, characterized, and tested for accelerated healing and healthy recovery of cells/tissues, derived from fish waste and modified with a polymer nanocomposite. The initiative aimed to contribute to waste management strategies by understanding waste generation volume and potential valorization. Highly pure collagen extraction from fish-based waste was achieved through a hybrid approach of enzymatic and chemical extraction techniques. The project's main novelty involved the development of novel Fish Collagen (FC) films modified with Mxene/ZrO_2-Cu polymer nanocomposite using an eco-friendly Gel casting technique. The as-developed patches underwent comprehensive characterization for their physio-chemical, mechanical, photo, and barrier properties. In vitro studies were conducted on the patches to heal human fibroblast cell lines, providing insights into performance and biocompatibility. Additionally, the realistic capacity of the wound dressing, including durability and antibacterial ability, was investigated in vivo using mice as a model for wound healing.

Keywords: *Fish collagen, Nanocomposite, Polymeric film and Skin regeneration.*

H 044

Formulation and Evaluation of Polyherbal Chewable Tablets for Soar Throat Infection Treatment

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ABSTRACT

The study was designed as formulation, standardization, and evaluation of polyherbal tablets prepared for the management of antioxidants. To overcome the problem of patients by the use of polyherbal tablets and powder formulations. Powder and tablets were prepared using aqueous root extract powder of the selected plant viz. Hibiscus rosa sinesis, and sorghum bicolor with the help of super disintegrant addition technique using crospovidone, sodium starch glycolate, and croscarmellose sodium in different percentages. Evaluation assessments such as the substantial test, weight variation, hardness, friability, content uniformity, disintegration, in vitro dispersion, stability study were carried out. Micromeritics of extracts powder were determined for all formulations, which signified good flow properties. A substantial examination was established, which comply with official requirements for uniformity test, and the drug content was close to 90% in all formulations. Disintegration time was observed for all formulations in which the polyherbal formulation-5 (F-5) showed 2.000±0.20 min; during in vitro dispersion time, all formulations showed appropriate dispersion in which the F-5 captivating 2.00±0.45 min only. The F-5 showed satisfactory disintegration and in vitro dispersion time due to crospovidone and was reported as the best formulation. It was achieved that the selected herbal plant have been developed into suitable composition which was tailored into unit single solid oral dosage form which pride patient- friendly usage for immediate relief form sore throat, cough and cold.

KEYWORDS: *Natural materials, polyherbal Tablets, Herbal medicine*

H 045

Efficient And Facile Synthesis of Pyrazole-Imidazole Hybrid Compounds

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ABSTRACT

In the era of black fungus like microbes based diseases, a huge demand of antimicrobial drugs has been raised. Pyrazole-imidazole hybrids are entrancing compounds on behalf of their effective antimicrobial properties. A new series of pyrazole-imidazole clubbed with heteroaryl have been synthesised efficiently in three steps involving click reaction and Debus-Radziszewski reaction. First step involves the synthesis of *N*-propargylated pyrazole carbaldehyde by nucleophilic substitution reaction. In second step, hybrid of heteroaryl pyrazole carbaldehyde were synthesised by click reaction, in this step pyrazole -1,2,3-triazoles hybrids formed. Finally, Pyrazole-imidazole heteroaryl was prepared using the well-known reaction called Radziszewski reaction. In this reaction, heteroaryl pyrazole carbaldehyde react with 1,2-diketones in presence of ammonium acetate in glacial acetic acid by condensation reaction and results into pyrazole-imidazole-triazole hybrid. Nuclear Magnetic Resonance (NMR), High Resolution Mass Spectrometry (HR-MS) and Fourier Transform Infrared Spectroscopy (FTIR) have been used confirm the structure of these newly synthesized. Results of these spectroscopic data are in full agreement with the proposed structure of pyrazole-imidazole compounds. Details of the current study will be presented in the conference.

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H 046

Improved Nonlinear Absorption Behaviour of Graphene Hybrid Interfaces for Neuro-regeneration

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ABSTRACT

Stimulated by the versatility, engineering advanced photonic materials made of graphene systems at various dynamic range for nonlinear absorption driven applications has a separate resurgence of interest. Graphene hybrids promotes greater advantage of tailoring and fine tuning NLO response, by rational modification of the chemical structure and through functionalization of appropriate materials. α-MnO_2 surface functionalized reduced graphene oxide nanocomposite with varying concentration of layered rGO was prepared by reduction method. XRD and Raman spectra confirms the formation of tetragonal phase α-MnO_2 and reduced graphene oxide. FESEM and HRTEM display the gradual transformation of surface morphology of α-MnO_2 from nanoclusters to nanorods then to nanowires upon the rGO sheets. Linear optical studies show absorption peaks at 266 nm (π-π* transition of the C-C aromatic bonds of graphene) and 270 nm (d-d transitions of MnO_2). Open aperture Z-scan technique using Nd: YAG laser (532 nm, 10 Hz & 9 ns) revealed an interesting switch over in the nonlinear absorption from saturable absorption (SA) to weak reverse saturable absorption (RSA) with surface functionalization. And MnO_2: rGO (20 wt %) displayed a stronger reverse saturable absorption ascribed to sequential two photon absorption. Influence of surface morphology on the optical nonlinearity and systematic transition from SA to RSA behaviour occurs mainly of rGO sheets and the MnO_2: rGO (20 wt %) involves superior nonlinear absorption and limiting response symbolizing potential use of the system in neuro-regeneration and laser safety device applications.

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H 047

Silver Incorporated Reduced Graphene Oxide-Molybdenum Disulfide (Ag-rGO-MoS_2)Hybrid Material for Bio-photonic Application

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ABSTRACT

Cancer is one of the pernicious diseases in the human life due to its high death rate and incurability. Thoughthere are several advances in treatment modalities, several factors like rapid metabolism, non-specific cytotoxicity and multi-drug resistance limits its effectiveness in therapy. In this regard, architecting novel advanced hybrid materials are the ultimatum entail for multifunctional traits and enhanced responses to thedesired inputs. The advent of exceptionally interesting class of 2D materials like graphene and graphene like materials has triggered a wide range of applications including bio-photonics owing to their unique properties. Further, the incorporation of metals to these organic-inorganic complex system enhances the effectiveness of anti-cancer activity due to their improved biocompatibility, pharmacokinetics and excellenttarget specificity. Thus, the present work is on preparation of multifunctional metal incorporated organic- inorganic hybrid nanocomposite (Ag-rGO-MoS2) suitable for laser based targeted cancer therapy. The limiting action of the Ag-rGO-MoS2 hybrid under 532 nm nanosecond green laser excitation was studied using Z-scan technique. MTT assay was carried out to study the antiproliferative action on MCF cancer cell line. The cytotoxicity studies revealed that the percentage of live cells decreased in the presence of hybridshowcasing higher percentage of inhibition. The morphological evidence for apoptosis and the detection ofnuclei alterations activated by the prepared hybrid were analyzed using AO/EB staining and Hoechst staining respectively. Earlier XPS, SEM and UV-Visible analysis were performed to illustrate elemental, morphological and ground state absorption studies. Thus, pleiotropic actions of Ag-rGO-MoS2 hybrid weredemonstrated for the possible use in laser bio-photonics applications.

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H 048

Optimization and Aalidation Process of Propranolol Hydrochloride Tablets

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ABSTRACT

To optimize and validate the process of propranolol hydrochloride tablets. Rationale behind the study: The formulation maintains the chemical and physical stability of propranolol hydrochloride tablets by optimizing the excipient concentration and their grades, ensuring uniformity, consistent manufacturing process validation, and ensuring safe patient formulation. Hypothesis: The study reveals that optimizing the excipient grades of propranolol hydrochloride tablets can overcome segregating conditions during compression, thereby enhancing product uniformity. The literature review suggests that particle size narrowing can reduce segregation, standard microcrystalline cellulose PH-101 with superseding microcrystalline cellulose PH-102, PH-105, and PH-200. Three successful formulations were formulated, with F1 reducing segregation and enhancing content uniformity, F2 increasing hardness and reducing friability, and F3 improving porosity and reducing weight variations. The enhancement of content uniformity, archived via F1 formulation, promotes better flowability and reduces segregation. The deviation caused by MCC was rectified by optimizing various excipient standards.

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H 049

Quantum Chemical Computations, Drug Likeness and ADMET Analysis on Antibacterial Compound Cadmium Chloride Adipic Acid

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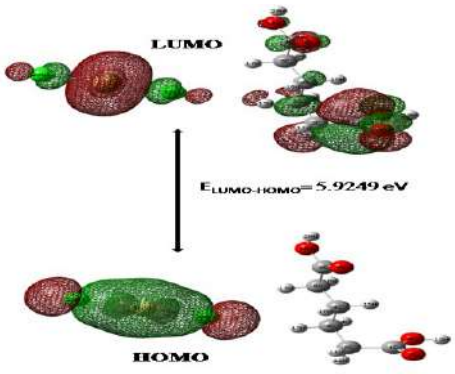
ABSTRACT

Density Functional Theory (DFT) quantum chemical computations of the antibacterial compound Cadmium Chloride Adipic Acid (CCAA) carried out at the B3PW91 level with LANL2DZ as the basis set. The chemical reactivity and charge transfer is elucidated by Frontier Molecular Orbital energy gap and the reactive sites were identified from the electrostatic potential map. The pharmacokinetic characteristics of the compound were investigated utilizing the Lipinski rule and Absorption, Distribution, Metabolism, Excretion, Toxicity properties and it shows that CCAA can be used as a drug because it is non mutagenic and does not impair the liver.



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H 050

Isomerization of Gamma-oryzanol in the mixed Langmuir monolayers

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ABSTRACT

Gamma oryzanol is extracted from rice bran oil and has potential applications in cosmetics industry with products like sunscreen products due to its photo-sensitive behavior. This makes it necessary to study the photo-chemical properties of gamma-oryzanol molecule in the presence of other biological lipids. In this work we have studied the quasi-2D phases exhibited by the mixtures of DPPC and gamma-oryzanol at the air-water interface and the isomerization of it in the mixed monolayer. The quasi-2D phases exhibited by the molecule are studied by surface manometry technique using Langmuir trough. The rate of photo isomerization and thermal isomerization was studied by shinning UV light of frequency 360 nm and in dark, respectively. The change in the surface pressure as function of time was measured. The data was fit to the equation given by raghavendra et.al . Using fit parameters the rate constants of photo isomerization and thermal isomerization are calculated. The rate constant corresponding to the isomerization is obtained for different mole-fractions of DPPC.

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H 051

Deep Convolutional Network for Cancer Type Identification

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ABSTRACT

Cancer is one of the present common causes for death in the world. The early recognition of the cancer and developing the new treatment techniques has been essential. The purpose of this project is to identify the type of cancer and provide information for the growing new techniques in treatment. The earlier we identify the easier the treatment could be. The trending and most reliable technique to follow in this identification is usage of Convolution neural network (CNN). Datasets of the required digital images are to be provided in this proposal model which helps in identifying the linear and nonlinear information from the input data. The required methodology also follows the mathematical and probabilistic formulae. In this model, training is provided at the beginning and followed by testing because any failure may lead to poor performance. The adaptive techniques help in improving the performance. Experimental result which is expected to show that our project can achieve required identification accuracy in an early stage.

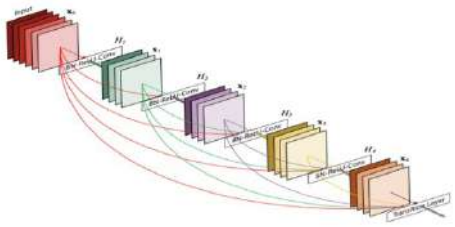

Fig (1): Dens net

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H 052

In Vitro and in Silico Approach Towards Biocidal Behaviour of Water-Soluble ChitosanDialdehyde Biopolymers

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ABSTRACT

Chitosan dialdehyde (ChDA) was prepared from a three-step process initiated by thermal organic acid hydrolysis, periodate oxidization, and precipitation from native chitosan (NCh). The developed ChDA resulted in an aldehydic content of about 82% with increased solubility (89%) and maximum yield (97%).The aldehydic (-CHO) group functional alteration in ChDA was established using vibrational stretching at1744 cm^{-1}. The increase in the zone of inhibition of ChDA than NCh has confirmed the inherentantimicrobial effect against bacterial and fungal species. The novel insilico predictions of the ChDA's biocidal activity were confirmed through molecular docking studies. The amino acid moiety such as ARG110 (A), ASN 206 (A), SER 208 (A), THR 117 (B), ASN 118 (B), and LYS 198 (B) residues of 7B53 peptide from E. coli represents the binding pockets responsible for interaction with aldehyde group of ChDA. Whereas, PHE 115 (E), ALA 127 (H), TYR 119 (C), GLN 125 (H), ASN 175 (E), ARG 116 (E), LYS 101 (H), and LYS 129 (H) of 1IYL A peptide from Candida albicans makes possible for binding with ChDA. Hence, the synergistic effect of ChDA, as a biocidal compound finds a plausible use in the drug delivery system for therapeutic applications.

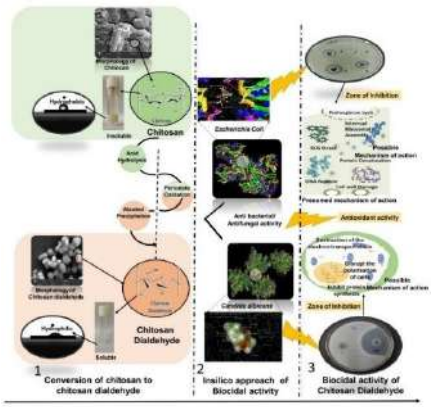

Figure 1: Graphical abstract

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H 053

Potential of particle size controlled (x)$CoFe_2O_4$ + (1-x) $BaTiO_3$ magnetoelectric nanocomposites in biomedical applications

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ABSTRACT

The role of pH variation and sintering temperature on $CoFe_2O_4$ (CFO) + $BaTiO_3$ (BTO) magnetoelectric nanocomposites and their potential use in biomedical applications is studied. Individual phases, such as CFO nanoparticles were synthesized by hydrothermal method whereas BTO nanoparticles by reflux method. The pH of the precursor is varied using ammonia during the synthesis. The final product obtained is sintered at different temperatures. The physicochemical properties of these materials were investigated by using different techniques such as X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX), and Fourier Transform Infrared Spectroscopy (FTIR). The composite of these phases (x) $CoFe_2O_4$ + (1-x) $BaTiO_3$ (x = 0.15, 0.30 and 0.45) were prepared by standard double sintering ceramic method. It is observed that as pH and sintering temperature increases the crystalline size also increases. SEM images revealed a granular surface shape, indicating the unique microstructure of the composite. The successful drug loading onto composites was clearly observed in FTIR analysis. Furthermore, the study investigates drug loading capabilities and drug release kinetics, offering information on potential for controlled and sustained drug delivery applications.

H 054

Evaluation of Titanium Dioxide-Incorporated Chitosan Nanoparticles for Synergistic Antimicrobial Activity

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ABSTRACT

The modern-day cosmetic products, with rich formulations of components, have become an ideal breeding ground for microorganisms. Titanium dioxide nanoparticles can decompose the outer membrane of microbial cells by producing free radicals such as hydroxyl and superoxide anion radicals. Chitosan and its derivatives have shown antimicrobial activities and are effective against gram-positive-, gram-negative bacteria and fungi. Chitosan-coated titanium dioxide (CS-TiO_2) nanoparticles were fabricated to analyse its antimicrobial efficacy against three bacteria and a fungal species *viz*. *E. coli, S. aureus, P. aeruginosa* and *A. niger* respectively. MIC_{50} and MBC will be used to identify the lowest concentration of CS-TiO_2 required to inhibit/kill the organism. Colony count analysis will be performed to evaluate the reduction in the number of colonies upon treatment with CS-TiO_2. Growth curve analysis to study if there are any alterations in the growth kinetics of the organism. Further, biochemical analyses, such as estimation of reactive oxygen species and lipid peroxidation will be performed to determine if oxidative stress contributes to the antimicrobial action of CS-TiO_2. Additionally, TEM imaging will be performed to obtain a microimage of the bacterial cell lysis.

Keywords: *Antimicrobial activity, Nanoparticles, Titanium dioxide, Medium molecular weight chitosan, Bacteria, Fungi*

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H 055

Evaluation of chitosan-coated titanium dioxide nanoparticle-induced toxicity using *Drosophila* as a model organism

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ABSTRACT

Nanoparticles, with an umbrella of applications, are widely used in the field of cosmetics as ingredients in products such as body creams, anti-ageing formulas, bath oils, anti-wrinkle creams etc. Titanium dioxide nanoparticles (TiO_2 NP) are used widely as a component in cosmetics, sunscreen, food and drug colourants etc. Chitosan is an ideal biomaterial due to its natural origin, availability, non-toxic nature, biocompatibility and biodegradability and is extensively used in cosmetics due to its intangible qualities. The toxicity of TiO_2 NP is debatable, and reports from previous literature state that TiO_2 toxicity can be modified by coating with a suitable material. Therefore, the present study aims to evaluate the toxicity of chitosan-coated TiO_2 composite using *Drosophila* as a model. Titanium dioxide nanoparticles were synthesised using titanium tetraisopropoxide as a precursor and fabricated using medium molecular weight chitosan as a coating material. The coated nanoparticles were characterised using XRD, FTIR, and UV-vis spectrometry. The toxicity of the coated nanoparticles will be assessed using *Drosophila melanogaster*. Behaviour and biochemical changes will be performed on both larvae and adult flies to evaluate the effect of the nanoparticle on the model organism.

Keywords: *Titanium dioxide nanoparticle, Chitosan, Drosophila melanogaster, Nanotoxicity Skin ageing*

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H 056

Remineralization of Enamel using Eggshell Derived Hydroxyapatite Nanoparticles with and without Carboxymethyl Chitosan- An *In Vitro* Study

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ABSTRACT

Enamel matrix proteins, particularly amelogenin play a major role in enamel biomineralization by controlling the hydroxyapatite crystal growth and orientation.[1] Recent research is focused on the development of therapeutic agents containing non-collagenous protein (NCP) analogs for rapid and effective enamel remineralization.[2] Carboxymethyl chitosan (CMC), a derivative product of chitosan with improved biological properties, is a widely studied NCP analog due to the abundance of both amino and carboxyl groups.[3] The objective of this preliminary *in vitro* study was to assess the synergistic effect of eggshell-derived hydroxyapatite nanoparticles (EnHA) and CMC on artificially induced enamel caries-lesions. CMC was commercially procured, while EnHA was synthesized using a microwave-irradiation method and subjected to characterization studies. 24 pre-demineralized coronal enamel specimens were randomly treated with the following test agents (n=6 each): artificial saliva (AS), EnHA, CMC, and EnHA-CMC, followed by pH cycling for 7 days. The surface morphology and elemental analysis was analyzed using HRSEM-EDX post remineralization. FT-IR and XRD results revealed that the prepared EnHA powder depicted the characteristic presence of phosphate and hydroxyl groups with high crystallinity. HRSEM and TEM analysis illustrated an irregular rod-like HA morphology with a particle size of 30–90 nm. After 7 days treatment, a layer of ordered crystals completely covered the surface of the demineralized enamel in EnHA-CMC group while other test groups revealed partial deposits. However, EnHA and CMC groups demonstrated increased apatite formation than AS treated specimens. The intensity of mineral peaks in the EDX spectra also supported these observations. Hence, within the limitations of this *in vitro* study, EnHA-CMC resulted in rapid and effective remineralization effect on artificial enamel-lesions.

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H 057

Anti-Bacterial Efficacy of Yttrium doped- Cerium oxide Electrospun Nanofibres against gram-positive and gram-negative bacterial strains

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ABSTRACT

Electrospinning can be used to create polymer fibres that possess antimicrobial properties. These fibers have distinct characteristics such as a large porosity, a high surface area-to-volume ratio, and a high length-to-diameter ratio. This chapter presents a comprehensive introduction to polymer nanofibers that possess antimicrobial properties. Microbial infections pose a significant risk to public health and are a prominent contributor to global mortality. The emergence of novel strains of pathogens, including drug-resistant types of viruses, bacteria, pathogenic fungi, and protozoa, is a matter of great concern. Traditional antimicrobial medicines have not demonstrated therapeutic effectiveness against multidrug-resistant variants of these diseases. This study presents the predominant applications of nanofibers in the field of antimicrobial medication delivery for the treatment of wound infections. The paper examines recent studies on microbial infections, microbial resistance, and the underlying mechanisms of antimicrobial treatment resistance. In this study, we have shown that metal nano-composites nanofibres made of the rare earth elements such as cerium and yttrium exhibited an excellent anti-bacterial activity against *Staphylococcus aureus, Enterococcus faecalis, Escherichia coli and Pseudomonas aeruginosa*.

Keywords: *Anti-bacterial activity, Cerium oxide, Nanofibers, Polymer, yttrium.*

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H 058

Towards Biocompatible Optical Imaging Agents: DNA-CTMA Enabled Metal-Enhanced Fluorescence

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ABSTRACT

Metal nanoparticles (NPs) with unique plasmonic properties offer a promising avenue for enhancing dye fluorescence through a phenomenon known as metal-enhanced fluorescence (MEF). In this study, we demonstrate that an intramolecular donor-acceptor system 2-(4-(dimethylamino) styryl)-1-methylpyridinium iodide (DASPMI), which is known to specifically stain mitochondria in living cells, can exhibit plasmon-coupling enhanced fluorescence. Gold nanoparticles (AuNPs) were synthesized in DMSO and ethanol by laser ablation. The fluorescent probe was DASPMI, and the nanostructures to immobilize the dye in the gap region of linked metal NPs were assembled using DNA-CTMA. Thin films of the complexes, with different enhancing substrates: dye only, dye @ Au, dye @ DNA-CTMA, dye@ Au @DNA-CTMA were fabricated by spin coating. The formation and optical properties of the fabricated nanohybrid system were analyzed using UV–Visible absorption spectroscopy, ellipsometer, fluorescence emission spectroscopy and fluorescence life time studies. The third order nonlinear optical behavior of the dye samples were investigated using open aperture Z-scan method. The nanohybrid of DASPMI dye modified by Au/DNA-CTMA display larger fluorescence enhancement effects compared to the other systems. Results show that this plasmon coupled fluorescence platform can be utilized for DNA visualization, highly sensitive sensing and imaging applications.

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H 059

Investigation of Anti-Bacterial Efficiency of Yttrium Doped Cerium oxide Nano-composites

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ABSTRACT

In the present circumstances, medical physicians use antibiotics to treat bacterial illnesses. However, relying solely on this class of treatments is unfavorable due to the emergence of antibiotic-resistant bacteria that have developed the ability to withstand their effects. Researchers are looking for alternatives to antibiotics. In this study, we have shown that metal nano-composites made of the rare earth elements such as cerium and yttrium exhibited an excellent anti-bacterial activity against *Staphylococcus aureus, Enterococcus faecalis, Escherichia coli and Pseudomonas aeruginosa*. The synthesis of yttrium-doped cerium nano-composite was achieved via co-precipitation method using hexamethylenetetramine (HMT). The physiochemical characterizations helped to determine the inherent characteristics of the composites including their size, shape, and composition. This information was crucial in understanding the chemical reactions and growth mechanisms involved. The most effective ceria nanoparticles for inhibiting the growth of *Staphylococcus aureus* without causing significant harm to human dermal fibroblast cells. This was determined through zone of inhibition (ZOI), colony counting and growth curve. The biocompatibility and antibacterial properties of yttrium-doped cerium oxide produced in different molar ratio. Hence, the present work validates that the use of nano-alternatives to antibiotics are not only possible, but also highly versatile and easily manufacturable. The clinical applications of rare earth metal nanoparticles are diverse, with ceria and yttria nanoparticles being recognized in the literature for their roles as potent antioxidants, regulators of tissue regeneration, and anti-cancer agents.

Keywords: *Anti-bacterial activity, Co-precipitation method, Cerium oxide, Nanocomposites, yttrium.*

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H 060

Synthesis, Characterization and Effect of Nano-Polydopamine on Enamel Remineralization

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ABSTRACT

Application of mussel adhesion phenomenon in nature derived by dopamine has been extensively used for biomaterial surface modification. Polydopamine(PDA) is the synthetic mimic of the specialized adhesive foot protein, Mefp-5(Mytilus edulis foot protein-5) in an oxidized form. PDA can induce the mineralization of tooth by binding to calcium ions and accumulating them at the interface thereby accelerating the formation of hydroxyapatite. Current research reports show extensive applications of PDA nanoparticles(nPD) in drug delivery and functional modification of biomaterial surface. nPD provide larger specific surface area to interact with more cells and bio-functional molecules with enhanced bioactivity. However, nPD application in dental field are not attempted yet. Hence this study aims to synthesize and characterize nPD using SEM-EDX and FTIR followed by evaluation of its tooth remineralization potential.. Enamel discs(10x8x2 mm) were obtained from extracted human mandibular teeth and baseline hardness values were recorded using Vickers microhardness(VMH) testing machine and SEM-EDX analysis was done for surface and elemental analysis. All the specimens were randomly divided into four groups(n=20); Group I-Positive Control(immersed in remineralization solution); Group II-PDA; Group III-nPD; Group IV-No treatment. Following this, respective experimental agents were applied on the enamel slabs and subjected to pH cycling regimen till 14 consecutive days followed by VMH evaluation, SEM-EDX, FTIR and XRD analysis at 7 and 14thday. The results were tabulated and statistically analyzed using One-way ANOVA and Multiple comparison Post-hoc Tukey's test. nPD showed higher remineralization potential on both mechanical and chemical analysis, Thus, nPD can serve as a novel remineralization inducing agent for dental applications.

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H 061

Simulation- A Novel Educational Approach in Nursing

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ABSTRACT

Simulation-based education is an educational or training method that is used to "replace or amplify real experience with guided experiences". It is not defined by technology but rather an educational approach grounded in learning theories. Simulation is meant to replicate aspects of the real world in an interactive manner that allows learners to be immersed in the learning environment. Simulation-based experiences (SBEs) occur in a simulation laboratory setting in which the UG students come for a defined period of time and engage in activities specifically designed around a set of learning objectives. These activities are developed into simulation scenarios. The scenario contains the learning objective, the patient information (e.g., background, current condition, medications, and other relevant information), actor scripts as needed, information for the high-fidelity simulator, a timeline for the unfolding of the scenario, cues needed by the facilitator to help the action flow along, and other essential information to ensure that the simulation-based learning education experience is successful. Simulation-based education is a learner-centered approach, grounded in learning theories based on constructivism. As such, learners create their reality and truth. To support this type of learning, activities include discussion, self-reflection, and questioning so that learners can engage actively in the learning process. Simulation has become a significant part of the UG curriculum. It is a theory-based, effective teaching method with a growing body of research evidence support. Simulation can be incorporated into the curriculum as a way to support student achievement of knowledge, skills, and attitudes (KSA) and competencies needed to attain the overall program goals set forth by the school curricular plan.

Keywords: *Simulation, Undergraduate nursing students, simulator, educational approach, scenarios, learning mannequins, virtual reality.*

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H 062

Advancements in Encapsulation Techniques for DHA (Docosahexaenoic acid) in Food Fortification: A Comprehensive Review

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ABSTRACT

Docosahexaenoic acid (DHA) is a carboxylic acid with a twenty two carbon chain with the first double bond located at the third carbon from the omega end. It is a long chain poly unsaturated (omega 3) fatty acid acid that contributes to the structural integrity of retina, skin and cerebral cortex. DHA's use in food fortification is constrained by its fishy smell, oxidative stability and low bioavailability. The key to extending its use in food and pharmaceutical applications is having a solid understanding of the variables affecting oxidative stability and the mechanisms that promote stability. The current review discusses various studies that has been conducted in the recent years that concentrates on the micro and nano encapsulation techniques such as nanoemulsion, nanoliposomes, emulsion gels, complex coacervation, solid lipid nanoparticles, electrospinning, electrospraying etc, using sodium alginate, zein, maltodextrin, soy bean lecithin, whey protein isolate and tween 80 as emulsifiers/ wall materials. Additionally, the impact of encapsulation on the physicochemical properties, oxidative stability and release kinetics of DHA in different food matrices is discussed. The enhanced stability of DHA opens doors for its incorporation into a wide range of fortified food products including infant formula, functional beverages, dairy products and baked goods thereby providing consumers with an accessible means to increase their DHA intake and improve overall health. This review also addresses the stability challenges of DHA and its potential to revolutionize the food fortification industry.

Keywords: *DHA, oxidative stability, bioavailability, fortification, encapsulation*

H 063

Optimization of the Extraction of Sulphated Polysaccharides from *Sargassum Polycystum* by using Response Surface Methodology BBD Experimental Design

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ABSTRACT

This study aims to optimize an alternative method of extraction of sulphated polysaccharides by using Response Surface Methodology Box–Behnken design (RSM). In order to explore an innovation in the isolation process, atomization drying was used reducing the time duration to obtain polysaccharide yield. The optimization study was carried out for the extraction of polysaccharides from *sargassum polycystum by* using RSM employing a BBD (four factors and three levels). Box-Behnken experimental design (BBD) with four factors and three levels was chosen to evaluate and optimize the influence of selected variables (extraction temperature (60, 70 and 80 ºC), pH (3, 5 and 7) and buffer to algae ratio (1:40, 1:50 and 1:60 g/dl), respectively on the extracted yield of polysaccharide properties were evaluated. Further, the extracted yield was examined to structural analysis, by fourier-transform infrared spectroscopy and nuclear magnetic resonance spectroscopy (1H-NMR). Results showed that the developed regression models adequately explained the data variation. Optimal extraction conditions were 70ºC, time duration 60 minutes, pH 5 and 1:40 g/dl. In these conditions, the yield polysaccharides extract properties determined by the polynomial model were 52.16±1.15%. The experimental were 50.73±2.17%. The nuclear magnetic resonance spectroscopy and infrared spectroscopy analyses showed that the crude polysaccharides extracted is composed mainly of sulphated polysaccharides.

Keywords: *Optimization, Response Surface Methodology, Box-Behnken Design, seaweed, polysaccharide.*

H 064

Banana Fiber-Chitosan-Guar Gum as a Composite for Wound Healing

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ABSTRACT

It is crucial to give proper attention to wounds, ranging from minor cuts to primary incisions, with a key aspect being the appropriate dressing of the wound. Currently, there are various materials for wound dressing under investigation. Recent research has seen a shift from synthetic fiber-based polymeric composites to natural fiber-based composites due to sustainability and environmental considerations. In India, banana fiber, considered waste biomass after harvesting by farmers, is abundant, making India one of the world's largest banana-farming countries. In our study, we utilized the herbal drug Vitex negundo Linn. (Verbenaceae) in banana fiber composites. The aqueous and ethanolic extracts of the leaves were employed for wound healing activities. Banana fibers, along with chitosan and guar gum as biopolymers, were used to create a patch with enhanced wound healing capabilities, incorporating Nirgundi as an herbal component. The purification of banana fibers involved a chemical treatment to form a film, and subsequent characterization revealed various properties. These purified fibers were then added as fillers to the biopolymers, creating bio-composites through solvent casting. Comprehensive characterization followed, including in-vitro drug release, anti-bacterial, and cell culture studies to assess the biocompatibility of the developed patches. The resulting composite patch holds promise for novel applications in biomedical fields, particularly in soft tissue engineering, offering potential benefits for wound healing and drug delivery.

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H 065

Bioactive behavior of TiO_2-modified 1393-B3 Borate Glasses

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ABSTRACT

Borate-based bioglass 1393-B3 (56% B_2O_3, 18.50% CaO, 11.10% K_2O, 5.50% Na_2O, 4.60% MgO, 3.70% P_2O_5) has received much attention recently due to its high bioactivity and fast biodegradability. Effect of selected cations substitution into the glass network has been studied as it renders beneficial properties to the glass. For instance, Ag^{+}, Zn^{+2}, Cu^{+2} and Ti^{+4} ions have resulted in antibacterial properties, and Sr-doped glasses are suggested for healing osteoporotic bone disease. Titanium and its compounds have shown best results in clinical fields due to its high biocompatibility, self-healing ability and superior osseointegration. Therefore, effect of TiO_2 (1,3,5,8, and 10 mol%) on the 1393-B3 bioglass are studied in this work. TiO_2-1393-B3 glass frits are prepared by melt-quenching process and their physical properties are studied using theoretical relations. In-vitro bioactivity of $TiO_2$1393-B3 glass compositions are tested in the simulated body fluids (SBF). Formation of hydroxyapatite (HA) phase over the glass surfaces is confirmed in X-ray diffraction and scanning electron microscopy studies. Pristine HA phase is also synthesized through precipitation process from the saturated SBF solutions for the comparative purposes. Our study indicates that bioactivity of the 1393-B3 glasses is enhanced upon the incorporation of Ti. Moreover, the surface reactivity and formation of HA layer on the surface of different materials (metal, glass, and polymer) is tested in order to understand the bioactivity behavior, whether it is simply a heterogeneous nucleation and growth over the foreign substrate or unique to the glass samples. We have confirmed that HA nucleation and its bond over the glass is unique to the glass samples. The bioactivity mechanism and physical properties are discussed and correlated.

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H 066

Development of Bombyx mori Silk Sericin-AgNPs Nanocomposite Characterizations and Dye Degradation Study

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ABSTRACT

This work focuses on developing a composite material that is both environmentally friendly and biocompatible. The *Bombyx mori* mulberry silk sericin protein (SSP) was used as a reducing and stabilizing agent for the synthesis of sericin protein-silver nano-composition (SSP-AgNPs) under UV-B environment. The synthesis takes advantage of redox reactions under UV environment to generate the composite. Surface plasmon resonance (SPR) from UV-Visible spectroscopic (UV-Vis) analysis confirms the formation of silver nanoparticles (AgNPs). The functional groups attached to the macromolecules, surface morphology, nanoparticle shape, crystalline nature, structural analysis, and luminousness properties were investigated using the techniques like Fourier transform infrared (FTIR), field emission scanning electron microscope (FESEM), X-ray diffraction technique (XRD) and photo-luminousness (PL) spectroscopy respectively. This work focuses on the adsorption of aquatic contaminants such as methylene blue dye (MB-dye) and uses biodegradable material in the context of environmental issues. Additionally, MB-dye photo-catalytic degradation employing biocompatible material and metal nanoparticles is investigated. In order to demonstrate the SSP-AgNPs' potential as a long-term remedy for pollutant removal or degradation, this paper focuses on their synthesis, characterisation, and environmental application.

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H 067

Electrospun Poly-ε-caprolactone/Gelatin Nanofibrous Mats Impregnated with Carrot Seed Oil – A Comprehensive Study on Characterization and Antibacterial Potential

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ABSTRACT

Burn Wounds are vulnerable to microbial invasion by both internal and external germs, which poses a serious risk to public health and results in significant financial hardship. There is a perceived need for the development of novel antimicrobial wound dressings that prevent bacterial colonization speed up the healing process, and ultimately enhance patient care. Historically, burn injuries have been treated extensively with herbal extracts, derived from medically significant plants. The goal of the current study is to synthesize, characterize, and study the antibacterial potential of carrot seed oil loaded nanofibers. Carotenoids, flavonoids, polyacetylenes, vitamins and minerals were the vital phytocompounds present in carrot seed oil determined by using Gas chromatography mass spectrometry. The synthesized nanofibers were characterized using scanning electron microscope, transmission electron microscope, fourier-transform infrared spectroscopy, UV-vis spectroscopy, and contact angle. MTT assay showed the carrot seed oil mats were biocompatible. Disk diffusion assay revealed the mats exhibited potent antibacterial activity against the tested pathogens. Overall, the developed nanofibers possessed the prerequisite properties to be an effective antibacterial wound dressing.

Keywords: *Electrospinning; Polycaprolactone; Gelatin; Carrot seed oil; Antibacterial wound dressing*

H 068

Biocompatible Nanofibrous Wound Dressings with Vetiver Components: Fabrication, Characterization, and In Vitro Evaluation

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ABSTRACT

Millions of individuals worldwide suffer from severe skin damage as a result of burns, infections, accidents, traumas, diabetic foot ulcers and other incidents and the cost of wound care is becoming a major economic issue. Novel antimicrobial wound dressing that prevents bacterial colonization and speed up the healing process are thought to be in high demand, as they would raise patient standards of care. In order to prevent the bacterial colonization at wound site, poly-ε-caprolactone/gelatin hybrid composite mats infused with natural herbal extract (Vetiver) was developed using electrospinning technique. Gas Chromatography Mass Spectrometry analysis was employed to determine the bioactive chemicals present in vetiver root extract. The nanofiber morphology and size were determined using scanning electron microscope and transmission electron microscope. Contact angle measurement was performed to determine the wettability of the synthesized nanofibers. The synthesized mats were non toxic and promotes the cell growth as tested against the 3T3 L1 fibroblast cells. In addition, the vetiver imbued mats showed potent antibacterial activity. Based on the findings, the vetiver impregnated PCL/gelatin nanofibrous mats can be a potent antibacterial wound dressing.

Keywords: *Nanofibers; Vetiver; Biocompatible; Antibacterial; Composite materials*

H 069

Chitosan Treatment Attenuates Acrylamide-induced Toxicity in the *Drosophila* Model

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ABSTRACT

Acrylamide (ACR) induced toxicity remains a significant concern globally, yet public awareness of its formation during common cooking practices is lacking. This study investigates the therapeutic potential of chitosan derivatives, known for their diverse beneficial properties, in alleviating ACR-induced toxicity. Specifically, the effects of chitosan derivatives on ACR-induced behavioral and redox parameters were evaluated in a *Drosophila* model. Results revealed promising outcomes, with significant improvements observed in locomotor functions and developmental indicators in flies treated with chitosan derivatives following ACR exposure. Additionally, analysis of redox parameters indicated a favorable modulation of oxidative stress, suggesting the antioxidant properties of chitosan derivatives. These findings emphasize the potential of chitosan derivatives as effective interventions against ACR toxicity, highlighting their importance in mitigating the adverse effects of environmental toxins on biological systems.

Keywords: *Acrylamide, Chitosan, Drosophila melanogaster, Toxicity*

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H 070

A Comparative Study on *Centella Asiatica* Mediated Green Synthesis of Silver and Copper Oxide Nanoparticles: Synthesis, Characterization, Antioxidant and Antibacterial Properties

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ABSTRACT

Centella asiatica, or Indian pennywort or gotu kola, is a petite perennial herbaceous plant belonging to the Apiaceae family. Triterpenoids, particularly asiaticoside and asiatic acid, are responsible for its medicinal qualities. These compounds have a wide range of uses in medicine, including for the prevention of ulcers, lupus, eczema, and other skin conditions. In the present study, Centella asiatica leaf extract has been conjugated with silver nanoparticles and copper oxide nanoparticles in order to enhance efficacy and bio-absorption. This comparative study proposes the tenacious vitality of a cost-effective, renewable silver nanoparticle (AgNPs) and copper oxide nanoparticle (CuO-NPs) biosynthesis for advantageous utilization. Green synthesis opens the door to a strategy that is efficient in terms of pharmaceutical biotechnology, eco-friendly, renewable, and biocompatible. The synthesised nanoparticles were put through GCMS to test for the presence of terpenoids, alkaloids and other bioactive compounds. The synthesised nanoparticles were characterized by employing FESEM, HRTEM, XRD, FTIR and UV spectroscopy were carried out separately. The nanoparticle's antioxidant content was evaluated using the DPPH assay to validate the effectiveness of its antioxidant properties. Furthermore, the antibacterial studies reveal that the synthesised nanoparticles were effective against both gram positive and gram negative bacteria

Key words: *Centella Asiatica, Ag-NPs, CuO-NPs, Green synthesis, antioxidant, antibacterial assays*

H 071

Chitosan-Coated Hydroxyapatite Nanocomposite as Safe Drug Carriers *In Vivo* Model of *Drosophila Melanogaster*

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ABSTRACT

Hydroxyapatite nanoparticles (HAp NPs) are widely utilized in dental implant coatings, bone tissue engineering, and drug delivery systems due to their exceptional biocompatibility and stability. Chitosan, a natural polymer sourced from crustaceans, possesses antioxidant, antimicrobial, and anti-inflammatory properties, making it a valuable component in drug delivery approaches. However, nanoparticles often exhibit an initial burst of drug release, prompting the investigation of sustained release strategies using polymers like chitosan. Despite their efficacy, the widespread use of nanoparticles raises environmental toxicity concerns, necessitating comprehensive safety assessments. In this study, we synthesized and characterized a Hydroxyapatite-Chitosan (HAp/CS) nanocomposite using various techniques, including Dynamic Light Scattering-Zeta potential (DLS-Zeta), Transmission Electron Microscopy (TEM), and Fourier Transform Infrared Spectroscopy (FTIR). Subsequently, we evaluated the safety profile of the HAp/CS nanocomposite in wild-type *Drosophila* through oral administration. Behavioral assays (crawling and climbing) and biochemical assays assessing Superoxide Dismutase (SOD) and 2,2-Diphenyl-1-picrylhydrazyl (DPPH) activities were performed in both larvae and adult male flies to assess the nanocomposite's impact. Our results demonstrate that the nanocomposite not only supports larval development but also enhances behavioral and antioxidant activities. Importantly, unlike previous studies utilizing HAp NPs, the inclusion of chitosan in our nanocomposite formulation contributes to these observed enhancements, likely due to its intrinsic antioxidant properties.

Keywords: *Hydroxyapatite Nanoparticles (HAp NPs), Chitosan, nanocomposite, Drosophila melanogaster*

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H 072

Synthesis of Yttrium Doped Cerium Oxide Nanocomposites and their In-vivo Toxicity Evaluation in Drosophila Melanogaster Model

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ABSTRACT

The nanocomposite and nanoparticles of cerium oxide, yttrium oxide, and yttrium-doped cerium oxide (Ce: Y) were synthesized using the Co-precipitation method, employing yttrium nitrate hexahydrate, cerium nitrate hexahydrate, and HMT as precursors. The resulting nanoparticles underwent characterization through UV-Vis spectra, XRD, FTIR, SEM, TEM, DLS, and Zeta potential analyses. The investigation of their toxicity at various compositions (0.9:0.1M, 0.8:0.2M, and 0.7:0.3M) and concentrations (1.25, 12.5, and 125µg/ml) involved exposing wild-type third instar larvae and adult male flies (Oregon K strain) to Ce: Y along with their food over a specific duration. Survival assay results indicated that, in comparison to the control, all concentrations (1.25, 12.5, and 125µg/ml) were non-toxic for the specified timeframe. Dietary administration of Ce: Y at these doses did not induce developmental or behavioural defects. Crucial biochemical parameters, including SOD activity and ROS generation, remained largely unaffected at the three doses of the nanocomposites, compared to the control. SOD activity in third instar larvae consuming nanoparticle-containing food also did not show significant alterations. The findings from these studies suggest that yttrium-doped cerium oxide (Ce: Y) at doses of 1.25, 12.5, and 125µg/ml did not exhibit significant toxicity in third instar larvae and adult flies when administered over a certain period. Additionally, this study proposes the potential use of Ce: Y as an antioxidant compound and a promising drug carrier in future studies involving Drosophila Melanogaster models.

Keywords: *Cerium oxide, Yttrium oxide, Yttrium doped cerium, Nanocomposite, Toxicity.*

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H 073

Moderating Acrylamide-Induced Toxicity in *Drosophila* Models through Nanoceria Co-Treatment

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ABSTRACT

Environmental toxins like acrylamide (ACR) found in high-temperature processed foods rich in starch and proteins are subjects of extensive research. ACR is suspected to induce harm by generating reactive oxygen species (ROS) within the cytosol, disrupting the redox balance. Such disruption can have detrimental effects as cytosolic redox rhythms play pivotal roles in regulating metabolism, cell division, and differentiation. Consequently, therapeutic approaches for ACR-induced toxicity primarily target non-toxic compounds capable of modulating oxidation mechanisms without adverse effects. Cerium Oxide Nanoparticles (nCeO2), a rare earth metal oxide, have garnered significant attention for their antioxidant properties and potential as drug carriers, owing to their mimicry of antioxidant enzymes. Given the suitability of the *Drosophila* model system for toxicological investigations due to its short lifespan and physiological similarities to humans, this study investigates the antioxidant efficacy of nanoceria against ACR-induced toxicity in the *Drosophila* model.

Keywords: *Acrylamide, Drosophila melanogaster, Nanoceria, Toxicity*

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H 074

Biocompatible Nanofibers Loaded with Papaya Seed Essential Oil as an Antibacterial Wound Dressing Material

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ABSTRACT

Wounds pose a significant health risk, affecting more than 8 million individuals in the United States. Due to the COVID-19 pandemic, the healthcare system is under pressure which is further aggravated by limited access to essential services. In the field of biomedicine, biomaterials have emerged as a viable candidate for wound care management. Bio nanomaterials are more likely to colonize with pathogenic microorganisms, which slows down the healing process. In this study, the synthesize, optimization of electrospinning parameters and characterization of poly-ε-caprolactone/chitosan blended nanofibrous mats containing papaya seed essential oils was reported. The as synthesized mats were investigated for their antibacterial properties, *in vitro* cell proliferation assays for skin cells. The FESEM and HRTEM results showed that the oil loaded mats were smooth, continuous, bead free, and randomly oriented. The FTIR analysis confirmed the successful incorporation of papaya seed essential oil in to the composite mats. Contact angle measurement unveiled the hydrophilic nature of the electrospun mats. The disk diffusion assay revealed the papaya seed loaded mats exhibited broad spectrum antibacterial activity. Furthermore, MTT assay showed the papaya seed containing PCL/chitosan mats were biocompatible and promotes the 3T3 L1 fibroblast cells proliferation. The obtained results demonstrated the PCL/chitosan hybrid system infused with papaya seed essential oil can be an effective antibacterial wound dressing.

Keywords: *Nanofibers; Chitosan; Papaya seed essential oil; Antibacterial; Biocompatible*

H 075

Biogenic synthesis and antimicrobial activity of silica-coated silver nanoparticles against cariogenic microorganisms

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ABSTRACT:

Development of biologically inspired green synthesis of silver nanoparticles is evolving into an important branch of nano-biotechnology. In the present investigation, we report the green synthesis of silver nanoparticles (AgNPs) employing the extract of Cissus Quadrangularis. This current study mainly focuses on synthesis of silver nanoparticles in an eco-friendly method using Cissus quadrangularis (CqNp), its characterization and understanding its potential biomedical applications. The CqNp's were confirmed using UV-vis spectroscopy, FT-IR and the structure of the nanoparticles were analysd by EDAX. The antimicrobial activities of green synthesized AgNPs and silica coated AgNPs have been evaluated against the dental caries causing microorganisms such as Strepto- coccus mutans and Lactobacillus acidophilus using agar diffusion method. The AgNPs and silica blended AgNPs resulted in significant antibacterial activity

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H 076

Formulation and characterization of 5-Fluorouracil Loaded Caseinate Nanoparticles for Drug Delivery

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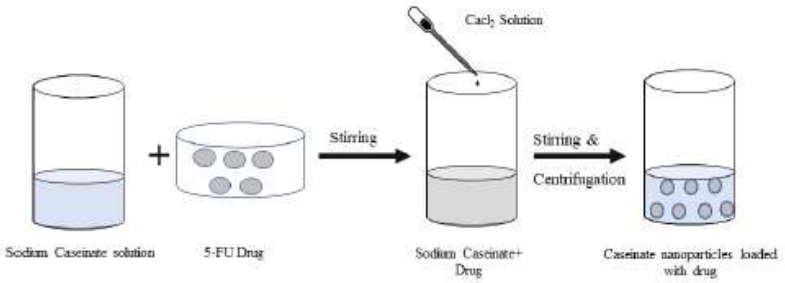
ABSTRACT

This study presents a simple method for the preparation of casein nanoparticles loaded with the anticancer drug 5-Fluorouracil (5-FU). Casein, a milk protein capable of self-assembling into micelles in water, exhibits binding properties to various drugs. The two-step coacervation method, employing different proportions of calcium chloride as a cross-linker brings soluble casein molecules in the solution together to form densely packed micellar nanoparticles. These natural protein-based nanoparticles hold promise as effective vehicles for delivering chemotherapeutic drugs. The resulting 5-FU loaded NaCas nanoparticles were characterized using X-ray diffraction, scanning electron microscopy, Fourier-transform infrared spectroscopy, and dynamic light scattering. The particle size ranges from 150-300 nm and the ability of Caseinate to encapsulate the drug was confirmed with X-ray diffraction and Fourier-transform infrared spectroscopy. Their morphology was observed through scanning electron microscopy and suggest nearly spherical particle.In-vitro release studies was also carried out.



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H 077

Synthesis and Characterization Cetrimide Templated Fine Nano β -TCP/HAp Biphasic Rods: Exploring Applications in Regenerative Medicine.

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ABSTRACT

Calcium phosphates like Hydroxyapatite (HAp), β-tricalcium phosphate (β-TCP) and their composites are significant materials for bone regeneration applications [1]. In this regard, their direct independent interaction with the biological system constitutes one stream of research; whereas, the interaction of their composites in various ratios forms the other. [1,2]. Hence, systematic studies on its preparation and influence of various parameters have been carried out globally. In this respect, biphasic transformation has been reported with varying Ca/P ratios (1.5 to 1.665) [3]. A study on the pH and temperature influence on the morphology has reported pure HAp phase at pH 6 [4]. However, the current study, conducted at pH 7.5 and consequent calcination (750°C), showed that the sample transformed to biphasic phase with 78% of β-TCP and 22% of HAp and its morphology has reformed from fibres to fine rods as confirmed by the TEM images. The XRD and the FTIR studies also confirm the same. The surface area (9.9 m^2/g), mesoporous nature and biocompatibility were also confirmed by BET and MTT tests respectively. Based on the CMC measurements, Gibbs free energy was calculated and the advantage of capping material has been revealed. This composite with fine morphology has a high potential in orthopedic and dental regenerative applications.

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H 078

Nanocrystalline Hydroxyapatite (HAP) for advanced biomedical applications

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ABSTRACT

Hydroxyapatite/HAP ($Ca_{10}(PO_4)_6(OH)_2$) is the most stable calcium phosphate ceramic at ambient temperature. Due to its excellent biocompatibility and physicochemical similarity to human bone and teeth, it has been used as an implant material for orthopedic, dental, and other biomedical applications. In this study, a high-energy planetary ball milling/mechano-chemical technique was used to synthesise nano HAP powder, as confirmed by the particle size analysis. At first, $CaCo_3$ and $(NH_4)H_2PO_4$ were taken as starting precursors and subjected to milling for 5 h with 300 rpm by using zirconium balls of 20 mm diameter as the grinding media. Field-effect scanning emission microscope, energy dispersive X-ray analysis, X-ray diffraction, and Fourier transform infrared spectroscopy, LCR meter were used for the characterization of surface morphology, elemental analysis, phase conformation, and electrical properties, respectively. The average particle size was found to be in the range of 65 nm to 109.8 nm. The pure phase of HAP was obtained at 800 ºC followed by 600 ºC for 4 h. The sintering was carried out at temperature values of 1200 ºC, 1250 ºC , and 1300 ºC for 4 h in a conventional furnace. Experimental densities of sintered HAP powders were found to be 2.8 g/cc, 3.03 g/cc, and 2.7 g/cc , respectively. The surface charge of HAP is another crucial parameter that assists the bone cell growth process. So, the electric properties need to be studied to understand the cellular behavior of bone. Microstructure and densification of sintered samples play a vital role in determining the dielectric constant of the system. The dielectric constant and dielectric loss of the HAP system at 1 kHz frequency were found to be ~29 and ~0.32, respectively. The bioactive material HAP can be used as a filler in polyvinylidene fluoride (PVDF) polymer matrix to enhance its bioactive nature.

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H 079

Effect of Mussel inspired Amorphous Calcium Phosphate Complex on Dentin Bio-remineralization

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ABSTRACT

Pathological conditions like caries, severe abrasion, can cause dissolution of dentin mineral phase, thereby leading to collagen matrix breakdown. Currently used remineralizing agents do not possess simultaneous collagen protecting effect. Biogenic Amorphous calcium phosphate (BACP) proved to have better bioactivity and enhance remineralization potential than synthetic amorphous calcium phosphate (SACP). Polydopamine (PDA) has been attempted to stabilize ACP which can also promote intrafibrillar mineralization with collagen stabilization effect. There are no literature studies on effect of ACP and PDA combination on dentin remineralization. Hence, this study aims to comparatively evaluate the effect of SACP and BACP -Polydopamine (PDA) combination on dentin remineralization and collagen degradation resistance. Around 90 coronal dentin slabs(5x5x1mm) will be obtained from extracted sound human molars or premolars. Prepared dentin slabs will be randomly divided into 6 groups (n=10). Group 1- control; Group 2 – PDA; Group 3 – SACP; Group 4 – BACP; Group 5 – SACP-PDA; Group 6- BACP-PDA. The samples will be then coated with the experimental agents followed by pH cycling for 14 days. Dentin samples will be then be evaluated for microhardness evaluation using Vickers Microhardness Tester followed by surface and elemental analysis using Scanning electron microscope- Energy Dispersive X-Ray (SEM-EDX) respectively. Remaining dentin samples (n=5) will be analysed for collagen degradation resistance analysis using Hydroxyproline and FTIR. The results will be tabulated and statistically analyzed using One-way ANOVA and Multiple comparison Post-hoc Tukey's test. BACP-PDA showed higher remineralization potential on both mechanical and chemical analysis. Hence, BACP-PDA combination can serve as remineralization inducing agent for dental applications.

I 001

Electrocatalytic CO_2 reduction on Bismuth cathode using Calix[4]imidazole catalyst

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ABSTRACT

Electrochemical CO_2 reduction reaction (CO_2RR) is the emerging method to reduce CO_2 into economically feasible liquid products includes formic acid, methane, ethane, ethylene, propylene, ethanol and methanol under different solvents and catalysts. Bismuth based electrocatalyst have been developed as a potential metal cathode for the electrochemical conversion of CO_2 to formate. Electroreduction of bismuth film electrode alone and presence of synthesized Calix [4]imidazole catalyst in CO_2 saturated electrolyte was studied from linear sweep voltammetry technique. The GC-Bi with CI-4 (2mM) catalyst in CO_2-saturated electrolyte (pH = 6.8) exhibit higher current densities than Bi modified and GC alone. The reduction peak current increases in the presence of Calix[4]imidazole express the catalytic support under CO_2 saturated electrolyte. The onset potential shift is observed at -1.4 V in the presence of catalyst. The controlled potential electrolysis was conducted to identify the reduction product. The product formed is confirmed from ^{1}H NMR analysis using the sample obtained from bulk electrolysis.

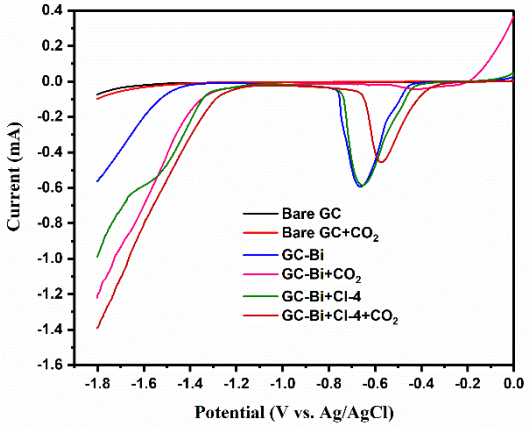

Fig. 1. LSV of Bi modified GC with CI-4 and without CI-4 under N_2 and CO_2 saturated 0.1 M $KHCO_3$.

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I 002

The Optimization of Water Bath Temperature for Electrodeposit-Cu_2O On TiO_2 Rod/FTO Substrate

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ABSTRACT

Titanium dioxide, TiO_2 rod structures are currently receiving a lot of attention as semiconductors thin film for stable and better efficient solar cell application [1]. This is because they provide a conductive pathway in the photovoltaic mechanism. However, due to its high bandgap and low-quality surface, the fabrication of cuprous oxide, Cu_2O is needed as an absorber layer in heterojunction thin film. Cu_2O is chosen as an absorbing layer because it helps TiO_2 collect more photons by broadening its light spectrum. In this study, a hydrothermal method is used to fabricate TiO_2 rods [2-3]. A hydrothermal etching is introduced to help increase charge transfer and encourage the uniform fabrication of the next layer, Cu_2O. Using the electrodeposition method, the Cu_2O will be developed on the TiO_2 layer. This research aims to study the effect of water bath temperature during the Cu_2O electrodeposition process to improve the properties of the p-n junction semiconductor material. With the increasing of the water bath temperature to 60 °C, the FE-SEM image shows that Cu_2O layers have a bigger grain size of three-side and has the highest structure of a (111) preferential orientation in XRD patterns. The AFM characterization also shows the roughness surface of the electrodeposited layers increases roughness for 41% when deposited at a water bath temperature from 40 to 60 °C. For the sample that deposited at 50 and 60 °C water bath temperature exhibited a stronger absorption at visible light region which could attributed by more Cu2O nanoparticles that loaded into the space of the etched rod structure. Therefore, finding the optimum water bath temperature can help to improve the crystallinity and roughness surface of the Cu_2O.

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I 003

Enzymatic Bioremediation of Insecticide using Cutinase Immobilized on Magnetic Nanoparticles

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ABSTRACT

Insecticide poisoning is one of the most common form of poisoning fatalities. It may occur due to accidental or occupational exposures. The most commonly used organophosphate insecticide i.e. Malathion has been associated with the increased risk of lymphoma and thyroid carcinoma [1]. In order to deal with the pollutants, use of enzymatic bioremediation techniques has been increased [2]. The present study explored the immobilization of cutinase on magnetic nanoparticles to enhance its enzymatic properties and catalytic applications. Maximum cutinase activity recovery (85%) was observed at 2% of magnetic nanoparticle concentration, 10 mM glutaraldehyde concentration and 90 min of cross-linking time. Cutinase immobilized nanoparticles (CMnPs) were characterized in terms of size, crystallinity, magnetic behavior, chemical composition and thermal stability. The CMnPs showed 94% activity even after five repeated washing and hence possess good reusability potential. The immobilized cutinase showed greater stability and significant insecticide degradation activity. GC-MS results confirmed the degraded metabolic products of malathion. In all, the immobilized cutinase was superior to free cutinase, showing promising structural and application characteristics.

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I 004

Microwave Assisted fabrication of Silver doped Yellow Carbon dot nanocomposite for effective photocatalytic degradation of cationic and anionic dyes

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ABSTRACT

A novel approach of reducing dye pollution leads to a sustainable environment for future generation. Photodegradation of dyes in presence of sunlight using carbon dot nanocomposite offers an effective and sustainable way to break down dye molecules, resulting in cleaner water and a pollutant-free environment. The primary objective of this research is to conduct the catalytic break down of organic dyes using nanocomposite. Solid Fluorescent Yellow Carbon Dots (SFYCDs) synthesised from Araucaria araucana impregnated with silver (Ag/SFYCDs NC) by microwave-assisted technique without the need of additional any reducing or stabilising chemicals is used for dye degradation studies. This nanocomposite exhibited high catalytic activity towards the complete reduction of both anionic and cationic dyes i.e., Methylene blue and Alizarin red S within 120 mins. The nanocomposite is found to be stable and reusable catalyst that it can be used up to five times without significantly losing its catalytic activity. This is due to their numerous applications, which include good light absorption, great photostability and potent catalytic activity. Multiple analytical techniques were used for the characterization of SFYCDs such as UV-Vis, XRD, FTIR, SEM-EDX, TEM and PL studies. The emission wavelength of SFYCDs in UV response is observed at 474nm and excitation at 350nm, which confirms that plant-based SFYCDs show maximum emission at excitations between 350 and 370nm.The SEM-EDX confirms the presence C and Ag and also a cubic morphology, the XRD response with 2θ=21° confirms the presence of CDs and the particle size is calculated to be 3.16nm. It is observed that the SFYCDs are able to degrade even nanomolar amounts of dye present in water sample. Thus, the synthesised nanocomposite is found to be an effective probe to detect and degrade the dyes under normal sunlight.

Keywords: *Carbon Dots, Methylene blue, Alizarin red S, Photocatalyst, Dye degradation.*

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I 005

Synthesis & Characterization of Fe_3O_4 magnetic nanoparticles for removal of heavy metal ions in waste water remediation

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ABSTRACT

Contamination of water bodies with toxic metal ions is a severe environmental & public health problem. Due to increase of industrialization & population, availability of safe & clean water is important not only for human life but also for the survival of aquatic lifestyle. Heavy metal ions like Cu, Cr, Pb, Hg, As, Ni, P, Cd etc. refer to those metals which are mixed in water bodies coming out from industries & other waste water releasing sources. These metals are toxic & harmful to humans if consumed above a certain limit. Now-a-days research is been carried out for use of Fe based magnetic nanoparticles to adsorb these ions in an efficient way to save the biotic life style. In this work, we report, magnetite (Fe_3O_4) nanoparticles synthesized using co precipitation method. These nanoparticles were further used for characterization like XRD, EDAX, TEM, FTIR techniques. The adsorption efficiency of various metals was estimated using Atomic Adsorption Spectroscopy (AAS). The major advantage of using magnetic nanoparticles is easy & efficient removal of nanoparticles from the treated solutions by using ordinary magnet.

I 006

Glucose Sensing, Photocatalytic and Super Capacitive Properties of ZnO Nanoparticles

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ABSTRACT:

Zinc oxide (ZnO) is a multifunctional material with wide applications in wastewater treatment, supercapacitors, gas sensors, and biochemical sensor devices. Nanoparticles of ZnO were synthesized by co-precipitation method for degradation of methyl orange, methylene blue, tetracycline as well as for supercapacitors and glucose sensors. The structural and morphological characteristics were investigated by X-ray diffraction, UV-visible spectroscopy, Fourier-transform infrared spectroscopy, Field emission scanning electron microscopy and High-resolution transmission electron microscopy. Degradation of waste in water was studied using UV-vis spectroscopy technique which shows degradation efficiency 57%, 74% and 90% for Methyl orange, methylene blue and Tetracycline respectively under UV irradiation. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were used for supercapacitors and biosensing applications. Detailed analysis of the experimental results demonstrate that zinc oxide nanostructure is a potential material to be used in waste water treatment, supercapacitor, and biosensing applications.

I 007

Biomineralization of Magnesium Doped Hydroxyapatite Nanoparticles using Lysinibacillus Fusiformis for Strontium removal

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ABSTRACT

Contamination of groundwater with strontium (Sr^{2+}) has been a serious issue in several Indian states, including Punjab, Andhra Pradesh, and a few locations in Assam, West Bengal, and Jharkhand.1 Industrial wastes, pesticides, and chemicals, all of which are released into the environment in one way or another, are the principal contributors to pollution. Strontium in water can cause renal difficulties and brain diseases if consumed in large amounts. Many people in Andhra Pradesh, India, have been diagnosed with chronic renal disease as a result of water pollution with silica and strontium. In order to remove Sr^{2+} from water, we have used biogenic hydroxyapatite (HAp) where the nanoparticles were produced by biomineralization of Lysinibacillus fusiformis bacterium via enzymatic process. The biomineralization of magnesium doped/incorporated hydroxyapatite (B-MgHAp) was mediated by phosphatase enzyme. As prepared B-MgHAp particles were characterized for their physicochemical characterizations. To evaluate the adsorption efficiency of B-MgHAp towards Sr^{2+}, the effect of contact time, adsorbent dosage, and pH range (3-11) were investigated. The adsorption behavior/pattern follows Langmuir and D-R isotherm model, the maximum adsorption efficiency (Q_0) was calculated to be 6.52 mg/g. Adsorption kinetics reveals that the B-MgHAp for Sr^{2+} obeys and follows the pseudo-second-order kinetic model. B-MgHAp was tested for its cytotoxicity towards MG63 osteoblast cells and found to be biocompatible with more than 88% viability at different concentrations. Herein the studies confirm that the synthesized B-MgHAp can be used as an efficient sorbent for Sr^{2+} removal.

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I 008

Silver Nanoparticle-Perforated Graphene Composite Produced from Horticultural Waste and Its Application in Ultraviolet Light Assisted Catalytic Dye Degradation

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ABSTRACT

Perforated graphene (PG) was produced by a one-step pyrolysis method from horticultural waste-dead Bougainvillea flowers.[1] Then, silver nanoparticles were attached to the PG by the reduction of a very small amount of silver nitrate (in a weight ratio of PG:Ag = 1:5) to form the PG@Ag composite.[2]. The structural, morphological and optical properties of as-synthesized PG and PG@Ag composites were characterized by various characterization techniques like X-ray diffraction, HRTEM, FESEM, EDX, UV-Vis DRS, etc. The photocatalytic activity of the as-prepared samples was examined using aqueous rhodamine B (RhB) and methylene blue (MB) dye under UV–visible light irradiation. It was found that the attachment of silver nanoparticles can noticeably enhance the photocatalytic potential of PG.[3, 4] The PG@Ag composite degraded the MB dye to ~93.4% within 90 minutes under UV-light radiation. Thus, this nanocomposite, PG@Ag, effectively derived from natural waste material, has proven to exhibit high photocatalytic and anticancer activity. Eventually, it may prove to be an effective tool for eradicating dye pollution from wastewater and a way to prevent cancer-mediated diseases in the cosmetics and pharmaceutical industries. The synthesized catalyst could be considered a potential photocatalyst for environmental remediation applications.

Keywords: *Perforated graphene (PG), PG@Ag composite, Photocatalysis, UV-light, Wastewater remediation.*

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I 009

Efficient Removal of Rhodamine B Using Graphene Oxide-Activated Carbon Composite

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ABSTRACT

This research is centered on the development of a nanocomposite that combines cost-effectiveness with eco-friendliness, specifically designed for optimal chemical adsorption performance. Recognizing the demanding criteria in this field, a one-step synthesis method was meticulously employed to produce a graphene oxide -activated carbon (GOAC) composite. This innovative and streamlined approach was supported by a comprehensive suite of advanced characterization techniques, which effectively verified the structural integrity of the constituent materials. Ensuring the preservation of the initial structural properties was identified as a crucial factor in facilitating efficient adsorption, and the successful confirmation of this preservation underscored the potential efficacy of the composite. The results were particularly promising, as the fabricated GOAC composite exhibited exceptional efficiency in the elimination of the organic dye Rhodamine B. Impressively, it achieved a maximum adsorption capacity of 90 mg/g within a remarkably short time frame of just 60 minutes. This quick and substantial adsorption capacity holds significant promise for practical applications where rapid purification or detoxification processes are required. The robust adsorption behaviour observed was found to closely align with the well-established pseudo-second-order kinetic model, providing additional evidence of the composite's efficacy and practical viability. By addressing both economic and environmental concerns, this research paves the way for the development of highly efficient and sustainable adsorption materials. Not only does it contribute to the growing demand for green and cost-effective solutions, but it also demonstrates the feasibility of using advanced materials science techniques to address pressing environmental challenges. As a result, the findings from this study offer valuable insights for the advancement of nanocomposite materials with enhanced adsorption capabilities, with potential applications in diverse industrial and environmental remediation settings.

I 010

Heavy Metal Removal from Waste Water by ZnO/rGO Composite

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Abstract

Heavy metals, such as Chromium and Cadmium, are highly carcinogenic and non-biodegradable pollutants released from various industrial activities. They are significant contributors to environmental pollution, posing serious health risks to living organisms exposed to contaminated water. Consequently, the need for treating heavy metal-polluted water is vital for ecological balance. The carbon-based composites were reported to be efficient adsorbers of heavy metals. In this study, we prepared ZnO/rGO composite by a single step eco-friendly method. Various characterization techniques confirmed ZnO/rGO composite formation. The prepared composites exhibited remarkable heavy metal adsorption capabilities and the adsorption studies were carried out by varying parameters such as adsorbent, adsorbent dose, pH, time, and concentration. The heavy metal adsorptive removal experiments were analyzed in batch mode using UV-Vis spectral analysis and Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-OES) analytical techniques. It was observed that the removal efficiency increased with higher adsorbent dosage and longer reaction times. The kinetic data were analysis through three distinct mathematical models: Pseudo 1st Order, Pseudo 2nd Order, and Intra-Particle Diffusion. Furthermore, the adsorption isotherm was explored using both Langmuir and Freundlich models. Detailed analysis using X-ray Photoelectron Spectroscopy (XPS) and Energy-Dispersive X-ray Spectroscopy (EDS) of the adsorbent after adsorption verified the effective adsorption of heavy metals on to the adsorbent. These findings suggest that ZnO/rGO composite is a cost-effective and efficient adsorbent for removing heavy metal contaminants from industrial effluents, making it a promising solution for addressing this environmental challenge.

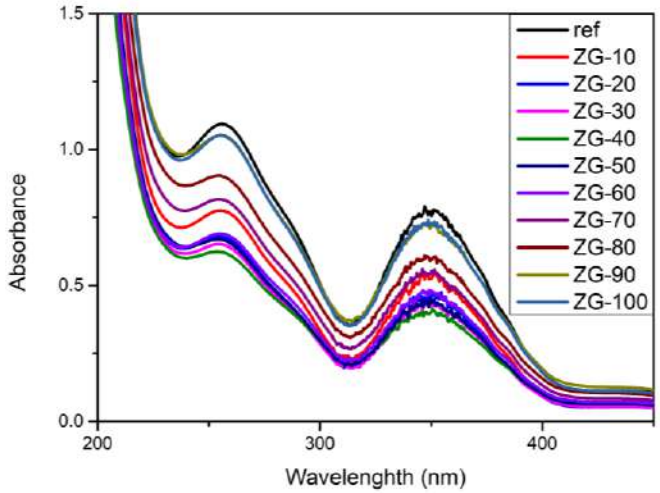

Figure 1 UV-Vis absorption spectra due to the adsorptive removal of Cr (VI) with various adsorbents in 1 hours.

I 011

Development of Molybdenum doped Cobalt Ferrite Nanoparticles Promoting the Heterogeneous Activation of Peroxymonosulphate for Rhodamine B removal

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ABSTRACT

Peroxymonosulphate (PMS) assisted advanced oxidation process (AOP) is one of the promising methods for the degradation of recalcitrant pollutants including organic dyes, pesticides, antibiotics and polychlorinated biphenyls (PCBs).1 The heterogenous activation of peroxymonosulphate to generate reactive radicals can be conveniently carried out with magnetic nanoparticle materials such as cobalt ferrites.2 Consequently, we have synthesised cobalt ferrite and molybdenum (Mo) doped cobalt ferrite nanoparticles in this work, adopting a urea-assisted hydrothermal method. X-ray Diffraction analysis verified the formation of pure crystalline spinel cobalt ferrite nanoparticles, and the Mo doping was confirmed from the FT-IR data, while the spherical morphology was revealed from the scanning microscopic (SEM) images where the particle sizes ranged from 15 to 34 nm. The Mo doping resulted in an increased surface area and the magnetic hysteresis curve indicated the ferromagnetic behaviour of Mo- doped cobalt ferrite. The catalytic efficiency of synthesized cobalt ferrite was estimated by conducting the PMS-assisted advanced oxidation of rhodamine B (RhB). In comparison with pure cobalt ferrite (CHr), Mo doped cobalt ferrite (MoCHr) revealed better degradation efficiency of 99.4% within 10 minutes when 5 mg of MoCHr and 5 mg of PMS were used. This suggested that the molybdenum doping might be having an important role in the degradation of Rhodamine B. The influence of various parameters including the concentration of catalysts, amount of PMS, pH, etc., was also studied. The radical scavenging experiments revealed that the sulphate radicals were the prominent active species generated., while the X-ray photoelectron spectroscopic analysis revealed the activation mechanism of PMS by Mo-doped ferrite nanoparticles.

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I 012

Effect of Y_2O_3 Addition on Photocatalytic, Antibacterial and anti-oxidant potency of ZnO nanoparticles

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ABSTRACT

Pure ZnO and Y_2O_3 doped zinc oxide nanoparticles were synthesized by the modified combustion method using hexahydrate nitrates of Yttrium and Zinc as starting materials. The structural analysis of the sample was performed with the aid of X-ray diffraction (XRD). The phase purity of the sample was confirmed using Fourier transform Infrared spectral analysis (FTIR). The surface morphology and particle size were understood from the high resolution Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (HRTEM). The photocatalytic activity of samples on azo and basic dyes were investigated in detail. The effect change in concentration and exposure time on the degradation rates of dyes were determined. The competency of the sample on antibacterial application for gram positive and gram negative bacteria through agar- well diffusion method. The antioxidant potency was estimated by measuring the scavenging activities of free radicals such as superoxide, hydroxyl, nitric oxide, and hydrogen peroxide.

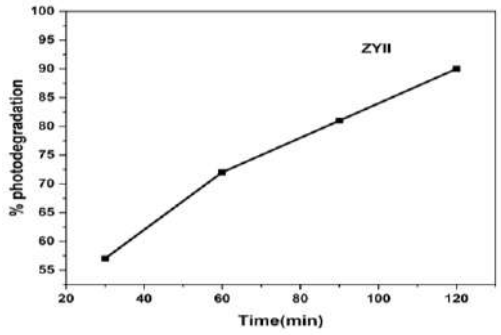

Fig.1. Rate of degradation congo red by Yttrium added ZnO(ZYII)

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I 013

Analysis And Application of Natural Wax Extracted from Colocasia Esculenta Leaves

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ABSTRACT

Colocasia esculenta, an edible aroid has superhydrophobic properties due to the presence of epicuticular wax present on its leaves. The hydrophobicity properties in these leaves are observed at contact angles greater than 150°. The epicuticular wax can be extracted by using polar and non-polar solvents with the maceration extraction technique. It was observed that non-polar solvents like Toluene, Xylene, Di-ethyl ether and Petroleum ether extracted the non-polar hydrophobic wax whereas polar solvents like ethanol, and ethyl acetate were not able to extract the same. The natural wax found in *Colocasia esculenta,* being non-polar in nature, dissolved only in non-polar solvents used in the maceration method. The percentageof the natural wax extracted ranged from 3-4% and mainly depended on the SPF factors.

I 014

Highly Efficient and Visible-Light-Driven Ni-doped V_2O_5 Photocatalyst for Degradation of Rhodamine B dye

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ABSTRACT

The development and application of Ni-doped V_2O_5 photocatalysts is an important field of investigation. In this work, the effectiveness of Ni doping in V_2O_5 for the degradation of Rhodamine B dye was investigated. X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), High-Resolution Transmission Electron Microscopy (HR-TEM), and Diffuse reflectance spectroscopy (DRS-UV) were carried out to identify the crystal structure, morphology, and optical properties respectively. The outcomes of XRD showed that the Ni ions had been successfully incorporated, which had caused a noticeable alteration of the V_2O_5 crystal structure and increased its ability to absorb UV light. Degradation of Rhodamine B dye was improved as the percentage of Ni doping in V_2O_5 was increased. The doping has enhanced the separation of electron-hole pairs and decreased charge carrier recombination. Photocatalytic degradation experiments were conducted under UV irradiation using Rhodamine B dye as a model pollutant. Ni-doped V_2O_5 photocatalyst demonstrated remarkably enhanced photocatalytic activity compared to pristine V_2O_5. The efficient degradation of Rhodamine B dye is attributed to the synergistic effect between Ni doping and V_2O_5, which facilitated the separation of electron-hole pairs and reduced charge carrier recombination.

I 015

Unraveling Cucurbit [7] uril's Potential In Biological Application And Dye Encapsulation

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ABSTRACT

Supramolecular chemistry, the world of non-covalent interactions, offers innovative solutions in biological systems with promising advancements in fields crucial to health and the environment. Cucurbit [7] uril, a versatile supramolecular host molecule, exhibits remarkable potential in biological applications and dye adsorption, making it a focus of research for its intriguing encapsulation properties. In the present work, (I)host CB [7], (II)the inclusion complex of Ionic liquid with CB [7], (III) host-guest complexes of thallium with CB[7] and ionic liquid, (IV) thallium with CB[7] were synthesized and analysed using spectroscopic techniques and biological, dye adsorption studies were conducted. The UV-Visible spectra of mixed ligand complexes show increase in absorbance at 225nm when compared with free CB [7] and IR spectra shows characteristic peak at 3394cm^{-1} which indicate the presence of intramolecular hydrogen bonding. The inclusion complex of CB [7] with ionic liquid showed a well-defined bacterial zone by resisting gram-positive and gram-negative bacterial growth and the inclusion complex of CB [7] with thallium showed higher antibacterial activity than its precursor CB [7] and mixed ligand complexes with metal. Tannery effluent water from a leather industry was collected and water-soluble cationic dye present in it was allowed to encapsulate into the inner cavity of cucurbituril. This dye molecule enters into the precipitate forming an inclusion complex with CB and allowing the filtrate to remain clear. The dye encapsulation was validated via colorimetric method where, absorbance decreases as time increases. The results show the potential for the supramolecule to contribute to sustainable and effective wastewater treatment solutions. The future work aims to compare different supramolecules for their encapsulation properties.

Keywords: *Supramolecular chemistry, Cucurbituril, inclusion complex , dye adsorption*

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I 016

Efficient TiO_2 Photocatalyst for Degradation of Organic Radioactive Wastes

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ABSTRACT

Quantum dots (QDs) have gained much as attention due to novel physical and chemical properties which find application in solar cells, photocatalyst, fuel cells, etc. TiO_2 is extensively used as photocatalyst because of its stability, economic and ecofriendly nature. Here we report a low temperature synthesis of anatase phase TiO_2 and demonstrates its efficacy as a photocatalyst for dye and Tri-Butyl Phosphate (TBP) degradations. Fast photocatalytic degradation of methylene blue has been observed using UV lights with k=0.03 min^{-1} compared to the commercially available P-25 photocatalyst. This understanding is extended to the degradation of TBP which is used in nuclear fuel reprocessing units to extract Uranium and Plutonium from the spent fuel. The continuous irradiation of TBP leads to formation of radiolysis products and as a result safe removal and controlled degradation of TBP is crucial. Photocatalytic degradation is found to be simple and effective approach towards its mineralisation process.

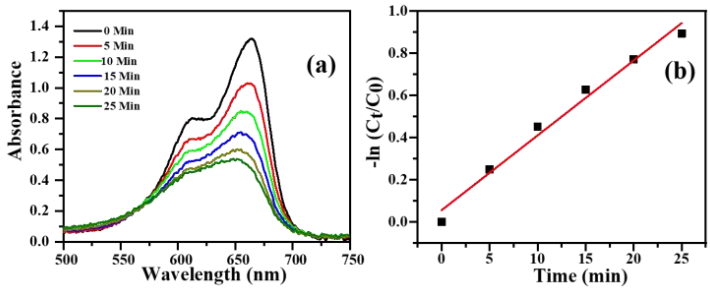

Figure 1 (a) The time dependent UV-Vis spectra Figure 1(b). The reaction kinetics for the degradation of MB dye under UV light by TiO_2 QDs.

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I 017

Nanotechnology -Enhanced Food Packaging: A Green Solution to Minimize Horticulture Waste

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ABSTRACT

Nanocomposite-based biofilms have garnered significant attention in food packaging due to their eco- friendly attributes, reduced toxicity, and potential to prolong the shelf life of food products effectively. In this study, we explore the development of innovative biofilms using fruit and vegetable peels in combination with functionalized silver nanoparticles (Ag-fHNT). The biofilms were meticulously prepared using the solvent casting method, resulting in three distinct categories: pectin biofilms, HNT- pectin biofilms, and Ag-fHNT-pectin biofilms. The comprehensive characterization of these biofilms encompassed various critical parameters, including moisture absorptivity, tensile strength, antimicrobial properties, DPPH (2,2-diphenyl-1-picrylhydrazyl) antioxidant assay, and FT-IR (Fourier-transform infrared spectroscopy) analysis, among others. The results obtained from our study revealed remarkable enhancements in the durability and antimicrobial efficacy of the Ag-fHNT-pectin biofilms, signifying their potential to not only extend the shelf life of food products but also reduce the risk of contamination, spoilage, and foodborne illnesses. This breakthrough offers a sustainable and eco-conscious alternative in food packaging, which could play a pivotal role in reducing environmental impact while ensuring the quality and safety of food throughout its storage and distribution. As we continue to address the challenges of modern packaging, this innovative approach using nanotechnology holds promise for a greener, more food-secure future.

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I 018

Sodium Borohydride-Assisted Catalytic Property of BiOCl Nanoparticles for Water Remediation

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ABSTRACT

The chemical catalytic property of the basic metal oxyhalides in the conversion of 4-Nitrophenol to 4-Aminophenol was observed [1,2]. The degradation efficiency for the most effective sample was about 100 %, and the rate kinetics was 1.88 min-1 within a 4-minute interval. The transformation process was performed at the ambient temperature and medium in the aqueous sodium borohydride solution. We reported an easy, cost-effective, eco-friendly hydrothermal synthesis of bismuth oxychloride (BiOCl) nanomaterials [3]. In addition to the synthesis assertions, efforts have been made to investigate the optical and electronic properties of nanomaterials by various sophisticated technics [4]. The tunability of band formation and phase equilibrium of nanomaterials, as well as the relationship between nanomaterials and catalytic activity, were examined [5]. The synthesized nanomaterials were very valuable for wastewater remediation in the aquatic environment.

Keywords: *Chemical catalysis, 4-Nitrophenol, 4-Aminophenol, Hydrothermal, Nanomaterials.*

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I 019

Development of Food-grade Bioplastics using Silk Sericin

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ABSTRACT

This research aims to develop a food-grade biodegradable plastic using silk sericin, which is a waste from the silk-based textile industry. Sericin is the second major protein after fibroin in silk cocoons. The degumming process of silk cocoons extracts silk fibroin, used by the silk-based textile industry, while sericin ends up mostly in wastewater streams. These waste streams from the silk industry have a chemical oxygen demand (COD) above 6000 mg/l and put a considerable load on the wastewater treatment plants. Silk sericin is a mechanically inferior and hydrophilic glycoprotein; therefore, no traditional use of silk sericin is present. India produces ~35 thousand metric tons of raw silk every year. By a rough estimate, ~9 thousand metric tons of sericin flows into water bodies. Therefore, the valorization of sericin for food-grade plastic (FGP) applications could have a substantial economic, social, and environmental impact. Silk sericin contains 18 types of amino acids, but it predominantly contains polar side groups, which give it strong hydrophilicity and changeability. It also has a wide range of physiological properties, including biodegradability, non-toxicity, UV resistance, and antibacterial activity. Substantial research efforts have exploited it in its pure form and modified forms, such as blends, crosslinked, and copolymerized with other macromolecules for applications in packaging, cosmetics, and wound dressing.; it. This work explores the protein crosslinking and plasticization approaches to create stable and flexible sericin films as bioplastics for FGP applications. The work also studies the properties required for FGPs, such as mechanical strength, solubility, and permeability, and to fabricate bioplastics.

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I 020

Oxidation of Rhodanide (SCN^-) in Micellar Media: A Kinetic Insight

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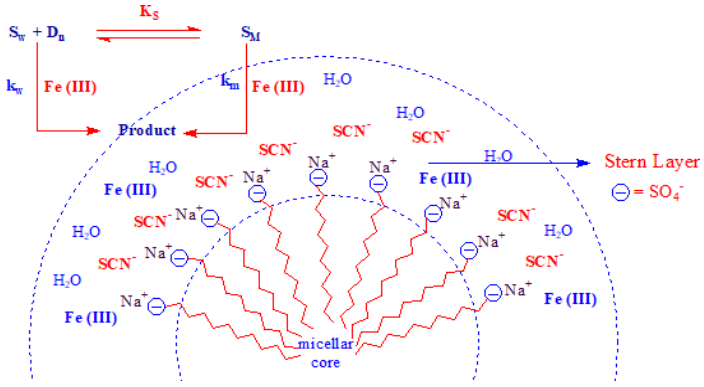
ABSTRACT

In continuation of our work on the kinetic studies in the oxidation of biologically, pharmaceutically, environmentally and industrially important organic substrates, in the present work we have extended our focus on rhodanide or thiocyanate (SCN^-) oxidation by iron(III) pyrophosphate in micellar medium. The study bears importance as SCN^- is found to catalyze electron transfer in cytochrome c and porphyrin compounds and is a main inorganic pollutant found in metallurgical wastewater. Moreover, redox processes in micellar media mimic biological processes and hence are considered significant. Micelles are organized assembly of surfactant monomers formed at a concentration regarded as critical micelle concentration (cmc). Progress of the reaction was monitored using a UV-VIS spectrophotometer maintaining pseudo first order conditions. Unit order dependence of rate on oxidant concentration was indicated by the linearity of plots between log (Absorbance) vs time. Detailed kinetic analysis revealed unit order dependence of rate on [SCN^-] and almost second order dependence on acid strength. Effect of other parameters like added salt and Fe(II) on the oxidation was also undertaken as a part of the study. In the micellar media although the main kinetic features remained somewhat similar compared to pure aqueous medium but presented some interesting results which calls for an explanation. We have considered Berezin model (Scheme-1) to explain our findings.



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I 021

Advanced Innovative SnO_2-Based Photocatalysts for Sustainable Wastewater Treatment and Advanced Environmental Cleanup

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ABSTRACT

Simultaneously removing antibiotics and heavy metal contaminants from wastewater without causing secondary contamination and ensuring easy recovery is a formidable challenge. To tackle this issue, we employed a hydrothermal method to create SnO_2-based photocatalysts with diverse morphologies. Our goal was to promote their valuable reuse and contribute to environmental protection. We employed various analytical techniques, including X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and High-resolution transmission electron microscopy (HRTEM) to confirm the formation of nanoparticles. We also used Raman, XPS, and Photoluminescence (PL) spectroscopy to explore their electronic, optical properties, and lattice defects. Furthermore, in this study, we also developed nanocomposites consisting of SnO_2 and graphene oxide to enhance their optical characteristics. These SnO_2/graphene oxide nanocomposites demonstrated remarkable catalytic performance, effectively degrading a 10 ppm RB dye solution in just 60 minutes under UV light exposure. Impressively, even after undergoing four cycles, the catalytic degradation activity remained consistently high, demonstrating exceptional structural stability. This improvement can be attributed to their enhanced adsorption capacity and the efficient separation of electron-hole pairs under light illumination. These findings underscore the potential of these composites as effective materials for breaking down harmful organic pollutants in wastewater treatment and for their application in spintronic devices. This opens up promising avenues for environmental remediation and advanced technology. Our current research is focused on identifying the structural, magnetic, and optical properties of various morphologies of SnO_2 NPs, as well as SnO_2/graphene oxide nanocomposites.

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I 022

Ambient-Temperature Synthesis of Molybdenum Disulfide (MoS_2) via Reaction-Diffusion Pathway: Morphological Control and Catalytic Implications

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ABSTRACT

A reaction-diffusion (*RD*) framework has recently been employed to synthesize thematerials with tailored properties.[1-3] *RD* offers apparent advantages over the conventional methods to synthesize the materials, such as hydrothermal, liquid phase synthesis, etc., in terms of precise control over shape and size running through nano- to microstructures.[2] Also, The synthesis of transition metal dichalcogenides (TMDCs) has been a subject of significant interest due to their unique properties and potential applications across various fields. Given this, our attention has focused on synthesizing Molybdenum Disulfide (MoS_2), a two-dimensional layeredmaterial from the TMDC family. The present study used a three-component 1D classical *RD* methodology to form the MoS_2. A test tube containing agarose gel immobilized with the inner electrolyte was clamped vertically. The outer electrolyte was allowed to diffuse in the gel overthe period to yield the product due to the *RD* phenomenon. The advantage of this methodology isa good yield of MoS_2 at room temperature. Material characterization techniques such as XRD, SEM-EDS, and IR were employed to confirm the formation of the product and check its purity. XRD technique confirmed the formation of hexagonal sheets, while SEM imaging verifiedspatially segregated hexagonal sheets from each other based on their size and shape. The ratio of Mo to S resulting from EDS analysis in our case is 1:1.9, which is close to the stoichiometry of MoS_2. The synthesized MoS2 was employed for the photocatalytic degradation of the organic dye methylene blue (*MB*). The *MB* reduction efficiency was found to be the function of the spatial formation of MoS_2. Given this, we believe that the *RD* methodology offers a promising and environmentally friendly route to synthesize MoS_2, making it suitable for various applications in the field of material science.

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Synergistic impact of metal-surfactant catalyst pair in the oxidation of cyclic alcohol: Interfacial-Surface adsorption kinetic view

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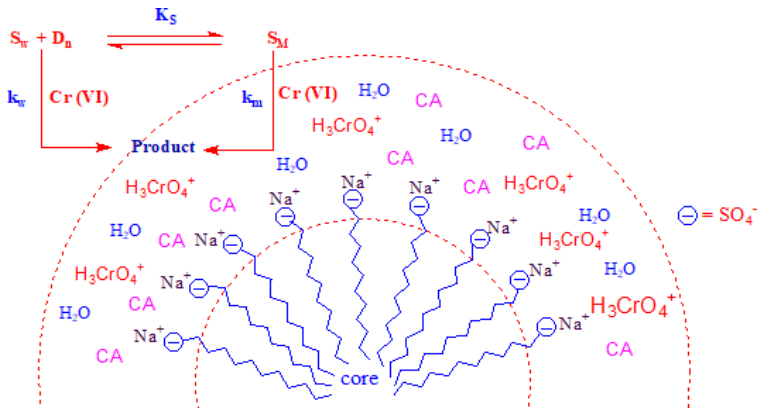
ABSTRACT

In view of the synthetic applications, oxidation of alcohols is considered as an important class of reaction [1]. Hexavalent chromium, Cr(VI) has been used extensively in its various forms as an oxidant to convert secondary alcohols to their respective ketones. To correlate the reactivity and conformation of cyclic alcohols (CA) and to study the influence of acidity of reaction conditions, the present work has been under taken. Recent reports on the oxidation reaction in presence of surfactants and micelles has opened new vistas in the field of electron transfer reactions [2]. The presence of surface-active agents containing a hydrophobic tail and a hydrophilic head group often brings acceleration of reactions. In the present work effort has been made to investigate the electron transfer mechanism of oxidation of cyclonols of importance by Ce(VI) in presence and absence of surfactant (Sodium lauryl sulphate, SLS) and develop a kinetic model. The progress of the reaction was monitored spectrophotometrically by measuring the fall in absorbance of Cr(VI) at its λ_{max}. The log(Absorbance) vs time plots indicates that the reaction exhibits a first order dependence with respect to Cr(VI). Unit order dependence of rate on [cyclonol], complex dependence on acid strength is what we observed. In presence of varying [SLS], rate marginally increases with increase in [SLS] until an optimum [SLS] which is around cmc and there after the rate decreases exponentially. In SDS medium partitioning of both the cationic Ce(IV) species and the substrate between water and micellar pseudo-phase is considered and accordingly Berezin model [3] (Scheme-I) is extended to explain the kinetic data.



(Scheme-1)

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I 024

Catalytic Insights into Methane Dry Reforming: Assessing the Influence ofNickel in Different Perovskite Environments

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ABSTRACT

Comprehending the physicochemical characteristics of catalysts is essential for establishing the "structure-activity/property" correlations, making it crucial for catalyst advancement and the elucidation of reaction mechanisms. In this study, we investigated nickel-based metal oxides, specifically perovskite $LaNiO_3$ and layered perovskite La_2NiO_4, for the first time in sustainable syngas synthesis via dry reforming of methane.Time-on-stream experiments revealed that the as-synthesized $LaNiO_3$ outperformed La_2NiO_4 initially. However, in the second time-on-stream experiment, the aged exhibited improved catalytic activity in CH_4 and CO_2 conversion and H_2/CO ratio beyond 800 °C. Furthermore, thermogravimetric analysis demonstrated insignificant coke formation over $LaNiO_3$ after 15h of time-on-stream testing. Detailed structural analysis unveiled the *in situ* formation of metallic Ni^0 during the reactions, which significantly influenced catalytic activity and was further substantiated by X-ray photoelectron spectroscopy. H_2 temperature-programmed reduction results strongly suggested that the greater reduction of Ni^{3+} to Ni^0 during dry methane reforming was a key factor contributing to the superior catalytic activity of $LaNiO_3$, even at lower temperatures compared to La_2NiO_4. In contrast, as-prepared La_2NiO_4, initially non-reducible in nature, exhibited poor catalytic activity but improved during the second time-on-stream experiment whena significant amount of Ni^0 was formed. *In situ* Fourier-transform infrared spectroscopy studies revealed the higher basicity of as-prepared $LaNiO_3$ compared to La_2NiO_4, enhancing CO_2 adsorption to a greater extent. This difference in reducibility, stemming from structural properties and availability of active basic sites, contributes to the distinct catalytic behaviors of both $LaNiO_3$ and La_2NiO_4.

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Multifunctional Fe_3O_4-Graphene Oxide-Ag-MoS_2 Composite Particles for Efficient Organic Dye Removal And Their Detection Using SERS

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ABSTRACT

Multifunctional nanomaterials can be engineered to possess a combination of different properties owing to which they find applications in different areas such as drug delivery, catalytic studies, imaging, optoelectronic devices, and magnetic storage. In particular, nanocomposites containing magnetic components have the advantage of external non-contact manipulation. In this work, we synthesize multifunctional magnetic-plasmonic composites with MoS_2 layer (Fe_3O_4@GO@Ag@MoS_2) and utilize them for efficient removal of organic dyes from aqueous solutions. The multifunctional particles were synthesized using the hydrothermal method. The samples were then characterized by using X-ray diffraction, Raman spectroscopy, UV-visible spectroscopy, SEM and a SQUID magnetometer. To demonstrate dye removal, we chose four different dyes including methylene blue (MB), methyl orange (MO), Malachite green (MG), Rhodamine 6G (R6G), and mixtures of these organic dyes in aqueous solutions. The removal of dyes by the adsorption process was monitored by UV-visible absorption spectrum of the dye in regular intervals after the addition of these as-prepared samples. All the experiments were carried out in the dark and at room temperature by stirring the dye magnetically after the addition of these samples. The adsorption kinetics and rate were then evaluated from the absorption measurements of the dye in the solution. Furthermore, we utilized surface-enhanced Raman scattering (SERS) to verify the dye removal. Here, aliquots of samples of the dye solution taken at two different times were taken after adding the multifunctional composite particles. They were mixed with gold nanoparticles and drop-casted onto a clean silicon substrate for Raman measurements at 785 nm. The results indicate efficient removal of the organic dyes from the aqueous solution. We believe that these composite magnetic-plasmonic materials are promising materials for environmental pollutant extraction applications.

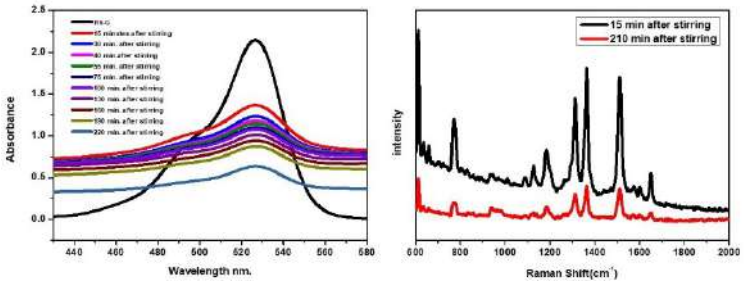

Figure: UV-Vis absorption spectra of R6G for various times after the addition of Fe_3O_4@GO@Ag@MoS_2 (left) and SERS spectra of solution samples collected after 15 min and 210 min.

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I 026

Synthesis and Applications of Ionic Liquids as a Catalyst and Solvent for Friedel Crafts Reactions And C-N Coupling Reactions

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ABSTRACT

Ionic liquids have emerged as versatile compounds with unique properties, making them promising candidates in various chemical processes. This study delves into the synthesis and multifaceted applications of ionic liquids as catalysts and solvents in key organic transformations, specifically acylation, alkylation, and C-N coupling reactions. By customizing the combination of cations and anions, ionic liquids can be tailored to exhibit specific characteristics that enhance their catalytic activity and solvation capabilities. The research investigates the impact of ionic liquid composition on reaction kinetics, selectivity, and overall efficiency in these crucial chemical processes. Through a comprehensive evaluation of various ionic liquid formulations, we aim to elucidate the optimal conditions for achieving enhanced catalytic performance and improved reaction yields. Furthermore, this study explores the potential of ionic liquids to facilitate environmentally sustainable practices in organic synthesis. Their non-oxidizing nature, stability, and ease of handling offer significant advantages over traditional solvents. This research endeavours to provide insights into the broader implications of employing ionic liquids in green chemistry initiatives. The outcomes of this study hold significant promise for advancing the field of catalysis and solvent design, with implications for a wide range of industrial applications. This research not only contributes to the fundamental understanding of ionic liquid behaviour but also underscores their pivotal role in sustainable and efficient chemical processes.

Keywords: *Ionic liquids, Catalyst, Solvent, Acylation, Alkylation, C-N coupling reactions, Green chemistry, Sustainable synthesis.*

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I 027

Removal of Arsenic Metal ions from Water using Salt assisted Chemically Exfoliated MoS_2 nanosheets

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ABSTRACT

The presence of highly toxic arsenic metal ions in drinking water even at low concentration is a very serious problem for human health. The utilization of nanomaterials with high adsorption capacities has created a possibility of removal of these ions. In present work, two dimensional MoS_2 nanosheets have been fabricated by systematic salt assisted exfoliation of bulk powder and tested for arsenic removal using various batch adsorption experiments. The synthesized nanomaterials were characterized using x-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), energy dispersive X-ray spectroscopy (EDS), Brunauer–Emmett–Teller (BET) and inductively coupled plasma mass spectrometry (ICP-MS) analysis. The interlayer spacing obtained from HRTEM analysis of exploited nanosheets is in good agreement interlayer planes spacing of the XRD analysis. The dependency of arsenic ions adsorbed by MoS_2 nanosheets on initial concentration, and adsorbent dosage were studied in detail. The obtained experimental data is statistically correlated with various adsorption isotherms and kinetic models. Our experimental results clearly reveal that 2D MoS_2 nanosheets could be used as effective adsorbents for the removal of arsenic ions from contaminated water.

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I 028

Biosynthesis of Reduced Graphene Oxide Nanocomposite Decorated with ZnS Nanospheres and its Enhanced Photocatalytic Activity

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ABSTRACT

The major part of the world consists of water. Water pollution happens when toxic substances enter water bodies that make the water unusable for drinking, cooking, cleaning, and other activities. The main issue of consumable water shortage in different regions of the world has stimulated the interest of researchers around the world in finding out novel, efficient and cost-effective means and techniques for the treatment of contaminated water. Motivated by these needs, here we report the bio synthesized Graphene Oxide Coupled ZnS Nanocomposite (GO-ZnS NCs), as applied to decontamination of water through Photocatalytic degradation. The high photocatalytic activity of these GO-ZnS NCs Photo Catalysts can degrade the pollutants in the contaminated water under UV and Visible light irradiation. The apparent rate constant of the catalytic reaction of contaminated water collected from the local area in the presence of GO-ZnS NCs is 0.011/min. 86 % of pollutants are degraded from the contaminated water because of excellent photo catalytic activity of GO-ZnS NCs under UV-light irradiation. 65 % of pollutants are degraded from the contaminated water under the illumination of visible light. It can be used to degrade the pollutants in real environmental samples. This study successfully demonstrated as a facile, sensitive, cost-effective method for the removal of toxic pollutants from the environment.

Fig.1 Preparation process of rGO

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I 029

MXene based Binary Nanocomposites for Effective Degradation of Antibiotics

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ABSTRACT

Water is the indispensable component for the survival of any life forms. However, owing to rapid development of industries and growing population, the water bodies are being polluted to greater extent. The contaminants include organic solvents, drugs, dyes, pesticides, fertilizers, large variety of organic intermediates, inorganic wastes, biological waste, medical wastes etc. Many of these wastes are highly toxic, carcinogenic, capable of spreading diseases, etc. There is a continuous quest for novel technology to treat this polluted water. However, several pros and cons associated with each technology. Photocatalytic treatment of water is promising technology that has the capability to treat wide variety of pollutants. Among various photocatalysts, recently, MXenes based photocatalyst are gaining limelight due to its outstanding properties. The current research work explores the synthesis, characterization and photocatalytic activity MXene/WO_3 binary nanocomposites. Mxene and WO_3 nanostructures were prepared distinctly by etching and hydrothermal method, respectively; whereas, binary nanocomposites is prepared using ultrasonication. The synthesized nanocomposites are characterized by X-ray diffraction analysis, Fourier transforms infrared spectroscopy, High resolution Scanning electron microscopy and Transmission electron microscopy. Optical properties were studied by UV–visible spectroscopy. The photocatalytic degradation efficiency was tested against tetracycline. The experimental results shows that the nanocomposites possess excellent degradation efficiency. It was also found that the composition of WO_3 has significant effect on photocatalytic of binary composites. Further, to have an insight into the photocatalytic activity, effect of various reaction parameters has been studied. Key species responsible for photodegradation of tetracycline is found by using radical trapping experiments. The synthesized catalyst possesses excellent stability and recyclability.

I 030

Synthesis of Fulevene-Based Ligands and Their Complexes for Investigating Diverse Applications

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ABSTRACT

This research endeavors to synthesize a series of fulevene-based ligands and their corresponding metal complexes, with the objective of exploring their multifaceted applications. Fulevene derivatives have garnered attention for their unique electronic properties and potential applications in various fields, including catalysis, materials science, and medicinal chemistry. The synthesis of these ligands involves a systematic approach, incorporating modifications to the fulevene backbone to fine-tune their electronic and steric properties. Subsequently, the resulting ligands are complexed with a variety of transition metals to generate a diverse set of coordination compounds. The study will comprehensively investigate the physicochemical properties, reactivity, and catalytic potential of these newly developed complexes. Additionally, their applications in areas such as homogeneous catalysis, luminescent materials, and biomedical sciences will be thoroughly examined. The research aims to provide valuable insights into the structure-property relationships of fulevene-based ligands and their complexes, paving the way for their tailored utilization in a range of cutting-edge applications.The outcomes of this study have the potential to significantly advance the field of coordinationchemistry and materials science, offering new avenues for the design of innovative materials and catalysts. Furthermore, the exploration of their applications in biomedical contexts holds promise for the development of novel therapeutics and diagnostics.

Keywords: *Fulevene, Ligands, Coordination Complexes, Catalysis, Materials Science, Medicinal Chemistry, Biomedical Applications, Structure-Property Relationships.*

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I 031

Efficient Adsorption Capacity of Hydrothermally Processed MoS_2 Nanoflower for Methylene Blue Dye Removal

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ABSTRACT

In this study, we explored the dye-adsorption capabilities of 2D transition metal dichalcogenide MoS_2 nanosheets. These nanoparticles were synthesized via a hydrothermal method at two different temperatures, 200°C (MS-200) and 220°C (MS-220). X-ray diffraction analysis confirmed the formation of hexagonal MoS_2 (2H-MoS_2), while Field Emission Scanning Electron Microscopy revealed their distinctive carnation flower-like morphology. The specific surface area was determined to be 9.290 m^2/g for MS-200 and 10.804 m^2/g for MS-220 using BET measurements. The synthesized nanoparticles were then evaluated for their ability to adsorb Methylene Blue (MB) dye, demonstrating adsorption rates of 94.45% for MS-200 and 96.40% for MS-220 within just 20 minutes. The study further explored the impact of contact time, adsorbent dosage, and initial dye concentration on the adsorption process. Results indicated that MS-220 nanosheets, synthesized at a higher temperature with a greater specific surface area, exhibited better performance in MB dye adsorption compared to MS-200. This suggests the potential of MS-220 for future research and practical applications in wastewater treatment as an effective MoS_2-based adsorbent.

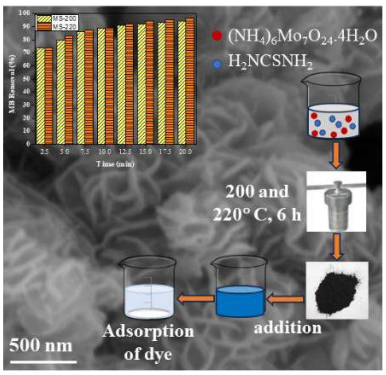

Fig. 1: FE-SEM image, synthesis steps, and bar diagram of MB dye removal percentage.

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I 032

A Novel Green Synthesis of Silver Nanoparticles for Photocatalytic and Antibacterial Activity

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Abstract

Green synthesis of AgNPs is carried out using the flower extract of Hibiscus vitifolius as the reducing agent and AgNO3 as the metal precursor. The color changes of the solution from yellow to reddish brown indicate the formation of AgNPs and are further confirmed by the characteristic SPR peak at 419 nm in UV-Vis spectroscopy. By comparing the FTIR spectrum of flower extract and AgNPs + flower extract, the shift in -OH peak and -C=C peaks suggests that polyhydroxy groups in the flower extract may have strong interactions with Ag ion during the AgNPs synthesis. Moreover, the capping behavior of flower extract imparts high stability to the synthesized AgNPs. The SEM analysis of AgNPs incorporated paper and chitosan beads reveals the particle size to be between 15 and 62 nm. XRD analysis of AgNPs incorporated paper showed four characteristic peaks at 38.1°, 46.1°, 64.5°and 77.3° corresponding to (111), (200), (220), and (311) planes for silver nanoparticles. The AgNPs incorporated paper shows excellent antimicrobial activity against Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Klebsiella pneumoniae. Besides, reduction of methylene blue dye is achieved by using AgNPs-coated chitosan beads. The concentration and pH studies show that 2 mg of AgNPs incorporated beads effectively reduce the 1.5 ppm methylene blue solution at pH 9.

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I 033

Synthesis of Mesoporous Ammonium Trivanadate ($NH_4V_3O_8$) Nanostructures for the Adsorption of Methylene Blue Dye

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ABSTRACT

In this work, we explored ammonium trivanadate ($NH_4V_3O_8$) nanomaterials for dye adsorption and analyzed their adsorption capacity considering the initial dye concentration as crucial parameter of adsorption. Hydrated $NH_4V_3O_8$ porous web-cage and $NH_4V_3O_8$ Niagara maple-like nanostructures (NSs) were synthesized via sol method with varying acidic strength at pH (1, 3, and 5) named as NVO-1, NVO-3, and NVO-5 samples. The structural, optical and morphological properties were investigated using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, UV-Vis spectroscopy (UV-Vis),Thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), Zeta(ζ) Potential, Field Emission Scanning Electron Microscopy (FESEM) and High Resolution Transmission Electron Microscope(HRTEM). It is evident that the variation in the pH, during synthesis has a significant impact on the crystallinity, surface charge, surface area, pore size, and morphological properties. To investigate the rate-controlling step and understand the adsorption mechanism, a number of kinetic models, including pseudo-first-order (PFO), pseudo-second-order (PSO), and intra-particle diffusion (IPD), and isotherm models such as Langmuir and Freundlich adsorption isotherm models were fitted to the experimental data. We found that the NVO-3 sample offers the higher adsorption capacity for initial dye concentration varied from 20mg/L to 500mg/L, with 90% removal efficiency within 5 minutes which is attributed due to strong electrostatic interaction with Methylene Blue (MB) dye as indicated by kinetic and isotherm study. On the other hand, NVO-1 sample offers best removal efficiency of around 99% (at 20mg/L) with good recyclability.

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I 034

Effect of Nb Doping on Structural And Spectral Studies of $SrTiO_3$

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Abstract:

$SrTiO_3$ is a perovskite oxide material with promising thermoelectric characteristics due to electronic band structure[1]. In this research, Nb doping was introduced to enhance the thermoelectric performance of $SrTiO_3$ with the formula $SrTi_{1-x}Nb_xO_3$ where x=0, 0.01, 0.02, 0.03 and 0.04. The compounds were prepared through solid state method. The experimental approach included X- ray diffraction (XRD) analysis to investigate structural changes in the material and understand the impact of Nb doping on the crystal lattice. XRD confirms the single phase of the compounds with the Cubic structure[2]. The obtained crystallite sizes are slightly decreases, the $Nb_{0.04}$ dopant value was increased compared to $Nb_{0.01}$. Ultraviolet-visible (UV-Vis) spectroscopy was utilized to assess the optical properties, including the modification of the material's band gap energy due to Nb incorporation. With the increase in Nb doping, the energy gap values are found to decrease. Fourier-transform infrared spectroscopy (FTIR) was employed to examine vibrational modes and chemical bonding in the doped SrTiO3, offering insights into the alterations in chemical structure induced by Nb doping. Raman spectroscopy complemented the analysis by providing information on lattice vibrations and crystal symmetry within the doped samples. The obtained Raman modes are well matching with the literature and the shifting of modes indicate the effect of Nb doping.

Keywords: *$SrTiO_3$, Nb-doped, X ray diffraction, Ultraviolet visible,*

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I 035

Solvothermal Synthesis of $Cu_{(1-x)}Zn_xBi_2O_4$ Nanostructures for Effective Degradation of Organic Dyes

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ABSTRACT

Due to rapid industrialization, environmental pollution is increasing day-by-day. Large quantities of pollutants are continuously discharged into water bodies which pose a serious threat to human and aquatic life. Photocatalytic technology provides an eco-friendly technique to deal with this issue which has led to intensive research in this field. Several strategies have been followed to achieve high photocatalytic efficiency, but some of them are expensive and non-renewable. Therefore, an inexpensive and easily prepare able catalyst is required to utilize solar energy effectively at a large-scale implementation of photocatalytic technology. In the present study, $Cu_{(1-x)}Zn_xBi_2O_4$ complex metal oxide nanostructures were synthesized by Solvothermal method and evaluated its photocatalytic activity under 50W LED. The concentration of Zn varied from x=o to x=1 (i.e.), the synthesized nanostructures range from pure $CuBi_2O_4$ to pure $ZnBi_2O_4$ nanostructures. The synthesized nanostructures were characterized by X-ray diffraction and UV-Vis spectroscopy and scanning electron microscopy. The electrochemical studies were performed using EIS and the photocatalytic degradation efficiency was tested against Rhodamine B. The photocatalyst, $Cu_{0.4}Zn_{0.6}Bi_2O_4$ exhibits best degradation efficiency in comparison with other catalyst and it degrades 59.9% RhB in 150 min under 50 Watts LED light, whereas, under the same condition, bare $CuBi_2O_4$ and $ZnBi_2O_4$ degrades 9.73% and 13.22% RhB, respectively. To have an insight into photocatalytic performance of catalyst, radical trapping experiments and kinetics studies were performed. All the nanostructures follow pseudo-first order kinetics. Overall, the current study displays a feasible and effective strategy to improve the photocatalytic performance of $CuBi_2O_4$ and $ZnBi_2O_4$ by modifying the extend of charge carrier separation.

I 036

2D MoS_2 layers: Outstanding candidate for Environmental Monitoring and Energy Harvesting

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ABSTRACT

The need of the hour is to explore new semiconducting materials which can perform at sub 10 nm regime with device performance. In the last decade, there has been significant research carried out on the layered structure (2D) materials where individual layers of covalently bonded atom/molecules are held together by van der Wal forces in out of plane direction such that layer by layer disintegration is achievable with ease. Out of known 2D materials, MoS_2 is the most prevalent and widely explored material for various application. It possesses an indirect band gap of 1.2 eV in its bulk form and become direct band gap (1.9 eV) semiconductor in its monolayer form due to quantum confinement effect. Since the invention of graphene and related quest of growing different 2D materials, one of the fundamental difficulties is to grow high quality 2D materials which can be used for realizing functional devices keeping scalability issues intact. To be realized in real applications at industrial scale, scalable synthesis method to grow high quality layered materials need to be adopted. Pulsed laser deposition (PLD) is a powerful bottom-up technique which is highly promising for growing stoichiometric and continuous 2D materials with great controllability. MoS_2 monolayers are grown using PLD technique. Different contact electrodes (Platinum (Pt)/Titanium (Ti), Silver (Ag)/Gold (Au) and Indium Titanium oxide (ITO)) are exploited with MoS_2 layers for the fabrication of efficient UV photodetectors. Power dependent experiment showed linear dependence of photocurrent values with varying power density suggesting that the photocurrent of the photodetector device is majorly attributed to the electron-hole pair generation upon light illumination rather than the trap centers. For the demonstration of FETs using MoS_2 layer as semiconducting channel, various metal contacts were deposited over the surface of trilayer MoS_2. To demonstrate the efficacy of optimized FET geometry, NO_2 gas sensor based on 90 nm thin Si_3N_4 as gate dielectric and Au/Ag (50/50 nm) as source drain contact and different number of MoS_2 layers as semiconducting channel were employed. Fabricated FET based gas sensor showed the sensing response of 59.4% towards 10 ppm concentration of NO_2 gas and limit of detection (LOD) of 1 ppm. Finally, optimized MoS_2 layers were also exploited for triboelectric energy harvesting applications based on motion of NaCl droplet on its surface. High voltage generations using monolayer MoS_2 nanogenerators and division of output voltage with increase in MoS_2 thickness are explained using equivalent circuit diagrams.

I 037

Unlocking the Potential: Advanced Thermoelectric Materials with Ca and Mn-doped $SrTiO_3$

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ABSTRACT

This study explores the fascinating world of advanced thermoelectric materials by investigating the impact of doping $SrTiO_3$ with calcium (Ca) and manganese (Mn) [1]. This research focuses on the intriguing realm of compound doping in $SrTiO_3$. In the pursuit of advanced thermoelectric materials, we investigated for $Sr_{1-x}Ca_xTi_{1-y}Mn_yO_3$ (x=0, 0.01, 0.02, 0.03 and 0.04) perovskite crystalline samples synthesized by solid state reaction method. The compounds were prepared through solid state reaction method. The X-ray diffraction results confirmed the single-phase cubic structure of the compounds [2]. The lattice parameters are calculated from Rietveld refinement method using Fullprof software. SEM images confirmed the dense structure of the compounds and EDX showed all the doped elements as per the composition. Three major Raman modes were observed in the room temperature Raman spectra of the compounds. The first one is located at 250-420 cm^{-1}, the second is situated in the 605-720 cm^{-1} range, and the third and smallest one is centered at 1020 cm^{-1}. Raman experiments provide evidence of the structural transformation in the doped compounds. Detailed analysis and origin of the modes are discussed in this work.

Key words: *$SrTiO_3$, Thermoelectric materials, X-Ray Diffraction, Raman Spectroscopy*.

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I 038

Mechanochemical Synthesis of MoS_2 Nanoparticles for Enhanced Photocatalytic Activity

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ABSTRACT

In this study, we present a novel approach to synthesize MoS_2 nanostructures through a grinding-sonication process, highlighting their remarkable potential as efficient photocatalysts. The synthesis method is cost-effective, environmentally friendly, and offers precise control over the nanostructure morphology. Structural characterization is carried out via X-ray diffraction (XRD), Scanning electron microscopy (SEM), UV-visible spectroscopy (UV-Vis), and infrared spectroscopy (IR). XRD analysis confirmed the formation of MoS_2 Nanoparticles. Our results demonstrate a substantial enhancement in photocatalytic activity compared to bulk MoS_2, which is attributed to the increased surface area and improved charge carrier separation achieved through the nano structuring process. The experiments for the photocatalytic degradation of Methylene Blue and Rhodamine B were carried out in sunlight, which gave degradation of 99.5 % and 99.8 % respectively.

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I 039

Study of Inorganic Minerals as Sustainable Flame Retardants for Leather

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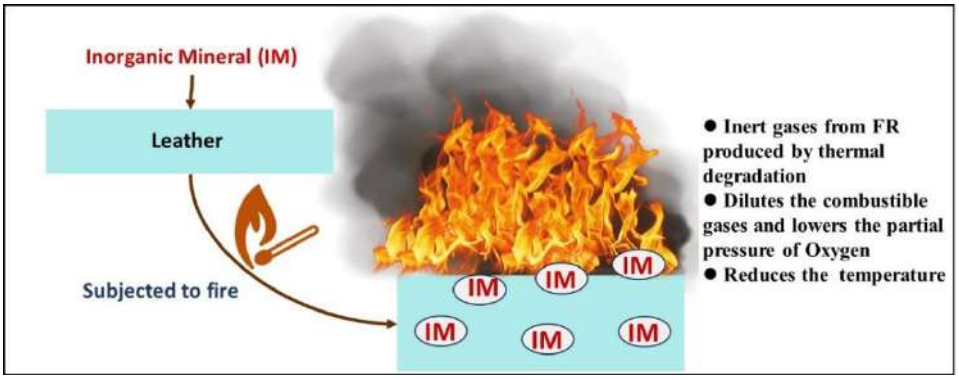
ABSTRACT

Leathers are natural fibrous materials widely used for making consumer articles/goods such as footwear, protective garments, fashion garments, upholstery, handbags, etc. Leather used in certain consumer products should pass the flame retardancy standard. Therefore, to enhance the flame retardancy of leathers, flame retardant (FR) chemicals are used during leather making or during finishing. Most of the FR chemicals available in the market are toxic in nature or generate toxic fumes on burning. In order to develop eco-friendly FR chemicals for leather, inorganic minerals (IM) such as Antimony pentoxide (SBO), aluminium hydroxide (AH), Mg-Al layered double hydroxide (MAH)), Mg-Al mixed metal oxide, ammonium polyphosphate (APP), and magnesium hydroxide (MH), have been studied in detail for their FR potential. The selected IMs were characterized by XRD, FT-IR, TGA, and DSC [1,2]. The preliminary FR activity of the IMs was assessed from the DSC thermogram, where an endothermic enthalpy change (ΔH) and a high ΔH value indicated the flame-retardant ability of the IM. The selected IMs were applied to leather (3% w/w of leather) during post-tanning operation and the flame retardancy was studied by horizontal flame retardancy test (ISO 17074) [3]. The flame-off time (FOT), smoke-off time (SOT), percentage weight loss, and flammability degree (FD) of the IM-treated leathers were recorded. The flammability degree of leather was improved by 13%, 17%, 12%, 4%, 4%, and 3% when treated with SBO, AH, MAH, MAO, APP, and MH, respectively. The present study indicated that aluminium hydroxide (AH) is the most potential flame retardant for leather.



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I 040

Enhancement Photoactivity of Sm-doped CuO Nanostructures toward Degradation of Organic Pollutant Under Solar Light Irradiation

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Abstract:

In this work, the influence of doped Samarium (Sm3+) metal ions on the structural, morphological, magnetic and photocatalytic activities of copper oxide (CuO) was investigated. A series of CuO, and Sm-doped CuO moieties were prepared in a facile hydrothermal manner. It was found that Sm^{3+} ions were effectively doped into the host CuO, and the photocatalytic performance of the Sm-doped CuO photocatalyst was significantly improved compared to pure CuO. The developed photocatalytic activity of Sm-doped CuO could be attributed to the natural absorption of sunlight and the effective charge separation of photoinduced electrons and holes. In addition, the probable photocatalytic mechanism of Sm-doped CuO nanostructures was also proposed. The resulting catalyst was extensively characterized using various techniques. The morphology and surface-dependent photocatalytic degradation of RhB and ciprofloxacin were studied under visible light irradiation. This work attempts to improve an efficient photocatalyst for the degradation of environmental pollutants.

Keywords: *Copper oxide, Nanostructure, Ciprofloxacin, Rhodamine B, Photocatalyst.*

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I 041

Visible-light-driven Efficient Catalyst of $LaCoO_3/NiS_2$ Nanocomposite as Reusable Photocatalyst for Removal of Organic dye Pollutants

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ABSTRACT

In recent decades, air and water pollution from organic dyes has become a serious problem due to their high toxicity. The removal of these organic dyes from polluted waters is a serious environmental problem, and the development of new advanced photocatalytic materials to decompose organic dyes can be a good solution. In this work, perovskite/layered nickel disulfide ($LaCoO_3/NiS_2$) nanocomposites with different NiS_2 content were synthesized by a one-step hydrothermal process. The X-ray diffraction pattern shows the rhombohedral and cubic crystal structure of $LaCoO_3$ and NiS_2, respectively. The morphological analysis confirms the formation of $LaCoO_3/NiS_2$ nanoparticle over the nanosheets. The elemental composition of the samples was determined using XPS, which shows a significant interaction between NiS_2 and $LaCoO_3$. The photocatalytic performance of $LaCoO_3/NiS_2$ nanocomposites was investigated by the antibiotic degradation of tetracycline (TC) and methylene blue (MB) dye. This work attempts to develop an efficient photocatalyst for the degradation of environmental pollutants and the possibilities of its application in wastewater treatment plants of the textile dyeing industry.

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I 042

Structural Analysis of Titanium Dioxide (TiO_2) Nanoparticles Prepared Via Chemical Route for Wastewater Management

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ABSTRACT

The utilization of sol-gel techniques has been explored in the preparation and application of titanium dioxide (TiO_2) in salinity and wastewater treatment processes. Scanning electron microscope (SEM) micrographs revealed the presence of TiO_2 nanoparticles (NPs) in a homogeneously dispersed state, exhibiting spherical forms. Furthermore, it was noted that the size of these nanoparticles decreases as the ageing period rises from 40 minutes to 60 minutes. The SEM graphs of nano powder with high transparency reveal their detectability in the visible spectrum. Furthermore, it is observed that the nano powder exhibits a shift in their highest wavelength as the period of ageing increases. This shift can be attributed to the improvement in the quality of water. Also, the nano sheet that was produced has an energy band gap exhibiting a reduction in width as the duration of ageing has been extended. This phenomenon can be attributed to the observed red shifting of the edges of the absorption spectrum within the nanosheet. The examination of the deposited NPs has been conducted to validate the presence of both anatase and rutile phases in the liquid state. The conclusions of the present study enabled us to ascertain the overall magnitude of the intensity. This study suggests that the utilization of photo degradation using a solar absorber could have significant implications in the fields of salinity and wastewater treatment.

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I 043

Tri-metallic Co/Zn/Ni-ZIF Mediated Synthesis of Nitrogen-doped S-scheme Heterostructure for the Detection and Photocatalytic Removal of Persistent Pollutants

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ABSTRACT

Transition metal oxides can be improved in their optoelectronic properties through various methods such as heteroatom doping, heterojunction creation, and defect engineering. To create durable and versatile materials, it is essential to develop a synthetic technique that unifies these different strategies. In this view, a bi-functional N-doped Co_3O_4/ZnO/NiO p-n heterostructure was formed, by calcining tri-metallic Zeolitic Imidazolate Framework (Co/Zn/Ni-ZIF). The high-temperature calcination of tri-metallic ZIF (600 $^{\circ}$C) resulted in the production of homogenously mixed metal oxides with abundant oxygen vacancies in the lattice. Furthermore, nitrogen substitution defects and zinc broken bonds were also confirmed in the semiconductor lattice through XPS investigations. UV-vis DRS testing was used to examine the opto-electronic characteristics of the materials. The prepared heterostructure exhibited enhanced photocatalytic degradation of doxorubicin (90%) and chlorpyrifos (80.5%) within just 120 minutes of visible light illumination, without the use of co-oxidants. Additionally, a detailed discussion of the proposed mechanistic pathway of photocatalytic degradation through the generation of reactive oxygen species has been presented. Besides photocatalysis, the fluorescent property of this bi-functional nanomaterial was also utilized for selective fluorescence sensing of doxorubicin, Cr^{6+} and chlorpyrifos. The proposed sensor displayed an extremely low detection limit, with values of 0.60 µM (doxorubicin), 5.01 µM (Cr^{6+}) and 15.4 µM (chlorpyrifos). The viability of the proposed sensor was further confirmed by real sample analysis.

I 044

Synthesis of mesoporous TiO_2 doped with La^{3+} for electrochemical sensor application

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ABSTRACT

This research presents the synthesis results using the hydrothermal method of mesoporous TiO_2 nanoparticles doped with La^{3+} ions at concentrations of 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, and 1.0. %. Several characterizations carried out were SEM, TGA, FT-IR, DRS, XRD, and ICP-OES. The goal was to detect the doping effect of La^{3+} on the parameters of optoelectronics, microstructural, and structural properties. The doping material was used to make a film on the conductive glass electrodes using the screen-printing method. The electrochemical characterization was done using the redox complex $[Fe(CN)_6]^{3-/4}$, with the modified electrodes with mesoporous TiO_2 at different doping concentrations in a three-electrode cell. The nitrobenzene (NB) sensor activity was tested in a 0.1 M Na_2SO_4 solution, where the TiO_2 film thickness was studied. An improvement in the detection was associated with an increase in the doping concentration of La^{3+}, improving the sensitivity up to 144.2 nA/ppm NB.

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I 045

Functionalized Biomass Derived Carbon Quantum Dots for Water Treatment

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ABSTRACT

Carbon quantum dots (CQDs) are amorphous nanoparticles that are exceedingly small and have excellent luminescence. The thermochemical conversion of biomass produces biochar, which is a green and sustainable starting point for the synthesis of various functional carbon compounds in anticipation of innovative applications. Either directly from the biomass or following physical and chemical activation of the biochar are followed . They differ in size from graphene oxide because they are quasi-spherical nanoparticles with a diameter of less than 10 nm. X-ray diffraction (XRD), Energy-dispersive X-ray spectroscopy (EDX), BET surface area, Raman spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM) was used to study CDs-nanocomposite. The naturally flexible physiochemical properties of these adaptable materials are extensively exploited for water treatment in the construction of membranes. One of the greatest ways to increase porosity nature while maintaining recyclability is to combine porous sheet materials with carbon quantum dots materials.

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I 046

Synthesis and Characterization of Poly (Glycidyl methacrylate)/Graphene oxide Nanocomposite for the removal of Rhodamine B – Adsorption and Toxicity Studies

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ABSTRACT

In this study, poly(glycidyl methacrylate)/Graphene Oxide (P-GO) nanocomposite was prepared by modified blending technique and used as an effective adsorbent for the removal of Rhodamine B (Rh B). The prepared P-GO was characterized by using Fourier Transform Infrared spectroscopy (FT-IR), X-ray Diffraction studies (XRD), Thermogravimetric analysis (TGA), Raman spectroscopy, scanning electron microscope (FE-SEM), energy-dispersive X-ray spectroscopy (EDAX) and transmission electron microscope (HR-TEM), to analyze the structure, thermal, morphology and composition of resulting material. The effects of pH, contact time, adsorbent dosage, temperature and dye concentration on the adsorbent for the adsorption of Rh B was studied. Pseudo-first-order and pseudo-second-order kinetic model were used to describe the adsorption process. Similarly, Langmuir, Freundlich and Temkin adsorption isotherm models were studied. The P-GO presents a promising solution for the removal of Rh B from wastewater due to its outstanding adsorption efficiency and rapid kinetics. This study not only contributes to the development of efficient dye removal materials but also offers a sustainable approach to address the growing concern of dye-contaminated effluents in various industries. The findings highlight the potential of P-GO as a cost-effective and eco-friendly adsorbent for the remediation of dye-polluted waters. The cytotoxicity assay of P-GO and dyes were studied using zebrafish gill cell lines by morphological alteration and cell survival. The dyes were treated and the secondary samples were also studied using *DrG* cell lines.

Keywords: *Adsorption, Polymer nanocomposite, Wastewater Treatment, Toxicity.*

Corrosion protection performance of Poly(PyM-co-GMA)/Graphene Nanocomposite coating on Mild Steel

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Abstract:

Corrosion of metal is a burning issue due to huge global economic and environmental concern. To overcome this, several researchers are working in designing and development of new materials as anticorrosive materials. Designing of a hybrid coating to improve the anticorrosive property and stability, attracts significant research interest in materials science. New hybrid polymeric materials that are non–toxic, bio–safe and ecofriendly are of high significance as protective coating in corrosion research. In the present work functional polymer Poly(PyM-co-GMA) was synthesized by free radical solution polymerization and the carbon based nanofillers were incorporated in the functional polymer to yield polymer hybrid material for anticorrosive application. The Poly(PyM-co-GMA) was structurally characterized using FTIR and XRD studies. The morphological changes were observed using FESEM and HRTEM. The Poly(PyM-co-GMA) and its nanocomposites were coated on Mild Steel (MS) substrates and their anticorrosive properties were analyzed by using Potentiodynamic Polarization and Impedance studies in 3.5% (wt/v) NaCl medium. The resultant hybrid material acts as a potential candidate in reducing corrosion rate even against stringent environment.

Keywords: *Polymers; Nanocomposite; Anticorrosion; EIS; Tafel plot.*

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I 048

Preparation of Reusable CuO-gC_3N_4 Nanoparticles Immobilized onto Calcium Alginate Beads for the Removal of Dyes

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ABSTRACT

The growing environmental concerns associated with the discharge of synthetic dyes into water bodies necessitate the development of efficient and sustainable material for their removal. In this study, we present a novel material for the removal of Methylene Blue (MB) using CuO-gC_3N_4 nanoparticles immobilized onto calcium alginate beads. The CuO-gC_3N_4/alginate composite beads were synthesized by a simple and cost-effective co-precipitation followed by deposition method. The resulting material possesses a unique porous structure favorable for enhanced the removal of dyes. The synthesized CuO-gC_3N_4 /alginate beads were characterized using various techniques, including Fourier-transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), scanning electron microscopy (SEM), confirming the successful formation of the composite. The effects of pH, contact time, adsorbent dosage, temperature and dye concentration on the adsorbent for the adsorption of methylene blue (MB) was studied. Pseudo-first-order and pseudo-second-order kinetic model were used to describe the adsorption process. Similarly, Langmuir, Freundlich and Temkin adsorption isotherm models were studied. The CuO-gC_3N_4/alginate composite beads not only used as an adsorbent but also facilitated the separation and recovery of the adsorbent over multiple cycles, making it a cost effective, sustainable and practical solution for wastewater treatment. This study provides valuable insights into the development of sustainable and reusable photocatalytic materials for the efficient degradation of organic pollutants and environmental remediation, aligning with global sustainability and pollution mitigation objectives.

Keywords: *Adsorption, Alginate, Kinetics, Wastewater Treatment.*

I 049

Wastewater Treatment Using Layered Double Hydroxide Nanocomposites and their Oxides

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ABSTRACT

Recently, Layered Double Hydroxides (LDH) and their calcined derivatives Layered Double Oxides (LDO) act as classic functional nanomaterials for removing different toxic materials from wastewater (1). LDH, which is also called anionic clay material or hydrotalcite is made of plate/sheet-like structures. These materials have a large surface area, unique crystallinity and porosity with good anion exchangeability which act as cheap and non-toxic materials for a wide variety of applications. Dyes are used in different industries such as textiles, leather, paper, printing etc. in order to colour their products. These dyes are toxic in nature, carcinogenic and mutagenic which affect human beings and aquatic species. Though various physical, chemical and biological methods are available to remove these dyes from wastewater, adsorption appears to be the most powerful technique due to its cost-effectiveness, simplicity and reusability (2-5). Herein, we synthesized flower-shaped Mg-Al Layered Double Hydroxides using the hydrothermal method and their oxides by the calcination process. These nanomaterials were characterized using SEM, XRD and FT-IR. Their specific surface area, pore size distribution and their thermal analysis have been studied. The fabricated nanomaterials are tested for the adsorption of dyes from wastewater. The adsorption behaviour of the materials was studied by varying different parameters such as the effect of contact time, temperature, pH, ionic strength, initial dye concentration and adsorbent dosage. The nanomaterial showed high adsorption capacity and fast adsorption kinetics towards methyl orange dye. LDO exhibited higher adsorption capacity over LDH within a short contact time. Moreover, the adsorption mechanism, kinetics and isotherms are also studied. Thus, these materials can act as promising adsorbents for the treatment of dyes from wastewater.

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I 050

Investigation of Optoelectronic and Gas Sensing behavior of CdO thin films as a function of Pb doping concentrations in final spray solution

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ABSTRACT

Cadmium oxide (CdO) and Lead (Pb) doped cadmium oxide thin films were deposited on microscopic glass substrates at 300°C by a homemade spray pyrolysis experimental setup. The deposited films were characterized for their structural, microstructural, optical and electrical properties. X-ray diffraction (XRD) characterization of CdO and Pb- doped CdO thin films reveal that films are of cubic crystal structure with Fm-3m space group (#225) on matching with the standard CdO. The intensity of the peak and crystalline size are improved by Pb- dopant concentration. The surface microstructures obtained from field emission scanning electron microscopy (FE-SEM) analysis revealed the information about the surface smoothness and micro morphology of CdO and Pb- doped CdO thin films. The XPS measurement shows the presence of Cd, O, C and Pb element and confirms that Pb-doped CdO thin films are Cd-rich. An excellent transmittance (ranging 72 – 86%) in the visible and NIR region and optical band gap energy values vary between 2.39 eV and 2.50 eV, depending on the Pb- doping concentration. The improved carrier mobility is (69 cm^2 / V·s - 86 cm^2/V·s) obtained for 0.25 wt. % of Pb- doped CdO thin films. The obtained result from the present work proved to select Pb as dopant to achieve the high mobility with good optical transparence for optoelectronic application in particular, as the window layer in solar cells.

Key words: *Spray pyrolysis coating; CdO; thin film; optical transmittance; carrier mobility; surface morphology*.

I 051

Effect of Ni^{2+} substitutions in $ZnWO_4$ phase for photocatalyst degradation of hazardous dye under natural sunlight

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ABSTRACT

Rapid industrialization has led to the contamination of water bodies due to the release of untreated water, which threatens the ecosystem due to its carcinogenic nature. The need for photocatalytic semiconductor technology to transform hazardous and organic pollutants into non-toxic products has increased. Here, we report improved heterogeneous photocatalysis activity of the Ni^{2+} substituted $ZnWO_4$ in rhodamine B (RhB) degradation due to the piezoelectric effect. Analytical techniques such as X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and UV-vis spectroscopy were carried out—photoelectrochemical activities to measure photocurrent density and electrochemical impendence response. The catalytic characteristics of the Ni^{2+} substituted $ZnWO_4$ were investigated by degrading RhB using sunlight. According to the findings, the 7% Ni^{2+} substituted catalyst exhibits better photocatalytic efficiency than pure $ZnWO_4$, with an apparent rate constant of 0.012657 min^{-1}. As the concentration of Ni^{2+} substitution rises, defects increase, stability and adsorption efficiency are improved, the charge transfer process is speed up, and the photocatalytic activity is effectively increased, Furthermore Ni^{2+} substitutions improve electronic conductivity and enhance photocatalytic activities.

Keywords: *$ZnWO_4$; visible light degradation; Co-Precipitation; Rhodamine B; Photocatalysts*

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I 052

An Environment-friendly $Na_{0.4}K_{0.1}Bi_{0.5}TiO_3$ Ceramic for One-to-One Replacement of PZT-based Ceramics in Multiple Applications

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ABSTRACT

The availability of advanced materials has enabled the development of new gadgets for household appliances, automobiles, and strategic/smart devices. In the race for such developments intertwined with commercial gains, toxicity of the component elements and resultant materials became secondary. One such successful example is the advent of Pb-based piezoelectric materials with its inherent toxicity effect on humans and the environment. In the functionality of inter-converting mechanical and electrical energy, commercially established piezoelectric materials like PZT address a wide range of applications, such as actuators, sensors, and transducer devices. Significant efforts have been directed in recent times towards eliminating lead from piezoelectric ceramics. However, to date, the best lead-free piezo ceramics synthesized in the research laboratories have not yielded compositions with useful piezoelectric properties so that they may readily replace the well-established commercial compositions of PZT. Thus, the problem of Pb pollution during fabrication, use and burial lingers on. In the present work, our efforts are focused on developing Pb-free piezoelectric material with properties matching closely with that of PZT and identifying the figure of merit for non-resonant applications similar to that of a PZT composition, for a direct and easy replacement of lead-based elements in existing devices, without entailing any other design changes and fabrication protocols. We have successfully demonstrated such one-to-one replacement in spark igniter and piezo buzzer devices.

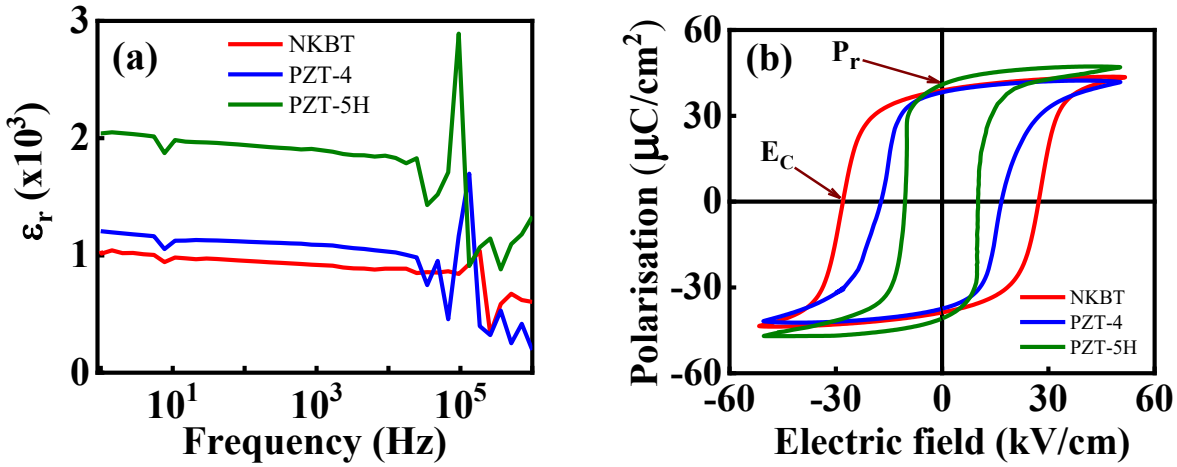

Figure 1. Comparison of room temperature data, (a) Dielectric constant; (b) PE hysteresis loops of NKBT, PZT-4 and PZT-5H ceramics.

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Synergistic powers of $ZnMoO_4$-g-C_3N_4: Unveiling a High-Performance novel nanocomposite photocatalyst for tackling antibiotic pollution

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ABSTRACT

This study investigated the potential of a $ZnMoO_4$ based g-C_3N_4 nanocomposite as a photocatalyst for the degradation of pharmaceutical pollutant - Amoxicillin (AXN) in waterbodies. The nanocomposite was synthesized and characterized using various techniques, including X-ray diffraction (XRD), high resolution scanning electron microscopy (HRSEM), X-ray photoelectron spectroscopy (XPS), photoelectrochemical, UV-visible spectroscopy and photoluminescence spectroscopy. The results indicated that the ZnMoO4 (ZMO) nanoparticles were uniformly dispersed on the g-C_3N_4 (gCN) sheets, and the nanocomposite exhibited enhanced photocatalytic activity compared to pure $ZnMoO_4$ or g-C_3N_4. This enhanced activity was attributed to the formation of a heterojunction between $ZnMoO_4$ and g-C_3N_4, which facilitated the separation of photogenerated electron-hole pairs, which was confirmed through the photoluminescence (PL) and photoelectrochemical studies (aimed at slowing down the recombination of these excited charges). The degradation of AXN followed pseudo-first-order kinetics, with the rate constant being significantly higher for the ZMO/gCN nanocomposite than for pure $ZnMoO_4$. The main active species involved in the photocatalytic degradation were hydroxyl radicals and superoxide radicals. Overall, the $ZnMoO_4$ based g-C_3N_4 nanocomposite demonstrated promising potential as a photocatalyst for AXN degradation in wastewater treatment applications.

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I 054

Chitosan-Crosslinked/Biochar Coupled Perovskite $BiFeO_3$ for Environmental Applications: A Comprehensive Study

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ABSTRACT

The growing demand for sustainable and efficient environmental remediation technologies has fueled research into advanced materials with multifunctional capabilities. This work unveils a novel approach involving the synthesis and characterization of Chitosan-Crosslinked/biochar-coupled perovskite $BiFeO_3$ for diverse environmental applications. The study employs a comprehensive set of analytical techniques, including X-ray diffraction (XRD), Rietveld refinement, Fourier-transform infrared spectroscopy (FTIR), high-resolution transmission electron microscopy (HRTEM), photoluminescence (PL), and explores its efficacy in dye degradation and heavy metal sensing. XRD and Rietveld analysis provide insights into the crystal structure, phase purity, and crystallite size of the synthesized material. The integration of chitosan and biochar into the perovskite structure is investigated using FTIR, elucidating the molecular interactions and chemical bonding within the composite. HRTEM imaging offers a detailed examination of the morphology and nanoscale features, providing crucial information for understanding the material's catalytic and sensing properties. The study delves into the photoluminescence properties of the Chitosan-Crosslinked/Biochar coupled perovskite $BiFeO_3$, shedding light on its electronic structure and potential applications in optoelectronic devices. Furthermore, the material's performance in dye degradation is evaluated, showcasing its potential as an efficient catalyst for environmental remediation. The conference presentation also highlights the heavy metal sensing capabilities of the developed material, emphasizing its utility in detecting and monitoring environmental pollutants. The integration of chitosan and biochar not only enhances the material's adsorption capacity but also contributes to its eco-friendly and sustainable nature. This multidisciplinary study bridges the gap between materials science and environmental engineering, presenting a promising avenue for the development of sustainable technologies for water treatment, pollution control, and environmental monitoring. The findings underscore the potential of Chitosan-Crosslinked/biochar-coupled perovskite BiFeO3 as a versatile and effective solution for addressing contemporary environmental challenges.

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I 055

Effectiveness of recovered Struvite ($MgNH_4PO_4.6H_2O$) from wastewater as fertilizer in the form of microcapsules, Struvite @alg-RHA

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ABSTRACT

Struvite, magnesium ammonium phosphate ($MgNH_4PO_4.6H_2O$), an alternative to rock phosphate-based fertilizer, has garnered considerable attention due to its production from N, P-rich wastewater. A single-step chemical precipitation of NH_4^+, PO_4^{3-} ions in domestic wastewater was carried out in a batch reactor at $Mg:NH_4:PO_4$ (1:1:1) in an optimized pH. Despite its notable fertilizing efficacy, powdered struvite exhibits a propensity to erode when in contact with soil, limit the nutrient availability. In view of this, the present study addresses this challenge by employing alginate, a biopolymer fortified with biomass, Rice Husk Ash (RHA), for the production of struvite micro beads. P release mostly influenced by the swelling of the microcapsule followed by breaking of the shell. Hence swelling study conducted and found that Struvite@alginate is harder, whereas the addition of RHA improved to 28-30% in the duration of 8-10 h. Furthermore P release kinetics results under different pH conditions in both water and soil environments revealed its slow rate of release and maximize to 98% for a study period of 30 days. By this way, it is very cost-effective, or otherwise amending of fertilizer is required twice a month to manage the P requirement.Successful encapsulation conformed from morphological images collected from High-Resolution Scanning Electron Microscopy (HR-SEM) with Energy-Dispersive X-ray Spectroscopy (EDS). Phase purity of struvite asserted from Powder X-ray diffraction and Fourier Transform Infrared Spectroscopy (FT-IR) data. The unaltered spectra of struvite in powder and beads conforming the physical interaction of core-shell. Inorganic-organic phase interaction inferred from BE lines of N, P, Si, Mg, and C from X-ray Photo electron spectroscopy (XPS). The hydrophilicity of the surface of beads due to the reinforcement of RHA augments the sustained release of P from struvite. On the whole, the micro encapsulation helped market value of struvite in addition, lessen the demand of rock based phosphate fertilizer.

I 056

Structural, Optical, Magnetic and Photocatalytic properties of α–Fe_2O_3@NiO nanocomposites for the treatment of hazardous Rose Bengal dye

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ABSTRACT

In this work, α–Fe_2O_3@NiO nanocomposites were synthesized by wet chemical co-precipitation method for wastewater treatment. These nanocomposites were characterized for their structural, optical, magnetic and photocatalytic properties using versatile techniques. XPS spectra was used to identify the defects/oxygen vacancies. The α–Fe_2O_3@NiO (1:2) sample shows maximum degradation of 93.5 % for RB dye. The increased photocatalytic activity can be attributed to synergistic contribution of α-Fe_2O_3 and NiO, which inhibits photo-generated charge carrier recombination and formation of highly active radical species (OH• radicals, and O_2• radicals). This study might help to design the effective photocatalysts for breakdown of organic pollutants in addition to providing insight into the photocatalytic mechanism.

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ZIF 8 as a functional material for CO_2 sensing and capture - A Review

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ABSTRACT

Zeolitic imidazole framework-8 (ZIF-8) has emerged as a promising functional material for CO_2 sensing and capture due to its high porosity, large surface area, and excellent thermal and chemical stability. This review provides an overview of the recent advancements in the synthesis, modification, and applications of ZIF-8 for CO_2 sensing and capture. Various synthesis methods have been developed for ZIF-8, offering control over its particle size, morphology, and crystallinity. Additionally, ZIF-8 can be modified to enhance CO_2 adsorption capacity and selectivity. ZIF-8 exhibits remarkable CO_2 sensing properties due to its reversible adsorption of CO_2. Various sensing mechanisms have been explored, including colorimetric, fluorescent, and electrochemical sensing. ZIF-based sensors demonstrate high sensitivity, selectivity, and fast response times, making them suitable for real-time CO_2 monitoring. ZIF-8 has shown promising potential for CO_2 capture from post-combustion flue gas, natural gas, and biogas. Its high CO_2 adsorption capacity and selectivity over other gases make it an attractive adsorbent. ZIF-8 can be integrated into membrane separation processes or used as an adsorbent in adsorption-based capture systems. ZIF-8 stands out as a versatile and promising functional material for CO_2 sensing and capture. Continued research efforts are focused on developing cost-effective synthesis methods, enhancing CO_2 adsorption performance, and addressing stability issues under operational conditions. ZIF-8 is poised to play a significant role in advancing CO_2 mitigation strategies and contributing to a sustainable future.

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I 058

Utilization of Synthesized Magnesium-containing Copper Ferrite for the Treatment of Water-containing Organic Dyes.

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ABSTRACT

Magnesium-containing copper ferrite nanoparticles were synthesized using a co-precipitation method and evaluated for their adsorption capacity towards congo red and methylene blue dyes in single and binary systems. The effects of various parameters, including contact time, dye concentration, pH, adsorbent dosage, doping percentage, and temperature, on the adsorption performance were investigated. The outcomes from the study showed that magnesium-containing copper ferrite exhibited high adsorption capacity for both dyes, with maximum adsorption efficiencies of 99.8% for congo red and 98.5% for methylene blue. The adsorption process followed the Langmuir isotherm model and pseudo-first-order kinetics, indicating the monolayer adsorption process. The results of regeneration trials showed that the adsorbent could be effectively regenerated and reused multiple times. The point of zero charge (pzc) was determined to be 6.5, suggesting that the surface of the adsorbent is positively charged below pH 6.5 and negatively charged above pH 6.5. Characterization studies using scanning electron microscopy (SEM) and powder X-ray diffraction (XRD) confirmed the formation of spinel ferrite nanoparticles with an average crystallite size of 25 nm. Overall, the findings demonstrate that magnesium-containing copper ferrite nanoparticles are promising adsorbents for the removal of congo red and methylene blue dyes from wastewater.

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I 059

New Insight into the Adsorption Behavior of Spherical Meso-porous Metakaolin Geopolymer for the Removal Colorant

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ABSTRACT:

A diverse variety of porous adsorbents are widely used in wastewater treatment for effective removal of organic and inorganic pollutants. This present work focuses on developing a spherical meso-porous geopolymer based on alkali-activated silica and aluminum-rich metakaolin clay to deploy in removing colorants from the aqueous medium. To prepare the beads, two step preparative methods were followed. Firstly, alkali silicate excited (SiO_2/Na_2O = 1.1) metakaolin geopolymer prepared by maturing them for a curing period of 28 days. In the second step, two set of spheres, namely porous (G), rigid (rG) geopolymer synthesized using matured samples with and without perioxide, a pore forming agent. Beads are generated by using sodium alginate and geopolymer in optimized ratio stabilized by Cross linking with calcium chloride. Morphological features and structural characterization of geopolymers were characterized by FTIR, XRD, and SEM. Porous spheres having a pore size distributed between 50 to 100 µm found to interconnected through micrograph analysis. Further, the Nitrogen adsorption-desorption isotherm analysis (BET and BJH methods) surface area was found to be 120 m^2/g and pore volume 0.10 cm^3/g. In this analysis conformed the higher intriguing surface area. Evaluation of the adsorption capacity of rigid and porous sphere evaluated the batch study using MB in cationic dye. The adsorption study enhances for 50-150 mg/g in porous sphere. A strong electrostatic interaction between the positively charged MB species and the negatively charged geopolymer sites established. A systematic study conducted on adsorption kinetics, isotherm and thermodynamics reported by fitting them into different models. The possible chemisorption with intra-particle diffusion mechanism derived.

Keywords: *meso-porous, non-porous, surface area, metakaolin, geopolymer*

I 060

Synergistic use of Metakaoline, Fly ash, and Ground granulated blast furnace slag for the development of Thermal and Fireproof porous Geopolymeric block

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ABSTRACT

The alkali-activated matrix of sole binders Metakaoline (MK), Fly ash (FA), and Ground granulated blast furnace slag (GGBS) in rigid and porous matrix did not show any significant fire resistance behaviour due to the loss of geopolymeric gel at elevated temperature exposure. The dehydration and dehydroxylation stages of the matrix upon thermal load can be controlled by the design of a matrix with a hybrid gel structure. In view of the above, this investigation aimed to develop the porous matrix by concurrent use of MK, FA, and GGBS through a chemical foaming method under optimised conditions. Developed geopolymers are subjected to fire situations directly and exposed to a thermal load up to 800 °C temperature and the results are discussed. A series of tests conducted to monitor the physical integrity of the block of size 30 x 30 mm through visual observations, mass loss under aggressive conditions, and residual compressive strength. The composite of weight ratio 1.5:1.5:2 of MK: FA: GGBS excited by sodium silicate of silica modulus 1.1 under ambient curing conditions outperformed with attained strength of 14.86 MPa with the density of 1040 kg/m^3 than other compositions. Upon elevated temperature exposure, the reduction of strength is 40% of the total strength but maintains the skeleton structure without any visual cracks. This matrix upon flame test, directly exposed to the one face of the cube to fire at 1050 ± 15^{o}C temperature for 1 h, did not degrade the internal structure. The temperature of the reverse side of the cube maintains the temperature of nearly 200 ± 7^{0}C with a drastic reduction of heat. The gel structural stability studied by micro characterisation of the sample before and after thermal load. Based on the results of powder XRD, Fourier transform infrared spectroscopy (FTIR), it is concluded that partial loss of hybrid gels due to the evaporation of occluded water, surface hydroxyl groups. Further transformation of the amorphous geopolymer gel into ceramide phases contributed to thermos mechanical strength. This resilience underscores the exceptional thermal properties of the ternary composites, positioning it as a highly promising material for effective fire protection applications.

Keywords: *Alkali activated material, porous block, compressive strength, fire resistance*

Room temperature Magnetocaloric Properties of the $D0_3$ Structured Ni_3Al Alloys.

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ABSTRACT

The current investigations are aimed at elucidating the structural, thermal phase transition, magnetic transition, and magnetocaloric properties of binary Heusler alloys crystallized in the $D0_3$ structure. The samples are synthesized using a vacuum arc melting furnace in an argon atmosphere. Subsequently, these samples are vacuum sealed in quartz tubes and subjected to thermal annealing for 72 hrs followed by quenching in cold water. The X-ray diffraction analysis confirmed the presence of the $D0_3$-type structure and the structural parameters were obtained after subsequent refinement of XRD profiles (1). Thermo-magnetic data analysis revealed that the sample exhibits magnetic entropy (ΔS_M) at near room temperature (2). Further, we have estimated the refrigeration capacity (RC) of Ni_3Al alloys based on thermo-magnetic data. Within the limits of our knowledge, this could be the very first report of magnetocaloric properties of Ni_3Al alloys in the literature (3).

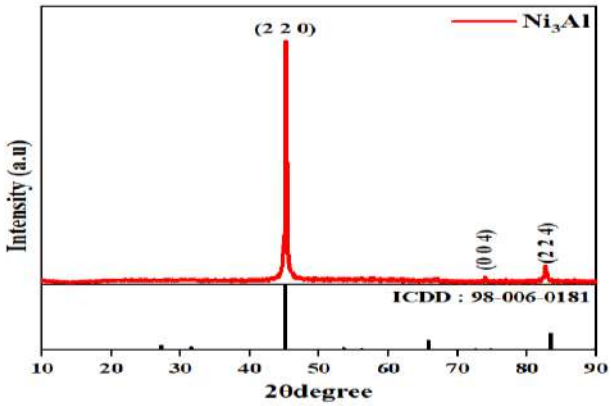

Figure: Xray Diffraction pattern of the prepared Ni_3Al.

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I 062

Magnetocaloric effect in Manganese - Nickel Binary alloys

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ABSTRACT

Mn_xNi (x=1,2,3) and Ni_3Mn binary alloys were prepared in vacuum arc melting under argon atmosphere, the samples were annealed for 72 hours at 950°C in a vacuum-sealed quartz tube. The critical refinement of the X-ray diffraction pattern shows that the Ni3Mn and MnNi belong to face- centered cubic (Pm-3m) and Tetragonal (I4/mmm) space groups respectively, and both Mn_2Ni and Mn_3Ni have Heuslar structure (Fm-3m space group). The thermo – magnetic properties were studied and calculated from the M – T and M – H graph. The austenite and martensite phase transitions were observed. Ni substitution at Mn sites shows promising magnetic properties. The structural, magnetic, thermal, and magnetocaloric characteristics of Mn_2Ni and Mn_3Ni are seldom Studied.

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Graphene Oxide / Copper Ferrite Magnetic Nanocomposite for Photocatalytic Degradation Of Antibiotics

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ABSTRACT

Antibiotic pollution has become a serious problem, posing a hazardous risk to the environment, owing to the significant discharge of antibiotic wastewater into aquatic and terrestrial ecosystems. In 2019 there were 297,000 deaths attributable to Antimicrobial Resistance (AMR) and 1,042,500 deaths associated with AMR in India. Various antibiotic removal investigations have been performed to address such concerns. Photocatalysis has gained an immense amount of attention considering its enormous potential for removing antibiotics from aqueous solutions in a inexpensive and ecologically conscious way. The present study investigated the photocatalytic efficiency of one pot Hydrothermally synthesized Graphene Oxide (GO)/Copper ferrite ($CuFe_2O_4$) nanocomposite with antibiotics such as Amoxicillin (AMX), Azithromycin (ATM), Cephalexin (CPL) which are the most common pollutant antibiotics in India. The nanocomposite was characterized using X-ray diffraction (XRD), Scanning Electron Microscope (SEM), Elemental Analysis (EDAX), Raman Spectroscopy, Fourier Transform - IR Spectroscopy (FTIR), Vibrating Sample Magnetometry (VSM) and X Ray Photoelectron Spectroscopy (XPS). The UV-Visible spectrophotometer was used to compare the photocatalytic efficiency of GO, Copper ferrite and GO/$CuFe_2O_4$ nanocomposite for the degradation of antibiotics. As GO/$CuFe_2O_4$ nanocomposite can be recycled and possesses magnetic and photocatalytic properties, it can be developed as an inexpensive substitute photocatalyst for antibiotic removal from pharmaceutical effluents and wastewater.

Keywords: *Graphene, Copper Ferrite Nanocomposite, Hydrothermal method, Antibiotic degradation, Photocatalytic degradation, Pharmaceutical degradation.*

I 064

Removal of organic pollutants by MoO_3 nanosheets

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ABSTRACT

Molybdenum trioxide (MoO_3), is a fascinating transition metal oxide that has remarkable features that make it useful in many different contexts. These include gas sensing, electrochemical capacitors, certain alloys, coatings, textiles, and the preparation of ceramics and glasses, among many others. MoO_3 is a key ingredient in molybdenum metal production. The synthesis of MoO_3 can be accomplished in a number of ways. In this case, we first synthesised MoS_2 using a straight forward hydrothermal process. Next, the MoS_2 powder was subjected to a three-hour heating process in a muffle furnace set at 500 ºC. The powder is analysed using FTIR, XRD, Raman, and SEM spectroscopies. The formation of MoO_3 has been verified. Using SEM spectroscopy, the nanosheet-like structure of MoO_3 was found. Careless disposal of many dyes, such as methylene blue (MB) and crystal violet (CV), poses serious risks to water bodies in the vicinity of these sectors because they are utilised in textiles and medicines, among others. Consequently, breaking down these harmful chemicals becomes an arduous effort. As a catalyst for dye removal from polluted water bodies, MoO_3 nanosheets can be useful in this effort. So, MB and CV dye degradation under natural and artificial visible light has been investigated with MoO_3 nanosheets. Degradation efficiency graphs, tauc plots for band gaps, pseudo-first order kinetic plots, and other graphs from the UV-VIS Spectroscopy data were compared to analyse the degradation activity. Both dyes are efficiently degraded by MoO_3 nanosheets, with a degradation efficiency of 98%.

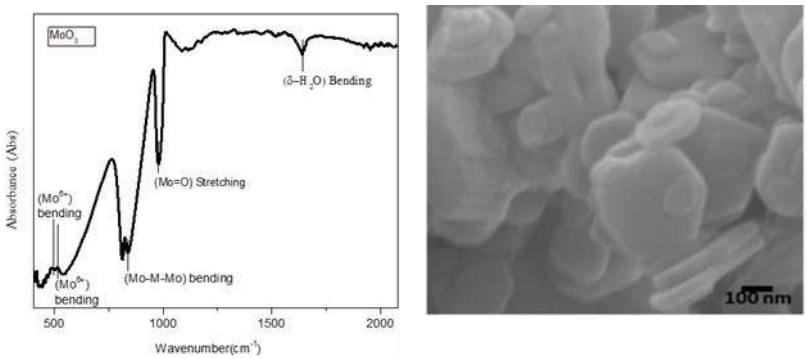

Figure 1. FTIR Spectra SEM image of MoO_3 Nanosheets.

Keywords: *MoO_3 (Molybdenum trioxide) nanosheets, Methylene Blue (MB), Crystal Violet (CV), catalyst, dye degradation.*

I 065

Exploration of Water Purification using Reviving Herbal Seeds to Remove Noxious Waste from Washing Machines

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ABSTRACT

Greywater from daily household activities is a substantial and reclaimable water resource, but traditional treatment methods often pose environmental and health risks due to chemical-laden and energy-intensive processes. This research focuses on examining physico-chemical parameters to evaluate the quality of greywater from washing machine discharge before and after treatment using Nirmali and Moringa oleifera seeds. Batch adsorption studies(adsorption) and Jar test (coagulation) were conducted, revealing a maximum sorption efficiency of 94.5% with a dosage of 5 grams and an agitation time of 30 minutes (140 rpm). The initial turbidity of collected water (200ml) was 56 NTU. Post-treatment with raw Nirmali and Moringa oleifera seeds at a 5g dosage, the turbidity removal capacity increased from 60% to 80% over 24 hours. Characterization studies, including FT-IR, SEM, and EDAX analyses, were performed to examine functional groups, morphology, and elemental composition in Nirmali and Moringa oleifera seeds. The results strongly affirm the seeds' effectiveness in eliminating turbidity and $PO4^{3-}$ from wastewater.

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6.

I 066

NanoSponge: Bismuth-Boosted Mg-Al LDH for Efficient Indigo Carmine Dye Sequestration in Water

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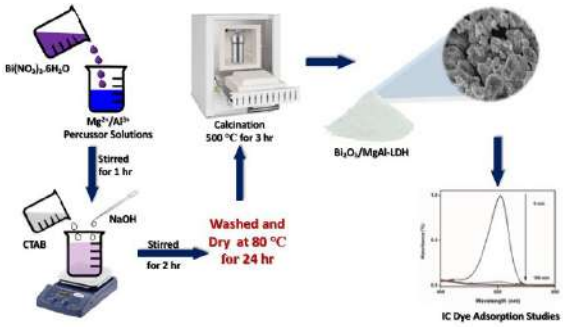
ABSTRACT

The escalating concern of water pollution, stemming from the continual release of organic contaminants like dyes and drugs into surface and groundwater, underscores the gravity of the issue. Metal-Layered Double Hydroxides (LDH) emerge as a pivotal solution, offering high efficiency and cost-effectiveness for the adsorption of these pollutants. Employing metals like Mg and Al for LDH synthesis, owing to their low toxicity and cost, results in Mg-Al LDH derived metal oxides with elevated porosity through calcination [1,2]. This study encompasses the synthesis of pure Mg-Al LDH and Bismuth (III) oxide-doped Mg-Al LDH by the co-precipitation method at a constant pH, where CTAB as a scaffold. To enhance the adsorption capabilities in wastewater, a facile surfactant-mediated sol-gel method is employed to synthesize the Bi_2O_3 impregnated MgAl-LDH nanocomposite. Investigating the adsorption of Indigo Carmine (IC), an anionic dye, from aqueous solutions is pivotal for advancing our understanding of efficient water treatment technologies, with the ultimate goal of providing clean and pollutant-free water to address the pressing global need for sustainable and safe water resources.



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I 067

Effective Detection and Removal of Hg(II) using Fluorescein (FL) Decorated Chicken Eggshell Derived Activated Carbon (ESAC) nanocomposite (FL-ESAC)

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ABSTRACT

Heavy metals, in particular mercury is considered as the most harmful pollutant in the environment which causes acute kidney failure, stomach diseases and even death in severe cases. Hence the present work aims at the preparation and characterization of chicken egg shell derived activated carbon based fluorescent probe (FL-ESAC) for the effective detection and removal of Hg(II) in waste water. where chemical activation method was adopted for the preparation of ESAC. The prepared FL-ESAC nanocomposite was subjected to XRD, FTIR, SEM, EDX, UV-vis and PL studies which strongly confirm the adornment of FL at the surface of ESAC. The Limit of detection and adsorption capacity of FL-ESAC towards Hg(II) was found to be 2.24 nM and 79.35 mg/g respectively. Even though the permissible limit for mercury ion concentration in drinking water is 10 nM according to U.S. Environmental Protection Agency, the prepared FL-ESAC probe could able to detect even below the permissible limit. Hence these results authenticate that the prepared FL-ESAC probe could serve as a better sensor material for the effective detection and removal of mercury in the realm of environmental remediation applications.

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I 068

Visible-Light-Driven Photocatalytic Activity of Hydrothermally Synthesized Copper Vanadate Nano-Pebbles Towards Environmental Remediation Applications

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ABSTRACT

The present work elucidates the synthesis, characterization and photocatalytic performance of copper vanadate nano-pebbles (CVNPs) towards the degradation of organic dye molecules present in wastewater. where a facile hydrothermal method was adopted for the synthesis of CVNPs. The structural, vibrational, morphological, elemental and optical properties of the prepared CVNPs were studied using XRD, FTIR, SEM, EDS and UV-Visible analysis. The XRD pattern confirms the monoclinic crystal structure of prepared CVNPs and it is well matched with JCPDS Card no: 01-073-1032. The characteristic vibrations of copper vanadate namely tetrahedral VO_4 and square pyramidal CuO_5 were observed from FTIR studies. The SEM and EDS results ensure the nano-pebbles-like morphology of CVNPs which comprises Cu, V and O elements only. From the UV-Visible analysis, the absorption peak appears in the wavelength range of 220 - 500 nm is attributed to the ligands to metal charge transfer (CT) transition of tetrahedral VO_4 coordination. In addition, the narrow bandgap of CVNPs (2.25 eV) may promote visible-light driven photocatalytic performance. The complete photocatalytic degradation of organic Methylene Blue (MB) dye aqueous solution was achieved under visible-light irradiation of 120 min. Moreover, there is a visible color change from deep blue to transparent was noticed in the MB dye solution. Hence it is strongly believed that the prepared CVNPs may serve as a potential photocatalyst in the realm of wastewater treatment in the near future.

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I 069

Enhanced Photocatalytic Activity of Biogenically Inspired γ-Fe_2O_3 Nanoparticles from *Mukia maderaspatana* Leaf Extract

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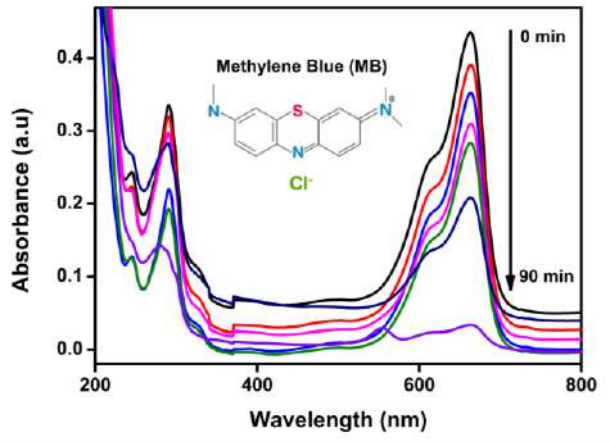
ABSTRACT

The growing demand for environmentally friendly materials in the field of environmental remediation has propelled research efforts to identify effective photocatalysts capable of harnessing natural sunlight to efficiently break down harmful and toxic substances into non-toxic counterparts. In this study, we successfully synthesized and characterized a graphitic nitride-based photocatalyst, employing various techniques including XRD, FT-IR, UV-DRS, Raman, PL, XPS, BET, TGA, SEM-EDAX, and TEM. The resulting catalyst exhibited outstanding photocatalytic performance of 92 % towards the degradation of methylene blue dye in 1.5 h. The catalyst's superior performance is attributed to its biogenic synthetic route with unique morphology of irregular cubical structure. Notably, a facile and straightforward biogenic method was employed to synthesize γ-Fe_2O_3, resulting in a photocatalyst with enhanced activity and stability.



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I 070

$CrNiNbTi_{1-x}Fe_x$ High Entropy Alloys: Enhanced Structural and Solid-State Hydrogen Storage Properties

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ABSTRACT

High entropy alloys (HEAs) $CrNiNbTi_{1-x}Fe_x$ (x = 0.1, 0.3, 0.5, 0.7, 0.9 mol%) have been investigated as promising candidates for hydrogen storage materials because of their quick hydrogenation rates, High energy ball milling is used to create these alloys, and then high-pressure torsion (HPT) is used. According to the results of XRD and elemental mapping, C14 Laves became the dominant phase in all $CrNiNbTi_{1-x}Fe_x$ alloys, and HCP also existed because of the abundance of Nd metal. Due to the high affinity between Nb and Fe, when Fe replaces Ti, the fraction of the C14 Laves phase rises while that of the HCP phase falls. This phenomenon is caused by the element Nb moving from the HCP phase to the C14 Laves phase. $CrNiNbTi_{0.5}Fe_{0.5}$ equimolar alloys have improved hydrogenation rates and capacities. Remarkably, even at ambient temperature and under 1 MPa, the $CrNiNbTi_{0.5}Fe_{0.5}$ alloy is able to reversely absorb 1.8 wt.% hydrogen. By reducing the H atom diffusion distance, the shortened inter-dendritic phase helps to increase the hydrogenation rates. The addition of Fe increases the amount of hydrogen that can be stored due to the movement of the hydrogen-absorbing element Nb to the C14 Laves phase and the rise in the proportion of the C14 Laves phase.

Keywords: *High Entropy Alloy, Ball Milling, C14 Laves phase, Hydrogen Storage Capacity*

Exploring the Adsorption and Desorption Properties of H_2 and D_2 in Sr based Metal-organic framework Materials for Storage Applications

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ABSTRACT

Hydrogen as a clean fuel offers zero-emission potential when utilized, contrasting with carbon- based fuels which release carbon dioxide and pollutants upon combustion contributing to environmental issues. Storage of hydrogen presents challenges due to its low density, requiring high-pressure or cryogenic conditions. The goal therefore is to design low-cost, light-weight materials that can reversibly and rapidly store hydrogen. Solid state adsorbents like metal hydrides, carbon-based materials (activated carbons and graphene), zeolites and metal organic frameworks (MOFs) offers distinct hydrogen adsorption properties. Among them metal–organic frameworks emerged as one of the most promising adsorbents for hydrogen storage.MOFs are crystalline porous solids whose structure is defined by metal ions or clusters of metals that are connected to bi or multipodal rigid organic linkers. They exhibit large surface area, adjustable pore size, high porosity, enabling efficient gas adsorption, storage and selective separations [1]. The surface area values of MOFs typically range from 1000 to 10,000 m^2/g, thus exceeding those of traditional porous materials such as zeolites and carbons. In the present study, MOFs were explored for hydrogen storage applications. Four Sr-based MOFs with different organic linkers containing diverse functional groups were synthesised by solvothermal method [2]. The synthesised MOFs were characterised by PXRD, FT-IR, SEM-EDX, TGA and BET. All the MOFs were investigated for adsorption and desorption properties of hydrogen. A volumetric gas absorption apparatus (Sievert) was employed to conduct hydrogen adsorption studies at different pressures at 77 K [3]. The influence of various of functional groups such as $–NH_2$, - COOH, $-NO_2$, $-SO_3H$ and isotope effect(H_2/D_2) was investigated on storage of hydrogen. Here, we also studied the adsorption and desorption behaviour of H_2/D_2 on all MOFs at different pressures at 77 K. Adsorption kinetics and isotherm studies for H_2/D_2 at different pressures were carried out to understand the adsorption behavior of MOF materials.

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I 072

Granular Activated Carbon and Iron Oxide-Modified Pervious Concrete for Pb^{2+} Removal

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ABSTRACT

This work reports the use of pervious concrete-based filters for removal of heavy metal ions from water. Pervious concrete filters were developed with partial replacement of the fine aggregates by granular activated carbon (GAC), iron-oxide-coated fine aggregates (IOA), and a hybrid of both. The prepared concrete had showed a 22% and 6% increase in compressive strength for the IOA and the hybrid systems, respectively, while GAC decreased the compressive strength by around 22% compared to control concrete specimens. Synthetic wastewater containing 15 ppm Pb^{2+} was trickled down through the modified pervious concrete filters for 8 hours. The overall lead removal efficiencies for the IOA, GAC and the IOA-GAC hybrid systems were 93.6%, 95.9% and 97.6% respectively, compared to an 87.4% removal for the control, unmodified pervious concrete filter. With a view of exploring reusability of the filters, desorption studies with 1M nitric acid were performed on the IOA, GAC and IOA-GAC systems and the reduction in the magnitude of leaching was observed. XRD, SEM and EDX results indicate evidence of physisorption and fixation of Pb^{2+} on the concrete by precipitation. These preliminary results demonstrate the utilization of pervious concrete as an economical, viable and sustainable option for heavy metal removal.

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Interpretation of Machining aspects of Silicon dioxide doped vegetable based nano fluids with Grey Analysis in Turning of AISI 316 Steel

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ABSTRACT

In the current engineering era, metal cutting emerges as an essential and broadly applied manufacturing process. It is vital in fulfilling the rigorous requirements of quality and productivity for machined parts, concurrently ensuring economic viability during the turning operation. The machining process is governed by a variety of factors, encompassing cutting speed, feed rate, depth of cut, and the geometry of the cutting tool, to name a few. This study delves into the machining aspects of Silicon Dioxide (SiO_2) doped vegetable-based nanofluids in the context of turning AISI 316 Steel. These nanofluids, employed as cutting fluids, are gaining traction owing to their environmentally friendly, sustainable, less toxic, and superior thermal and tribological attributes. The research concentrates on the impact of these nanofluids on performance indicators such as surface irregularity, machining force, tool wear, power consumption, and the temperature generated during the machining process. The exploration also extends to the application of Minimum Quantity Lubrication (MQL), a method known for its efficiency and eco-friendliness in applying cutting fluids in machining processes. The findings indicate that the utilization of an eco-friendly Nano-machining fluid leads to enhanced surface features, reduced tool wear, lower cutting force, decreased power requirement, and a reduction in the temperature of the machining zone. This can be attributed to the superior cooling and lubrication properties of the fluid. This project offers a comprehensive analysis of the machining aspects of SiO_2-doped vegetable-based nanofluids by using grey analysis, thereby making a significant contribution to sustainable development in the manufacturing industry.

I 074

Deterministic Seismic Hazard for Ranchi Districts, Jharkhand,India, by Estimation of Peak Ground Acceleration

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ABSTRACT

The most industrially advanced city area in Jharkhand, India is Ranchi, which is located in 23.3441° Nto 85.3096° E. Earthquake-resistant structures must be designed because of the importance of industryto city dwellers. The site-specific peak ground acceleration (PGA) for the Ranchi (23.3441° N to 85.3096° E) must be determined by engineers using a deterministic seismic hazard assessment (DSHA).Additionally, research must be done to create a seismic hazards map for the Ranchi by using different seismic parameters like the maximum earthquake magnitude for that area, appropriate ground motion prediction equations (GMPEs), the idea of a logic tree, and an appropriate weight factor for this particular selection areas. For this, 213 grid points of size (0.054°x0.054°) have been placed throughoutthe selected area. Every grid point takes the site position into account. With the help of the Seismotectonic ATLAS of India. Linear sources and seismic events are taken with the help of Arc- GIS software, in which Georeferencing and digitizing process within an 800km radius in which Ranchicity is considered as a center point. Maximum magnitude has been calculated based on observed maximum magnitude by using an application of National Disaster Management Authority (NDMA),P Anbazhagan (2015), Wells & Coppersmith (1994), and Nowroozi (1958) methods. The result ofMaximum peak ground acceleration is 0.241g for the study region elongated along the middle portion of the region from the east side (TAMAR, BUNDU, RAHE important location place) to the west side(NAGRI, BERO, as well as RANTU) also small region show higher value in a southeast corner (RARGAON place). Now the result is validated with IS: 1893 code and EN1998 Eurocode8.In my study, the calculated maximum spectral acceleration coefficient (SA) is 0.8g for a predominant frequency of 0.25 (1/t) at the bedrock surface.

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I 075

Polystyrene and Polyethylene microplastics alter *Drosophila* Behaviour and Development

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ABSTRACT

Plastic use and production have been major concerns for decades, and global governments have taken many initiatives to curb its use and formulate suitable disposal agendas. However, despite the policies against plastic production and disposal, it is inevitable to fully eradicate its presence from the ecosystems or develop effective and cost-efficient replacements. One of many prominent plastic-associated concerns involves the formation of microplastics (MPs) from plastic degradation in marine or terrestrial ecosystems. In addition to this, intentional use of microplastics has become a common practice for the past five decades. Plastics in the form of microbeads have been extensively used in toothpaste, cleansers, paint, detergents, and cosmetics. These particles eventually end up passing through a multitude of wastewater processing systems and end up contaminating aquatic ecosystems. Polystyrene (PS) and polyethylene (PE) are commonly used to produce food packaging materials, automobile parts, medical supplies, casings, etc. Therefore, the chances of improper disposal strategy and subsequent neglect increase the presence of polystyrene and polyethylene microplastics in the environment. In this study, we have assessed the toxic effects of PS and PE MPs on *Drosophila melanogaster* behaviour and development.

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I 076

Nonlinear viscoelasticity of fungal biofilm-based membranes after uptake of excess nitrogen and phosphorous in wastewater

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ABSTRACT

Biofilm is a living material consisting of microbial cells embedded in a self-secreted extra-cellular matrix (ECM) of polymers: This arrangement helps them stave off environmental assaults. We recently discovered that the porous air-liquid interface filamentous fungal biofilms of *Neurospora discreta* can efficiently uptake excess nitrogen and phosphorous – environmental assault - commonly found in industrial wastewater [1]. Here, we report the resultant changes to the viscoelasticity of the biofilms by subjecting them to large amplitude oscillatory shear flow and monitoring the microstructure using field-emission scanning electron microscopy before and after the shear flow. The main finding is at large strain amplitudes, the biofilms display a weak strain overshoot in the loss modulus signifying a yielding transition from elastic to plastic deformation state: Resistance to yielding transition is determined by a rich interplay between filament orientation and ECM composition. Yielding transition is quantified by the dimensionless parameter, β, a measure of the intensity of the weak overshoot: Changes in filament orientation distribution before and after shear flow is determined by a new measure called orientation complexity function $|\Delta OCF|$: Changes to the ECM composition is measured through proteins and polysaccharides per unit dry biomass. Figure 1 shows that β is positively correlated with protein and polysaccharides concentrations per unit biomass and inversely related to $|\Delta OCF|$. The results have implications for rational design of fungal biofilms as membranes with tuneable mechanical properties.

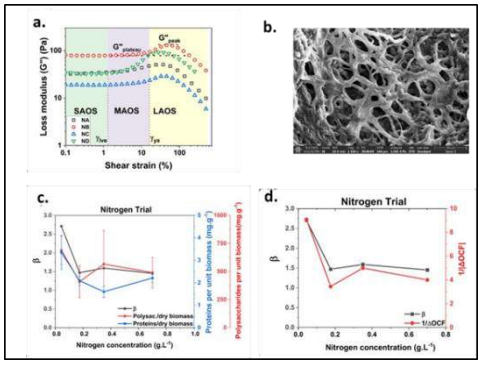

Figure 1: a) Loss modulus as function of shear strain illustrating weak overshoot behavior;b) SEM image of porous biofilm; c) β and ECM composition relation for nitrogen trial;d) β and $1/|\Delta OCF|$ relation for nitrogen trial

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I 077

Methylene Blue Dye Degradation Using Hydrothermally Synthesized V_3O_7 Nanostructures

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ABSTRACT

In this work, V_3O_7 nanostructures were synthesized by simple and low-cost hydrothermal method and is used as a catalyst for the degradation of methylene blue in the absence of light. The prepared nanostructures were characterized by X-ray diffraction, Ultraviolet- Visible absorption and FTIR spectroscopy. The catalytic effect of V_3O_7 nanostructures were studied by adding 20mg of the prepared sample into 50ml of 20ppm of methylene blue solution in distilled water. The catalytic degradation was observed both in light and dark conditions. In 110 minutes, catalyst showed a degradation efficiency of 95.1% and 94.8% in presence and absence of light respectively. Later 0.1M of $NaBH_4$ was added to the dye-catalyst solution to study the effect of reducing agent on the degradation of dyes and a degradation efficiency of 95% was observed in just 10 minutes. To verify V_3O_7 nanostructures are the one that is responsible for dye degradation, the degradation of dye-$NaBH_4$ solution is studied in the absence of V_3O_7 for 120 minutes and no significant degradation of dye was observed.

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I 078

Evaluating the Toxicity of Polyethylene Microplastics Using the *Drosophila melanogaster Model*

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ABSTRACT

Microplastics, ubiquitous plastic particles less than 5mm in size, have become a major environmental concern. Among them, polyethylene (PE), the most commonly used plastic, is particularly worrisome due to its widespread distribution and persistence. Studies have highlighted the adverse effects of microplastics on aquatic organisms, but research on their impacts on terrestrial organisms is still limited. *Drosophila melanogaster* offers a unique opportunity to explore the toxicity of microplastics on a representative terrestrial organism and the model has functional homologs for over 75% of the genetic material responsible for human diseases. Therefore, the model is considered to test the potential toxicity induced by microplastic exposure. The effects of MP exposure will be evaluated at behavioral, biochemical, and gene expression levels. The study will focus on evaluating the expression levels of genes that are crucial in cellular stress response, antioxidant defense, and embryo development process. Biochemical assays will be conducted to understand the molecular responses of organisms to stressors like microplastics. This study will provide new information on the toxicity of PE microplastics in terrestrial organisms and help to understand their potential ecological and health implications.

Keywords: *Drosophila melanogaster*, Gene expression, Microplastics, toxicity.

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Non-Thermal Plasma-Induced Surface Modifications on ZnO for Improved Photocatalytic Performance

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ABSTRACT

Photocatalysis, a promising technology for environmental remediation and energy conversion, relies on efficient semiconductor materials. Zinc oxide (ZnO) has gained attention due to its excellent photocatalytic properties; however, its performance can be further improved through surface modifications. In this study, we explored the potential of non-thermal plasma (NTP) treatment, as an innovative approach, to enhance the photocatalytic efficiency of ZnO. The NTP treatment led to surface modifications, including the creation of active sites. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) analysis showed distinctive spherical-shaped, slightly agglomerated nanoparticles of 74 nm particle size, compared to the non-treated particles measuring 131 nm. UV-DRS analysis indicated a decrease in bandgap energy from 3.4 eV (non-treated) to 3.1 eV (plasma-treated). X-ray photoelectron spectroscopy (XPS) analysis confirmed the alterations in crystal structure and chemical composition after plasma treatment. In conclusion, the study demonstrated significant changes in the surface characteristics, crystal structure, and chemical composition of ZnO nanoparticles after NTP treatment. Characterization using x-ray diffraction (XRD) revealed a reduction in crystallite size from 28 nm to 18 nm after 60 min of plasma treatment at 15 kV, and 50 Hz. Therefore, this study centres on examining the photocatalytic activity of plasma-treated ZnO using organic dye under visible light conditions. The results indicate that the crystal violet degradation occurs at a time of 1h and low catalyst weight 5mg, highlighting the efficacy of the plasma-treated ZnO in facilitating efficient photocatalytic degradation.

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I 080

Visible-light-promoted C-C and C-N bond formation: $Mn_2(CO)_{10}$ catalysed multi-component sustainable approach for the synthesis of novel 1*H*-pyrazole-4-carboxamides

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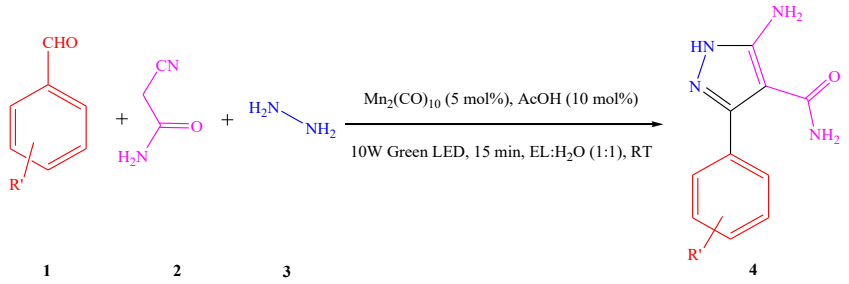
ABSTRACT

Multicomponent reactions play a pivotal role in the synthesis of 1*H*-pyrazole-4-carboxamides, underscoring its significance in sustainable organic synthesis. These compounds, valued for their diverse biological activities, have garnered substantial attention in the realm of pharmaceutical research. Herein, we employ a facile, rapid one-pot strategy to access an extensive array of 1*H*-pyrazole-4-carboxamide derivatives, utilizing substituted aldehydes, cyanoacetamide, and hydrazine hydrate as substrates and a readily accessible $Mn_2(CO)_{10}$ as photocatalyst in EL: H_2O (1:1). The current method is characterized by its affordability, non-toxicity, easy access to starting materials, and notably with minimal waste generation. Additionally, remarkable aspects include its mild operating conditions, environmentally friendly nature, and the ability to accommodate a wide range of both electron-donating and electron-withdrawing groups.



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I 081

A Metal-Free Green and Sustainable stepwise addition of Phenacyl Bromides, Aryl Amines, and Potassium Thiosulphate for the Rapid Synthesis of Novel 1*H*-Imidazole-2-Thiols under ultrasonication

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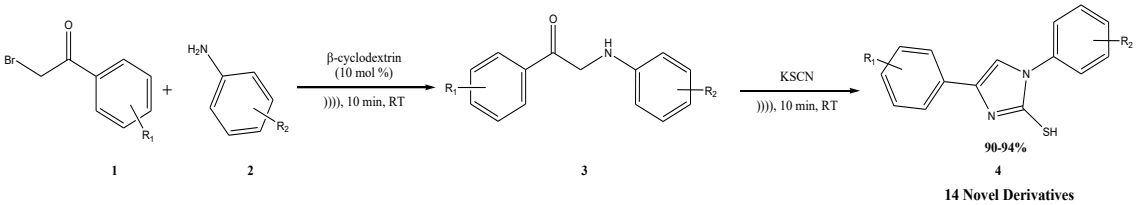
ABSTRACT

Organic Chemistry plays a crucial role in advancing society towards the achievement of Sustainable Development Goals (SDGs). The imperative for new chemical research, environmentally friendly and sustainable chemical synthesis, and a commitment to social responsibility is pivotal for both current and future chemists as we collaborate in safeguarding the planet. In the realm of contemporary organic chemistry, the utilization of metal-free catalysis processes assumes a key role in aligning with green chemistry principles. The synergistic blending of substrates like phenacyl bromides, aryl amines, and potassium thiocyanate under ultrasonication presents an efficient approach for synthesizing innovative 1*H*-Imidazole-2-Thiols in the presence of *β*-cyclodextrin. This method not only provides a practical and sustainable means to obtain diverse derivatives of 1*H*-Imidazole-2-Thiol but also enhances overall synthesis efficiency. Furthermore, it upholds green chemistry tenets by minimizing waste generation and reducing the number of reaction steps. Consequently, organic chemists and researchers striving to innovate novel molecules increasingly rely on ultrasound techniques for their synthesis.Our method offers several advantages, such as secure handling, impressive yields, shortened reaction duration, and a straightforward purification procedure. All the resulting derivatives undergo comprehensive spectral analysis for characterization.



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I 082

Electrochemical Reduction of Hexavalent Chromium in a Dual-Chambered Redox Electrochemical Cell

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ABSTRACT

Rapid industrialization has resulted in the direct or indirect release of wastewater containing harmful heavymetals into the air, soil/sediment, surface water, and groundwater. Hexavalent chromium, Cr(VI), presentsa significant risk to human health and environmental safety due to its high mobility and solubility across awide pH range. It is being discharged from various industries, including electroplating, chrome plating, metal finishing, and tanneries. Several researchers have reported the reduction of Cr(VI) to Cr(III) using conventional methods such as chemical reduction, photocatalytic degradation, electrochemical techniques,and biological approaches. Electrochemical techniques offer numerous advantages over conventional methods, including the absence of chemical requirements, ease of operation, and no residual contamination.On the other hand, elevated levels of ammonia nitrogen can intensify water body contamination, while a high N/C ratio could lead to a significant nutritional imbalance proportion. Although methods to eliminate ammonia nitrogen are effective, they require a significant amount of energy. Recently, great interest has been shown in extracting the inherent chemical energy in wastewater and using it for self-treatment through non-energy-intensive processes, such as microbial fuel cells and redox fuel cells. Generally, contaminantswith a low redox potential in aqueous solutions can function as fuels, oxidizing on the anode to produce electrons, while those with a high redox potential serve as electron acceptors, being reduced on the cathode.In this work, a novel chromium-ammonia redox system was explored that can simultaneously reduce hexavalent chromium at the cathode and oxidize ammonia nitrogen at the anode without any external energyinput. Experiments were conducted in a dual-chamber cell with carbon felt as cathode and nickel as anode.Around 71% Cr(VI) reduction efficiency was achieved within 36 h in this system.

I 083

Viologen based Covalent Organic Networks as Metal free Bi-functional Electro-catalyst

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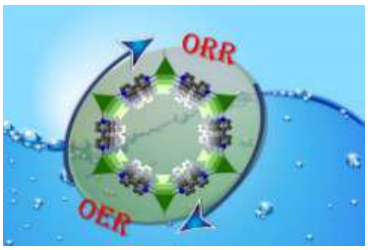
ABSTRACT

The development of energy storage technologies such as fuel cells and metal-air batteries rely heavily on bifunctional electrocatalysts that can catalyze both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) events. Here, we report for the first time a new series of viologen based cationic covalent organic networks (vCONs) - a metal-free electrocatalysts toward the bifunctional ORR and OER applications. These vCONs (vGC, vGAC, vMEL, and vBPDP) were synthesized by the solvothermal- assisted Zincke's reaction. The redox-active viologen moieties inside the extended covalent network play the role of displaying high ORR and OER activity. Among these four vCONs, vBPDP has the highest ORR activity with a half-wave potential of 0.72 V against a reversible hydrogen electrode in 1 M KOH electrolyte. The combination of high nitrogen content and inherent radical nature of vBPDP is the crucial key factor for achieving an effective ORR catalyst through a four-electron pathway. On the other hand, vMEL demonstrated high OER electrocatalytic activity, with an overpotential of 320 mV at a current density of 10 mA cm2, and a Tafel slop of 109.4 mV decade-1 in 1 M KOH solution electrolyte. This work is one of the rare reports in metal-free ionic covalent organic networks which are useful as bifunctional (ORR and OER) electrocatalysts in wider pH windows (acidic to basic).



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I 084

Infrared active narrow bandgap Ni doped $LaFeO_3$ nanoparticles for desalination and decontamination of water leveraging interfacial solar steam generation.

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ABSTRACT

Photothermal Ni-doped $LaFeO_3$ (NLFO) ($LaFe_{1-x}Ni_xO_3$, x=0, 0.2, 0.3, 0.4, and 0.5) microspheres composed of nanoparticles synthesized by hydrothermal method are utilized for interfacial solar steam generation (ISSG) of salty and contaminated water. The orthorhombic () to rhombohedral () phase transition of $LaFeO_3$ (LFO) at morphotropic phase boundary (MPB) flattens the free energy profile, and high absorbance in the 800-2000 nm Vis-NIR region arises due to the creation of intra-band gap states are accountable for superior activity towards the ISSG for desalination. The La, Ni, and Fe possess the oxidation states of 3+, 2+, and 3+/4+, respectively, showing successful doping of Ni^{2+} at the Fe^{3+} sites that produce lattice distortion at La/FeO_6 octahedra. $LaFe_{0.5}Ni_{0.5}O_3$ (NLFO5) sample exhibits surface temperature of 50.4 °C due to heat localization and produces evaporation flux of 2.89 kg/m^2h under IR illumination at the air-water interface. Importantly, NLFO5 loaded cellulose paper shows good repeatability and cyclic stability for 10 consecutive cycles under IR illumination and equivalent evaporation flux of 2.4 kg/m^2h under direct sunlight illumination. Moreover, 3.5 wt% saline water shows a drastic decrement in ion concentration after ISSG, as confirmed by atomic absorption spectroscopy. NLFO5 possesses good evaporation flux of 2.27 and 2.20 kg/m^2h for water contaminated with RhB and MB organic dye. Our results propose the NLFO as distinguished photothermal material for ISSG application and wastewater purification by means of evaporation.

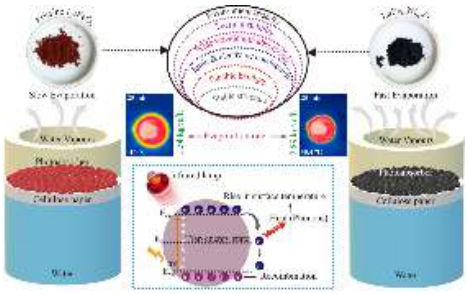

Fig.1 Schematic representation of Ni-doped $LaFeO_3$ photothermal materials for real-time applications in interfacial solar steam generation

I 085

Investigation of Adsorption Properties of Novel Magnetic Cellulose Nanofibers - Reduced Graphene Oxide (MCNF-rGO) Nanocomposite for Dye Elimination

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ABSTRACT

Dye removal from industrial wastewater is a serious environmental issue that is a global concern. In the present study, a novel and facile magnetic cellulose nanofiber-reduced graphene oxide (MCNF-rGO) nanocomposite was synthesised and characterised for the removal of dye from wastewater. The nanocomposite was characterised using scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy to investigate the morphology, crystallinity, and chemical structure of the nanocomposite. In this study, the central composite design (CCD) based on the response surface methodology (RSM) was used to evaluate the operating parameters and identify the ideal conditions for the removal of dyes by MCNF-rGO. The maximum adsorption capacity of this nanocomposite was determined using adsorption isotherm models. The results showed fast adsorption kinetics, easy magnetic extraction, renewal, good stability, and removal efficiency, making (MCNF-rGO) nanocomposite a cost-effective and promising adsorbent for the removal of organic dyes, offering a promising approach for wastewater treatment and environmental protection.

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I 086

Enhanced Photocatalytic Activity of Electrodeposited Cu-Zn BMNPs for the Sustainable Treatment of Industrial Wastewater

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ABSTRACT

The development of environmentally friendly photocatalytic nanomaterial has gained valuable insights for the effective alternate for the wastewater treatment. This investigation demonstrates the photocatalytic applications of copper-zinc bimetallic nanoparticles (Cu-Zn BMNPs) electrodeposited onto the graphite surface with perfect cubic morphology. Cu-Zn BMNPs were characterized for the structural and morphological properties using powder X-ray diffraction (PXRD), high resolution transmission electron microscopy (HRTEM), high resolution scanning electron microscopy (HRSEM) and X-ray photoelectron spectroscopy (XPS). The results also includes the characterization of copper and zinc nanoparticles for comparison. Photocatalytic analyses were carried out in the sun light and characterized using UV-Visible spectroscopy. These findings validated the catalytic efficiency of the electrodeposited metal nanoparticles. These results proved the enhanced photocatalytic efficiency of Cu-Zn BMNPs for the minimum load (15 mg) compared with CuNPs and ZnNPs which can be used as an eco-friendly material in the wastewater treatment for the effective removal of toxic compounds.

I 087

Efficient Photocatalytic Degradation of Cr(VI) using (Ag-Cu) Bimetallic Nanoparticles Through Electron Transfer Reactions

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Abstract

Removal of toxic pollutant such as Cr(VI) from waste water has become a great challenge which causes significant impact on the ecosystem destruction. However, precipitating the toxic Cr(VI) by reducing it to Cr(III) by the simple electron transfer reactions make the Cr(VI) removal process easier. Here we demonstrate the one step process for the reduction of Cr(VI) to non-toxic Cr(III) using silver-copper (Ag-Cu) bimetallic as an efficient photocatalyst synthesized via cost-effective electrochemical route. The photon (sunlight) induced reduction of Cr(VI) to Cr(III) was carried out with the linear increase in the concentration of (Ag-Cu) bimetallic phtotocatalyst with the irradiation time. Ag-Cu bimetallic NPs exhibt high recyclability for more than four cycles with significant stability. Ag-Cu bimetallic NPs demonstrated the efficient catalyst for the treatment of Cr(VI) in the wastewater treatment.

I 088

Efficient Removal of Microplastics from Water Using Reduced Graphene Oxide-Based Nanocomposite

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ABSTRACT

Microplastics (MPs) represent a critical and emerging environmental hazard, posing threats to both aquatic ecosystems and human health. This study investigates the applicability of a reduced graphene oxide(rGO) based nanocomposite for the removal of challenging microplastics from water through adsorption mechanism. The method involves subjecting an aqueous solution containing microplastics and rGO based nanocomposite to a magnetic field for a brief duration, resulting in the successful extraction of microplastics from the water. The nanocomposite is comprehensively characterized using various techniques, including x-ray diffraction (XRD), Transmission Electron Microscopy (TEM), and Raman spectroscopy. Analysis of Scanning Electron Microscope (SEM) images reveals the effective adsorption of microplastics onto the rGO based nanocomposite. Adsorption kinetics and isotherms are employed to elucidate the adsorption mechanism. In summary, our findings underscore the promising potential of the rGO based nanocomposite as an environmentally friendly and efficient solution for the removal of microplastics from water

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I 089

Conducting Polymers as Flexible Thermoelectric Materials

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ABSTRACT

Conducting polymers owing to their intrinsic low thermal conductivity and tunable electrical properties are being looked as promising thermoelectric materials. Their solution processability and flexibility provide facile integration with inorganic materials to combine advantages of both the organic-inorganic realms. Polymers such as PEDOT:PSS and poly(3-hexylthiophene) P3HT exhibited remarkable improvement in their electric conductivities on doping. Treatment of PEDOT:PSS films by organic solvents dimethyl sulphoxide (DMSO) resulted in enhancement of electrical conductivity from ~1.6 S/cm of pristine to ~150 S/cm without much affecting the Seebeck coefficient (~11-15 μV/K). Further, incorporation of Bismuth Antimony Telluride nanoparticles in DMSO mixed PEDOT:PSS not only changed the morphology of films to free-standing but also enhanced the Seebeck Coefficient upto 17 μV/K. Conducting polymers in such a flexible free-standing form can be utilized for irregular target surfaces. The enhancement of electrical conductivity has been attributed to better chain ordering and to the conductive pathways provided by metallic nanoparticles in between the polymeric chains as depicted in Figure 1 (a & b).

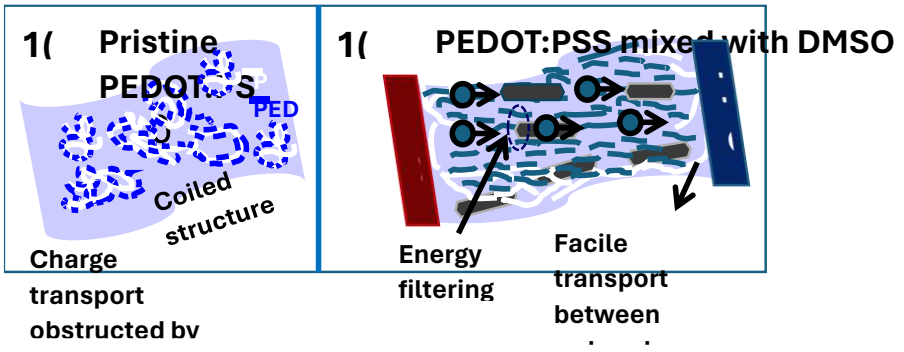

Figure 1: (a) Pristine PEDOT:PSS; (b) Alignment of PEDOT and PSS chains under the effect of organic solvent and energy filtering provided by nanoparticles in between chains

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I 090

Red Graphitic Carbon Nitride Embedded Floating Photocatalyst for Simultaneous Removal of Binary Water Pollutants

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ABSTRACT

Graphitic carbon nitride is a versatile polymeric semiconductor nano photocatalyst which is oftenconsidered as the representative material for visible light photocatalysis[1]. The colour of the conventionally synthesised graphitic carbon nitride varies from off-white to faint yellow. In this work, red-coloured graphitic carbon nitride was synthesised and embedded in an environmentally benign buoyant base, thereby fabricating a floating photocatalyst with supreme visible absorptivity and catalytic properties. The synthesised floating catalyst was utilized for theremoval of environmental pollutants from the aquatic environment. The detailed characterizationof the catalyst provided valuable insights into the development of floating photocatalysts capableof mitigating a multitude of environmental pollutants. The fabricated catalyst showed good recyclability for up to five cycles without noticeable catalyst loss from the surface of the buoyant support. The schematic representation of the synthesised photocatalyst is given in Figure 1.

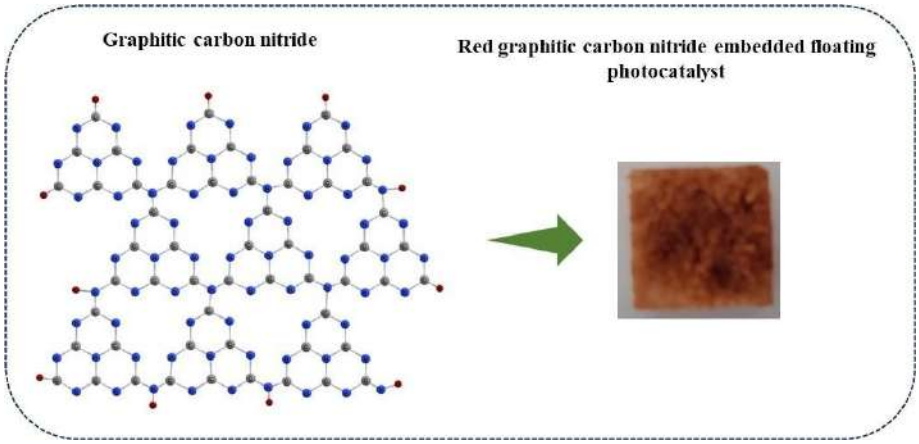

Figure 1. Schematic representation of the red graphitic carbon nitride embedded floating photocatalyst.

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I 091

Investigating The Thermoelectric Performance of Lead-Free Manganese Telluride Via Substitution of Zn for Mid-Temperature Application

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ABSTRACT

The p-type Manganese telluride (MnTe) is a potential candidate for thermoelectric application in mid-temperature range. Herein, the thermal conductivity of 1.26 W/mK at 703 K for $Mn_{1.07}Zn_{0.05}Te$ was achieved due to the substitution of Zn in MnTe, according to the stoichiometric ratio of $Mn_{1.12}Zn_xTe$ (x =0, 0.025, 0.05, 0.075, 0.1) samples were prepared via vacuum sealing and hot press methods. The incorporation of Zn drastically reduces the total thermal conductivity by contributing to the phonon scattering through point defects. Moreover, the substitution of Zn atoms which possess the oxidation state of Zn^{2+} occupancy in Mn site, examined by X-ray photoelectron spectroscopy (XPS). The increase in the carrier concentration at the elevated temperature leads to enhance the electrical conductivity to 1100 S/m at 703 K for $Mn_{1.07}Zn_{0.05}Te$, as a result the maximum power factor of 161 $\mu W/mK^2$ at 703 K is obtained for the same sample. The synergistic effect of low thermal conductivity and high electrical conductivity increased the zT value to 0.08 for $Mn_{1.07}Zn_{0.05}Te$ at 703 K.

Key words: *Phonon scattering, Point defect, Co- substitution, Thermal conductivity*

I 092

Materials for Environment and Sustainable Development Goals Mineralization of Alizarin Red Using Visible-Light-Driven Catalyst: Bismuth Aluminium Tungstate ($BiAlWO_6$)

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ABSTRACT

Twenty percent of the water pollution in the world comes from the textile industry, which is the same as 110 million people using less water for a year. 60% of azo dyes, 20% of vat dyes, and 20% of acid dyes that are carcinogenic to humans—are present in textile wastewater. When released into the environment untreated, these dyes disrupt the aquatic ecology and damage the soil. Recent studies have shown that heterogeneous photocatalysis is a versatile method for breaking down azo dyes. This work reports the degradation of Alizarin red under visible light region using Bismuth Aluminium Tungstate ($BiAlWO_6$). The photocatalyst was prepared by co-precipitation. The structural, morphological, and photophysical behavior of the materials were confirmed using FTIR, XRD, DRS, PL, FESEM, and EDAX. The optical studies showed that aluminum-doped bismuth tungstate had a reduced band gap compared to bismuth tungstate. The HRTEM exhibited a range of particle sizes from 15 nm to 30 nm, whereas the FESEM images displayed spherical morphology. The effects of various reaction parameters, such as the initial concentration of the dye solution, the amount of catalyst, and the effect of solution pH on the rate of photodegradation were optimized using Design Expert software. The degradation results revealed that the nano-catalyst removed around 85% of the AR dye in 90 mins under visible-light irradiation. The photodegradation rate of $BiAlWO_6$ was three times greater than pure $BiWO_6$ which proved the reduced recombination rate of the electron-hole pair.

Keywords: *doping, $BiAlWO_6$, photocatalysis, Azo dyes.*

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I 093

The Mechanical Properties of M30 Grade Concrete in An Underground Drainage System

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ABSTRACT

Due to significant advancements in the construction industry, the demand for river sand is outpacing its availability. Top countries are experiencing a heightened need for river sand, primarily due to rapid infrastructure development in areas such as railways, bridges, high-rise structures, and roads, as well as the production of building materials like lightweight aggregates and blocks. M sand has been recommended as an alternative to natural river sand, as it enhances the robustness of concrete and contributes to increased strength in the overall concrete structure. This research centers around conducting experimental investigations on the utilization of M sand in M30-grade concrete. The mechanical properties of concrete were studied by examining the effects of replacing river sand with M sand in 25%,50%,75%, and 100%. The compressive strength, split tensile strength, and flexural strength were studied and reported. The optimum percentage of replacement was 100% in M30 grade concrete. Using M sand in concrete helps to reduce the use of natural materials and save natural resources.

Keywords: *Compressive strength, M sand, Split tensile strength, and flexural strength.*

I 094

Bioremediation Using Microbial and Plant Lectins - A Comparative Study

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ABSTRACT

Anthropogenic activities have triggered unprecedented changes at a global scale that may lead to the mass extinction of species and the destruction of biodiversity. Bioremediation aims to partially cleanse the environment of the recalcitrant heavy metal waste generated by humans. Bacterial isolates and seedpods of Moringa oleifera obtained from heavy metal contaminated sites were tested for their ability to produce lectins for biosorption of heavy metals. Out of the 20 bacterial isolates, CuB1; PbS1 grew in M9 media supplemented with 10 to 40 ppm of heavy metals such as Cu, Cd, Pb, Sn and Hg. The bacterial and plant pod isolates were screened for lectin production activity via hemagglutination assay and the HA titres were determined. Bacterial isolates CuB1 and PbS1 exhibited high HA titre values of 256 and 512 respectively. Whereas, the seed pods of Moringa oleifera exhibited a higher titre value of 1024. A significant drop in heavy metal concentration was observed for the plant-based lectins as compared to the bacterial lectins which was confirmed using Flame Atomic Absorption Spectroscopy (FAAS) due to lectin-mediated biosorption. SEM analysis revealed the morphology and size of the isolates. CuB1 and PbS1 to be 2.43µm and 2.07µm respectively. Lectins from the seed pods of Moringa oleifera were also characterized via SEM. Further, the molecular weight of lectins was studied using SDS PAGE.

Keywords: *Bioremediation, Lectins, Moringa oleifera, Heavy metals, FAAS*

Deciphering Pollution Patterns with Cutting-edge Image Classification and Deep Learning.

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ABSTRACT

The menace of air pollution poses a grave risk to both human well-being and the ecosystem. This study harnesses the power of advanced deep learning techniques to anticipate pollution levels through image classification. Employing the EfficientNetB3 architecture, pre-trained on the extensive ImageNet dataset, serves as an adept feature extractor, capitalizing on its adeptness in learning intricate representations. The model undergoes rigorous training on a diverse dataset, embracing images that encapsulate varying pollution intensities—ranging from Moderate Pollution and No Pollution to Severe Pollution. The project unfolds through meticulous phases, encompassing the intricacies of data preprocessing, the thoughtful design of model architecture, and intensive training . An insightful evaluation of the compiled model is conducted, gauging its efficacy through metrics such as categorical cross entropy loss and accuracy. A significant facet of this endeavor lies in the creation of a predictive function. This function empowers users to input new images, receiving prompt, real-time predictions pertaining to pollution levels. Such functionality enhances the model's pragmatic utility in the realm of environmental monitoring. The culmination of this project reveals compelling insights into the efficacy of deep learning for predicting pollution levels through meticulous image analysis. The developed model stands testament to its accuracy in categorizing pollution levels, laying the groundwork for future exploration and practical applications in the domains of environmental monitoring and public health.

Keywords: *Deep learning ,EfficientNetB3,Pre-trained model,Image classification,ImageNet dataset,Pollution prediction.*

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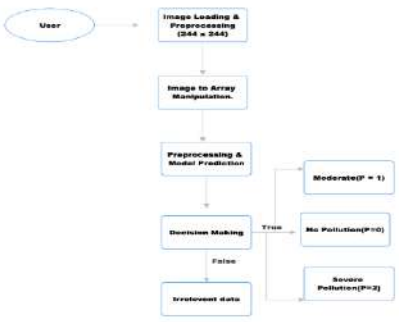

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I 096

Nanostarch: Sustainable Production and Food Industry Applications

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ABSTRACT

A fair amount of attention has been paid to sustainable production techniques recently because they are eco-friendly and can be used. As starch is inexpensive, renewable, and non-toxic, research on creating nanoparticles from it is gaining momentum. There is a dearth of literature reviewing the eco-friendly manufacturing process and potential food applications of nanostarch. The present article elucidates the environmentally friendly synthesis of nano starch, with a particular focus on its significant application in the food industry as a thickening agent, reinforcement agent in food packaging, emulsion stabilizer, and nanoencapsulation system for bioactive constituents found in food and nutraceuticals. This review provides an overview of environmentally friendly methods utilized in the synthesis of nanostarch. These methods include electrospinning, enzyme hydrolysis, high-pressure homogenization, cold plasma treatment, ball milling, ultrasonication, extrusion, and high-pressure homogenization. Using sustainable techniques to make nanostarch gives it special qualities like being biodegradable, biocompatible, and having better barrier properties, which makes it a great choice for use in the food industry. The health and security implications of administering green-synthesized nanostarch have been carefully investigated. This article provides an overview of the environmentally friendly synthesis of nanostarch and how it is used in the food industry to help the sector develop sustainably.

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I 097

Synthesis of Solar Light Driven Copper Oxide and Cerium Oxide Co-Doped with Conducting Polymer for Better Photocatalytic and Antimicrobial Activity in Water Treatment Process

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ABSTRACT

Scientists have suggested numerous research projects including the use of nanocomposites to remove different types of pollutants from water. Previous studies using copper oxide and cerium oxide as semiconductors have demonstrated the ability to degrade dyes and kill water-borne microorganisms when exposed to sunlight and visible light. The capacity of copper oxide, cerium oxide, and dopants in the treatment of waste water against the deterioration of different contaminants and microorganisms has been amply shown by these works. In this sense, the research project presented here will use a straightforward precipitation technique to create a nanocomposite made of conducting polymer (p-n-p combination), copper oxide, and cerium oxide. The resulting p-n-p material underwent extensive physicochemical studies to clarify its properties. Additionally, in comparison to the performance of a typical p-n (CuO/CeO) combination, the mechanism was supported for the optimum photocatalytic activity under visible light stimulation for the breakdown of azo dyes and killing of microorganisms. So as to demonstrate that the nanocomposite was created as one of the greatest combinations for the water treatment procedure.

Keywords: *visible light; copper oxide; cerium oxide; antimicrobial activity; azo dyes; water treatment*

I 098

Predictive Modelling of Air Pollution Using Deep Learning Techniques

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ABSTRACT

Air pollution poses a significant threat to public health, serving as a contributing factor to various diseases with fatal consequences. Consequently, the imperative to monitor and predict air quality has become extremely important in developing nations. Machine learning methodologies have arisen as sophisticated and effective tools, outperforming conventional approaches, to systematically investigate and confront the complex challenges presented by latest environmental hazards. Conducting insightful exploratory data analysis identifies pollutants directly impacting the air quality index. In this paper, we have incorporated deep learning methodologies, namely LSTM, CNN, and a hybrid CNN-LSTM model, leveraging their inherent capabilities to capture temporal dependencies, spatial patterns, and complex relationships in data. The incorporation of advanced deep learning methodologies demonstrates notable success in precisely forecasting air quality. The algorithms excel in discerning subtle patterns, recognising correlations, and extracting features from diverse sources, leading to improved precision and reliability in predicting air quality levels. The experimental findings suggest that our proposed approach, the "hybrid CNN-LSTM multivariate" model, outperforms other models in achieving more accurate predictions.

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I 099

The role of AI in circular economy and environment sustainability

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ABSTRACT

Effective utilization of available nonrenewable energy resources, pollution control, recycling and reusing of plastics are the major requirements today. The circular economy is the model designed to achieve all the above requirements through waste reduction, reusing and it concentrates from material input to disposal of contents. But the replacement of existing linear economy with the limited technologies is the tedious task. Artificial intelligence is an umbrella term with machine and deep learning as subordinate techniques plays a major role to obtain the goals of circular economy. AI offers sustainable improvements in areas such as product design, optimization, operations and infrastructure. The sectors like space, manufacturing, production, transport, energy are utilizing the benefits of AI. Resilient growth; advancements towards the Sustainable Development Goals (SDGs); green development and Lifestyle for Environment (LIFE); technology transformation and public digital infrastructure are among the other points of emphasis of the most recent G20/2023 summit, which was hosted in India and included worldwide participation. There are still certain obstacles in the way of applying AI because of data scarcity, implementation costs, and the need to integrate different industries and technology. This study examines how artificial intelligence (AI) is affecting the circular economy across many industries, as well as its benefits and drawbacks. It also looks at potential integration and usage of related technologies to help achieve more sustainable future objectives.

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I 100

Efficient Textile Wastewater Treatment Using Electrocoagulation Methodology with an AC@MgO Catalyst-Loaded Al Foam Electrode: A Comprehensive Study on Purification, Disinfection, and Removal of Heavy Metals

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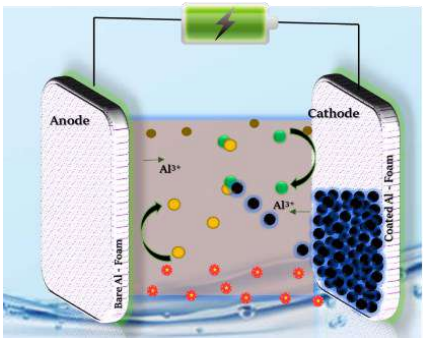
ABSTRACT

Textile wastewater can be treated efficiently by the electrocoagulation (EC) process, utilizing an aluminium (Al) foam electrode. Here, we present the green synthesis of MgO@nitrogen-doped biochar-derived activated carbon from date seeds, denoted as activated carbon/magnesium oxide (AC@MgO) catalyst. Further, the catalyst was loaded firmly at the Al-foam electrode by the spray pyrolysis process (Al-F/AC@MgO) for the EC study. The results of the lab-scale EC-treatment using an Al-F/AC@MgO electrode showed notable variation with a short retention period (20–30 min) in the wastewater composition collected from the textile industry. Importantly, the complete bleaching of colour from textile effluents was studied by UV-Vis spectra. Moreover, the total organic carbon (TOC) value has decreased from 1280 to 230 mg/L. In the EC process, lead (Pb), copper (Cu), and other suspended particles were significantly reduced from textile industry wastewater. In comparison to the results of the bare Al-F electrode in textile effluent treatment, the Al-F/AC@MgO-coated electrode greatly enhanced its efficiency. Additionally, the modified catalyst has excellent disinfectant performance, as demonstrated by the removal of S. aureus and E. coli. Thus, the proposed methodology could be applied to minimize the environmental toxicity and in the advancement of wastewater reuse and in biomedical areas.



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I 101

Metal Particle Modified Silicon Nanowires for the Removal of Textile Dyes from Water

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ABSTRACT

Water contamination from significant industrialization and urbanization has drawn the attention of numerous researchers to water remediation techniques like photocatalysis. The intriguing characteristics of silicon nanowires (SiNWs), like light trapping and catalytic activity for the removal of textile dyes, have drawn attention to this material. In this work, the synthesis of SiNWs and their modifications with metal particles like copper or silver with different concentrations has been reported. Metal-assisted chemical etching (MACE) method was used to synthesize SiNWs with an optimized aspect ratio as the method was easy and cost-effective. The as-prepared material was studied by X-ray diffraction, electron microscope, Fourier transform infrared spectroscopy, and UV-visible spectroscopy. The XRD confirms the deposition of the silver and copper particles on SiNWs. The FESEM image reveals the formation of network-like structures for silver and flower-like structures for Cu-doped SiNWs. The as-prepared samples have shown efficacy in removing textile dyes like Rhodamine B by the process of photocatalysis under irradiation with UV light. It has been shown that when the concentration of the copper nanoparticles was increased, a significant increase in the photocatalytic activity was obtained. The removal efficiency, when calculated came out to be laying within the range between 50 -65 %. So far, the authors are concerned there are no reports related to the application of Cu/Ag decorated SiNWs in removing different textile dyes from contaminated textile affluents.

Keywords: *Silicon nanowires, Photocatalysis, Rhodamine B dye, Metal assisted chemical etching*

I 102

Studies on the Photodegradation of Antibiotic using III-Nitride Semiconductors

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ABSTRACT

In present scenario, dyes and effluents are released into the environment as pollutants rom textile and pharmaceutical industries. Photocatalytic dye degradation is crucial for environmental protection, as it effectively removes synthetic dyes and pharmaceutical residues from wastewater. Ciprofloxacin, a broad- spectrum antibiotic, is commonly found in rivers in India with median concentration level of 275.2 ng/L, posing risks to aquatic ecosystems and potentially contributing to antibiotic resistance [1-4]. The study focuses on the photocatalytic degradation of these pollutants, utilizing InGaN photocatalysts to develop effective and sustainable methods for their removal from wastewater, addressing environmental and water quality concerns. In this work, gallium nitride and indium gallium nitride [$In_xGa_{1-x}N$ (x= 0 to 1)] alloy was synthesized using chemical co-precipitation technique with indium nitrate and gallium nitrate as precursors followed by ammonolysis. Gallium Nitride nanoparticles was found to have lattice parameters of a = 3.157Å and c = 5.135Å. The composition of indium in InGaN nanoparticles was calculated using Vegard's law. The crystallite size of gallium nitride nanoparticle was found to be around 10 nm, which was found to increase with indium content to around 20 nm. The bandgap of GaN nanoparticles was calculated to be 3.34eV, which decreases with increasing indium content. The optical and morphological properties were studied using photoluminescence spectroscopy and scanning electron microscopy (SEM) studies. The degradation of ciprofloxacin using InGaN nanoparticles is fivefold efficient than GaN nanoparticles under UV radiation.

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I 103

Application of Nanocrystalline Spinel MFe_2O_4, (M = Co and Cu) In Wastewater Treatment

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ABSTRACT

Transition metal spinel ferrites of the formula MFe_2O_4 (M = Cu and Co) were successfully synthesized following co-precipitation method and the structural, optical, photocatalytic, antimicrobial, and toxicity studies have been carried out. The characterization of the title compound has been carried out using XRD, SEM, EDS, FT-IR, PL, and UV analyses. The XRD studies confirmed a cubic spinel structure with the Fd-3m space group, indicating that copper and cobalt ferrites exist in the nanocrystalline size of 43 nm and 17 nm, respectively. The SEM images revealed the agglomerated nature of the ferrite nanoparticles, and EDAX spectrum confirmed the elemental compositions present in the samples and their purity. The FT-IR spectra indicated the presence of metal–oxygen stretching bands. The antimicrobial properties were investigated using the agar well diffusion method. Drosophila, an invertebrate fly model, has been used to study the in- vivo toxicity of synthesized nanoparticles. The ferrite samples demonstrated photocatalytic performance in the visible active region, as assessed by the degradation of methylene blue (MB), a cationic dye, in aqueous solution under visible irradiation. After 105 minutes, $CuFe_2O_4$ and $CoFe_2O_4$ catalysts exhibited degradation percentages of 72% and 56% for the MB solution, respectively, affirming their potential utility in treating wastewater containing organic dyes.

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I 104

Ameliorative Effect of Biogenic Iron Oxide Nanoparticles on Microplastic Stressed Azolla

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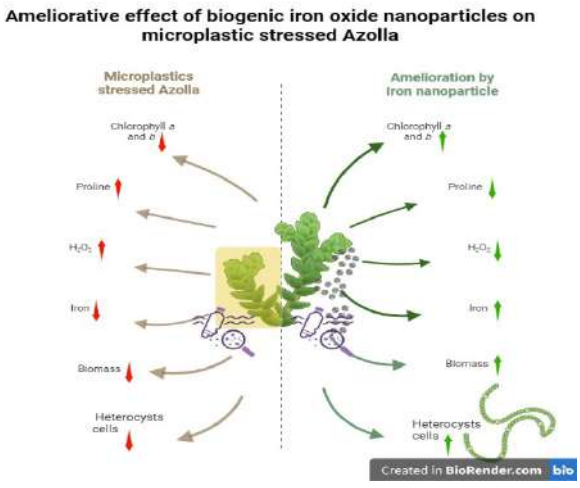
ABSTRACT

This study explores the potential of biogenic iron oxide nanoparticles (FeNp) in alleviating the detrimental impacts of microplastic pollution on azolla—an aquatic fern serving as a model for plastic-induced aquatic pollution. Green-synthesized iron oxide nanoparticles, utilizing Chaemotomorpha antennina, were prepared and characterized. The application of these biogenic FeNp to microplastic stressed azolla resulted amelioration of the stress responses. A substantial reduction of stress markers was quantified through diverse biochemical assays. Assessments of chlorophyll, soluble sugar, iron, and amino acids in the FeNp treated microplastic stressed azolla revealed a noteworthy increase with respect to the control plants. However, some stress markers such as proline, H_2O_2, exhibited up to a twofold reduction. These findings hold significance for the agricultural industry, which contends with diminished yields due to microplastic contamination. Furthermore, given azolla's role as an excellent biofertilizer, this research suggests a potential solution to enhance agricultural productivity while addressing the challenges posed by plastic-induced stressors.



Keywords: *iron oxide nanoparticles, microplastics, azolla, biogenic, microplastic amelioration.*

Harnessing Solar Energy for Photocatalytic Degradation of Toxic Azo Dyes and Antibacterial Efficacy via Cr-doped α-Fe_2O_3 Nanoparticles: Real-Time Monitoring and Mechanistic Insights

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ABSTRACT

Pristine and Cr-doped α-Fe_2O_3 nanoparticles are synthesized using low-cost and simple one-step hydrothermal method without any precipitating agent. Cr-doped α-Fe_2O_3 was found out to be a promising candidate for recyclable photocatalytic application for Congo-red degradation under normal sunlight irradiation along with excellent antibacterial properties. Addition of Cr shows a significantly improved degradation rate from 20% to 96% in just 20 minutes, which was also monitored in real-time using IoT. Also, a high degree of mineralization was achieved (~85 %), which was confirmed using (Total Organic Carbon) TOC content. In parallel, BOD_5/COD ratio confirmed the fast degradation efficiency using a small amount of catalytic dosage (~ 0.35 g/L). Moreover, Cr-doped α-Fe_2O_3 displays excellent antibacterial activity towards E.coli and E.Faecium. Major factors involved in sunlight driven photocatalytic activity for example absorbance range, porosity, separation between e^--h^+, charge transfer property were surprisingly improved by Cr doping and henceforth increased photocatalytic activity and antibacterial property. This work highlights the potential utilization of Cr-doped α-Fe_2O_3 for the purification and disinfection of industrial waste water.

Keywords: *Waste-water treatment, Photocatalytic, nanoparticles, antibacterial, Cr doped α-Fe_2O_3.*

I 106

Synergistic Photocatalytic Effect of Zn-Doped Co_3O_4/g-C_3N_4 Nanocomposite for Efficient Removal of Cationic Dyes

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ABSTRACT

In this study, Zn doped Co_3O_4 was prepared by using a co-precipitation method, and a simple pyrolysis method was adopted to obtain g-C_3N_4. Consequently, Zn doped Co_3O_4/g-C_3N_4 nanocomposite was synthesized by using a sonication method. Zn-Co_3O_4/g-C_3N_4 nanocomposite have been employed for selective removal of cationic dyes from aqueous solution. The synthesized nanocomposite was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM), High-resolution transmission electron microscopy (HR-TEM), UV-visible spectroscopy (UV-Vis), Raman spectroscopy, Photoluminescence (PL) and BET analysis to investigate the structural and morphological characteristics of the materials. Zn-Co_3O_4/ g-C_3N_4 nanocomposite exhibit excellent potential in removing cationic dyes such as Rhodamine B (RhB) and Malachite green (MG) via photocatalytic degradation under sunlight. Variables such as pH, catalyst dose, dye concentration, and time were used to test the photocatalytic efficiency of the catalyst. In this study, Zn-Co_3O_4/ g-C_3N_4 nanocomposite demonstrated maximum degradation of 98% against MG dye in 150 minutes whereas a maximum degradation of 90% was evidenced in 120 minutes in case of RhB dye, making it an excellent photocatalyst. Furthermore, Zn-Co_3O_4/ g-C_3N_4 nanocomposite illustrated high photo-stability for cationic dyes degradation during five consecutive cycles, with little effect on the photocatalytic activity.

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Interface engineering at 2D/2D $CaTiO_3$/protonated g-C_3N_4 nanosheets for enhanced photocatalytic hydrogen evolution through efficient spatial charge separation

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ABSTRACT

Photocatalytic water splitting is one of the promising approaches to address the energy crisis and environmental pollution which are regarded as major obstacles to the growth of modern society [1]. Perovskite materials with the formula ABO_3 have garnered much interest for their multifunctional properties, including applications in fuel cells, solar cells, supercapacitors, and environmental remediation. Among the various perovskites, $CaTiO_3$ is a favorable material for water splitting as it is a common cheap semiconductor in industry and possesses high thermal stability, stable crystal structure, favorable conduction and valence band positions, and good catalytic properties [2]. In this work, both amorphous and crystalline $CaTiO_3$ photocatalysts were prepared and a novel $CaTiO_3$/PCN heterojunction was successfully constructed using the self-assembly method for photocatalytic hydrogen production applications. To gain a deeper understanding of the impact of crystallinity on photocatalytic hydrogen generation, we performed a comprehensive comparative analysis of the amorphous $CaTiO_3$/PCN and crystalline $CaTiO_3$/PCN composites. The as-synthesized amorphous $CaTiO_3$/PCN exhibited a promoted hydrogen evolution activity of 550 µmol/g/h, surpassing its crystalline counterpart. This superior performance is attributed to the high specific surface area of amorphous materials, facilitating catalytic reactions. In summary, our study suggests that amorphous materials hold significant potential for efficient photocatalytic production of hydrogen and the synthesis methods employed for these materials present a promising alternative to traditional high-temperature approaches.

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I 108

Efficient Solar light induced Photo degradation of anionic Congo Red Dye Utilizing Ce@Co_3O_4-$BiVO_4$ Catalyst: A Sustainable Approach for Wastewater Treatment

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ABSTRACT

A new modified Ce@Co_3O_4/$BiVO_4$ p-n heterojunction photo catalyst is synthesized employing a one-step technique for photo catalytic degradation of Congo Red (CR) dye. The structural, morphological, optical, and electrical characteristics of the doped catalyst were investigated using XRD, FTIR, FE-SEM, HR-TEM, PL, EIS, TGA, XPS, UV-DRS, and BET analysis. The band gap energy of modified $BiVO_4$ decreased from 2.9eV to 1.95eV while the absorption peak was shifted to the visible light range. The photo catalytic activity of the developed catalyst was investigated by degrading CR dye under various conditions such as pH, beginning dye concentration, catalyst dosage, time, temperature, and seasons. The maximum degradation was seen at acidic pH with a catalyst dosage of 0.06g/L in 60 minutes under sun light. The photo degradation of CR dye followed pseudo-1st order kinetics. The lower intensity in PL spectra indicated the reduction in charge carrier recombination, and the higher surface area from BET analysis assisted the superior photo catalytic activity. The reusability investigation displayed the presence of crystallinity and phase of catalyst that may be employed for practical applications.

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Synergistic Boost in Photocatalytic Activity of Interfacial 2D-2D $ZnNiInS_2$:In_2S_3/g-C_3N_4 Nanosheets for Photocatalytic Hydrogen Production and Degradation

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ABSTRACT

The pursuit of efficient and sustainable photocatalytic materials for hydrogen production and organic pollutant degradation has gained significant attention in recent years. In this study, we explore the synergistic enhancement of photocatalytic activity achieved through the integration of interfacial 2D-2D $ZnNiInS_2$:In_2S_3/g-C_3N_4 nanosheets. Through a comprehensive characterization approach combining X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS), the structural morphology and elemental composition of the nanocomposite are thoroughly examined. Our investigation focuses on assessing the photocatalytic performance of the synthesized nanomaterials for both hydrogen evolution and degradation of organic pollutants under simulated solar irradiation. The results reveal a remarkable synergistic boost in photocatalytic activity, attributed to the unique interfacial interactions between the $ZnNiInS_2$:In_2S_3 and g-C_3N_4 nanosheets. The interfacial integration of these two-dimensional materials facilitates efficient charge separation, enhances light absorption, and promotes the generation of reactive oxygen species, crucial for photocatalytic reactions. Furthermore, the intimate contact between the $ZnNiInS_2$:In_2S_3 and g-C_3N_4 components creates active sites and accelerates interfacial charge transfer processes, contributing to the overall enhancement of photocatalytic performance. The promising results obtained from our study underscore the potential of interfacial 2D-2D nanocomposites as advanced photocatalytic materials for sustainable energy generation and environmental remediation applications. The synergistic effects observed in this study provide valuable insights for the design and development of next-generation photocatalysts with enhanced efficiency and functionality. Overall, the synergistic boost in photocatalytic activity demonstrated by the $ZnNiInS_2$:In_2S_3/g-C_3N_4 nanosheets holds great promise for addressing pressing global challenges related to energy sustainability and environmental pollution mitigation.

Keywords: *g-C_3N_4, $ZnNiInS_2$:In_2S_3, Photocatalyst, Water splitting, Degradation*

I 110

Photocatalytic Hydrogen Production Activity of Nanostructured ZnCuOS Supported Graphitic Carbon Nitride

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ABSTRACT

This study investigates the photocatalytic hydrogen production activity of a novel composite material composed of nanostructured ZnCuOS supported on graphitic carbon nitride (g-C3N4). The synthesis of the ZnCuOS/g-C_3N_4 composite was achieved through a facile and cost-effective approach, combining hydrothermal synthesis and a subsequent calcination process. The resulting material was characterized using various analytical techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Fourier-transform infrared spectroscopy (FTIR), to elucidate its structural and morphological properties.The photocatalytic performance of the ZnCuOS/g-C_3N_4 composite was evaluated under simulated solar irradiation. The results demonstrate a significantly enhanced hydrogen evolution rate compared to individual ZnCuOS and g-C_3N_4 counterparts. The synergistic effect of the composite structure promotes efficient charge separation and migration, leading to improved photocatalytic activity. Additionally, the stability and recyclability of the catalyst were investigated over multiple cycles, affirming its robustness and potential for practical applications. The study provides valuable insights into the design and fabrication of composite photocatalysts for enhanced hydrogen production, contributing to the advancement of sustainable and renewable energy technologies. The synergistic combination of ZnCuOS and g-C_3N_4 opens new possibilities for developing high-performance photocatalytic materials with implications for environmental remediation and clean energy production.

Keywords: *sulfide-based material, Water Splitting, Photocatalytic Hydrogen Production, Nanomaterials.*

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Bio Blended Epoxy Coatings for Anticorrosion Applications

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ABSTRACT

Epoxy has become a conventional choice for protective coatings, which is a petroleum-based product. Nevertheless, these epoxy and PU (polyurethane) polymers encompass Bisphenol-A (BPA) and isocyanates, which possess the potential to endanger humans and other organisms upon exposure. The continuous utilisation of these polymers leads to a rise in the concentration of BPA in the environment. Additionally, these polymers necessitate the use of Volatile Organic Compounds (VOCs) as solvents to maintain their fluidity, hence posing a threat to the environment. Vegetable oils (VOs) are a type of hydrocarbon substance obtained from plants that can serve as an alternative to traditional hydrocarbons. They possess several advantageous qualities such as being non-toxic, reasonably inexpensive, biodegradable, and renewable. Vegetable oils (VOs) typically consist of double bonds, hydroxyl groups, and ester sites, which can be altered to produce polymers suitable for coating applications. Epoxidized vegetable oils (EVO) can undergo modification to produce non-isocyanate polyurethanes (NIPU) through the process of CO_2 fixation under high pressure. These NIPUs can be conveniently cured at room temperature. The objective of this study was to examine the use of bio-blended DGEBA/CSBO-based NIPU coatings in order to increase the bio-content of epoxy. Various weight proportions of cyclic-carbonated soya bean oil (CSBO) were incorporated into epoxy (DGEBA). Tri ethylene tetraamine (TETA) was applied as a curing agent and deposited onto aluminium substrates at ambient temperature. The coatings were examined using FTIR, FESEM, contact angle goniometer, and TG-DTA. Polarisation and electrochemical impedance spectroscopy (EIS) studies were conducted to gain further insights into the corrosion characteristics of the material.

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Photocatalytic Degradation of Cationic Dyes Using Green Synthesized Copper-Doped Cerium Oxide Nanoparticles

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ABSTRACT

Cerium oxide nanoparticles have emerged as promising candidate for photocatalytic degradation of cationic dyes due to their unique properties such as high catalytic activity, large surface area, switchable redox reactivity. In this study, we have investigated the efficacy of copper doped CeO_2 nanoparticles (Cu-doped CeO_2 NPs) synthesized using Actinidia deliciosa peel extract as a reducing and stabilizing agent for photocatalytic effect of cationic dyes. The green synthesized nanoparticles were characterized by X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, and UV-visible spectroscopy (UV-Vis). XRD pattern revealed the cubic phase of Cu-doped CeO_2 NPs with a crystallite size of 6 nm, whereas FESEM images indicated the grain size of 65 nm. The characterization techniques confirmed the successful synthesis of the Cu-doped CeO_2 NPs. The photocatalytic activity of the nanoparticles can be attributed to their unique structural and optical properties, facilitating efficient degradation of cationic dyes. The synthesized Cu-doped CeO_2 NPs exhibited remarkable efficiency in degrading methylene blue (99%) and brilliant green (96%) dyes under solar light. This study emphasizes the potential of Cu-doped CeO_2 NPs synthesized via greener routes as efficient photocatalysts for environmental remediation applications.

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Synthesis and Characterization of Zn-doped SnO_2 Nanoparticles and their Photocatalytic Activity

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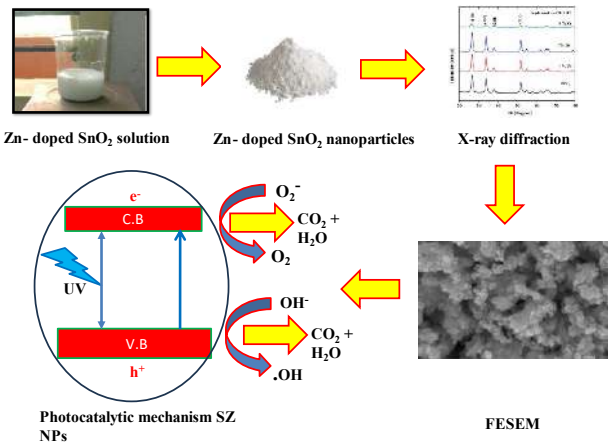
ABSTRACT

This study investigates the synthesis of Zn-doped SnO_2 (Zn-SnO_2) nanoparticles using the co-precipitation method for the photocatalytic degradation of malachite green dye. The resulting Zn-doped SnO_2 nanoparticles exhibit a tetragonal structure and spherical agglomerated morphology, confirmed by X-ray diffraction (XRD) and field-emission scanning electron microscopy (FESEM) analysis. The Fourier-transform infrared (FTIR) spectrum reveals the vibration of the Sn-O-Sn bending bond in the range of 608 cm-1. Optical studies show that Zn-doped SnO_2 direct transitions occur with bandgap energies in the range of 3.35-3.09 eV. The photocatalytic activities of the pure and Zn-doped SnO_2 samples were evaluated by degrading malachite green dye in an aqueous solution under UV light irradiation. This research contributes to materials for reducing water pollutants and environmental cleanup.

Keywords: Co- precipitation; Zn-SnO_2; Malachite green; Photocatalytic degradation.



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I 114

SnS Thin Films Deposited at Room Temperature – Efficient and Reusable Dark Catalyst for Water Remediation at Ambient Conditions

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ABSTRACT

Dark catalytic degradation of organic water contaminants has become a practical, affordable, and energy effective method for treating wastewater. This study describes the catalytic degradation of textile dyes under dark ambient conditions using SnS thin film as a catalyst without the assistance of any external stimuli. The thin films were deposited by a modified SILAR method at room temperature and characterized using XRD, XPS, FESEM, TGA, and UV-VIS spectrophotometers. Tin chloride, sodium sulphate and triethanolamine were used as tin source, sulphur source and complexing agent, respectively. Characterization revealed polycrystallinity, orthorhombic crystal structure, absence of impurity phases, presence of constituent elements, panchromatic optical behavior, thermal stability, and so on. The dark catalytic degradation of methylene blue dye was investigated using a spectrophotometer and validated by LCMS analysis and an adsorption desorption test. The decrease in degradation rate in the presence of isopropanol indirectly demonstrated the role of the hydroxyl radical in dye degradation, which was confirmed by the terephthalic acid test. The role of dissolved oxygen in the degradation process is also investigated, and a dye degradation mechanism is proposed. A kinetic study revealed that dark catalytic degradation follows pseudo-first-order kinetics. The influence of initial dye concentration, magnetic stirring, and stoichiometry of the catalyst on the degradation efficiency was also studied. The same catalyst was used five times in succession to test its reusability, and it was then structurally and thermally characterized to test its stability. SnS thin film catalysts have shown the ability to degrade anionic (methyl orange) and cationic (rhodamine B, methylene blue) dyes, as well as a commercially available dye. This study emphasizes the possible use of SnS thin film as an effective, reliable, and reusable around-the-clock catalyst for the degradation of dye-contaminated waste water without the assistance of light or any chemical additives.

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Catchment Erosion and Degradation study for Pawna-Indryani Sub-basin, Maharashtra –A case study on Integrated Geo-informatics Technology and Remedial measures

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ABSTRACT

Geo-environmental Hazards refers to natural or human-induced phenomena which pose a threat to environment, human and ecosystem. The Pawna-Indrayani sub-basin is the part of Bhima River basin which is region of Pune and Raigrah district of Maharashtra and is a part of Western Ghats. In the present study, Geo-environmental hazards like erosion and forest degradation have been perceived and analyzed. Geological mapping, hydrological modeling and spatial analysis techniques were employed to understand the spatial distribution and the severity of these hazards within the sub-basin. Various thematic layers, such as slope, geology, soil, drainage and landuse/landcover were integrated through GIS platform to find out various geo-environmental hazards. In addition to hazard assessment, this study proposes a set of remedial measures to mitigate the identified environmental risks. The results indicated that there is around15.79% (233.699 sq km), 22.63% (334.925 sq km), 19.83% (293.519), 26.85% (397.315 sq km), 27.34% (404.689 sq km) of soil erosion . Similarly, 10.45% (154.74sq km), 18.95% (280.498sq km), 6.61% (97.817sq km), 15.01% (235.104 sq km), 2.878% (42.598 sq km) of Forest degradation and natural vegetation in year 2002, 2003, 2015, 2019, 2022 respectively. Overall this study underscores the importance of geo-informatics technology with traditional environmental assessment methodology to address complex geo-environmental hazards effectively. According to the Sustainable Development Goal number 13, to take urgent action to combat climate change and its impact remedial measures have been applied to reduce these hazards.

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Climate Change Impact on Agriculture for Kiliyar Sub Basin, Tamilnadu - An Integrated Study Through Geoinformatics Techniques

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ABSTRACT

Climate change poses highly challenges to Agricultural production, particularly in regions like kiliyar sub- basin, the livelihoods is heavily depended on agriculture. This study deals with advanced techniques like remote sensing (RS), geographical information system (GIS), and global positioning system (GPS) techniques to assess the impact of climate change on agricultural productivity. Through the analysis of satellite image and non-spatial data changes in land cover and land use are evaluated by year. The Objective of this study is to carry out the analyses of climate change and its impact on agriculture for Kiliyar Sub Basin and to develop sustainable agriculture land management model through Geoinformatics technique. In recent years GIS has provided spatial dimension to natural resource management and planning. To adopt smart agriculture to address the climate change challenges that adversely affect crop productivity and livelihoods of the farming community. The analysis through geospatial technique gives better yield cultivation in agricultural management. The finding of this study contributes to the understanding of how climate change is affecting agricultural production in kiliyar sub-basin, and the implementation for achieving sustainable development goals (SDGs). By RS and GIS techniques, stakeholders can identify areas most susceptible to climate change impact, prioritize adaptation and mitigation strategies. Furthermore, this research aligns with several SDGs, including SDG – 1 (No Poverty), SDG - 2 (Zero Hunger), SDG - 13 (Climate Action), SDG – 15 (Life on Land).

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Amidoxime Functionalized Zinc Oxide Nanoparticles for the Effective Adsorption of Endocrine Disrupting Pollutants

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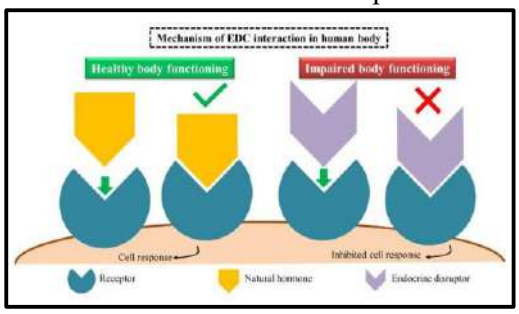
ABSTRACT

Endocrine disruptors are chemical agents from cosmetics, fertilizers, plasticizers, etc., that interfere with the functioning of hormones causing detrimental effects in humans and animals. The most abundant endocrine disruptors are bisphenol A (plastic containers), parabens, phthalates (cosmetics and body care products), triclosan (toothpaste), etc. In this study amidoxime functionalized zinc oxide nanoparticles (ZnO-AO NPs) were used as adsorbent for the removal of endocrine disruptors and the model pollutant is Bisphenol – A. ZnO NPs were synthesized by chemical method and functionalized with amidoxime in series steps of reactions. The nanoparticles were characterized using FE-SEM, XRD, and EDS to confirm the crystalline structure, composition, and morphology. ZnO nanoparticles of 70 nm size with high crystallinity were obtained. Functionalizing the NPs with amidoxime helps in increasing their affinity towards the endocrine-disrupting pollutants due to the interaction by attachment of specific ligands onto the nanoparticle surface. Amidoxime also helps enhance the formation of pores on the nanoparticles' surface to favor adsorption. Batch adsorption studies were performed to investigate the effect of pH, adsorbent dosage, contact time, and concentration, on adsorption of BPA in aqueous solution. ZnO-AO nanoparticles exhibited a maximum adsorption efficiency of 90.1% at pH 8 for an adsorbent dosage of 50 mg/50 mL containing 30 ppm concentration of BPA.



Keywords: *Adsorption, amidoxime, endocrine disruptors and zinc oxide nanoparticles*

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Ice Bath Assisted Low Temperature Synthesis of Bismuth Ferrite Nanoparticles and its Sono-pyro Catalysis of Dyes

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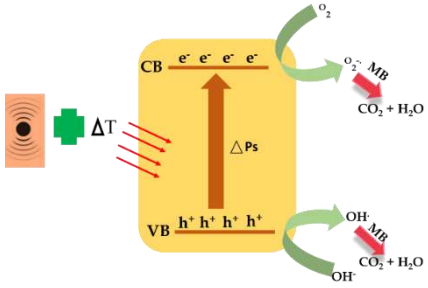
ABSTRACT

Strong synergistic pyro-sono catalytic dye degradation was notified with novel low temperature ice bath assisted synthesis of $BiFeO_3$. Ice-bath assisted synthesis at 4^0C yielded phase pure forms of highly crystalline $BiFeO_3$. The prepared nanomaterials were studied for their physicochemical, morphological dielectric and magnetic properties with sophisticated analytical instruments. Pyro catalysis was held with the hot-cold alternating cycles with the bath sonicator under the absence of ultrasound excitation. It emanated from the conjugation of pyroelectric effect with electrochemical process of oxidation/reduction mechanisms. Sono-pyro catalysis was rendered to create the piezo-ferro-pyroelectric catalytic properties of $BiFeO_3$ to aggravate the reduction process. The adopted process achieved higher degradation efficiencies of textile dyes of MB, RhB and MO under study with the mechanism of synergistic effect of piezo-pyro-ferroelectric behavior of $BiFeO_3$.

Keywords: *Bismuth ferrite, sonocatalysis, pyro catalysis, synergism, ice bath, phase pure.*



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Adsorptive Removal of Nitrate Ions from Aqueous Solution by Mesoporous Metal Oxide nanoparticles

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ABSTRACT

Global nitrate contamination, spurred by agricultural and industrial activities, poses severe risks togroundwater. The World Health Organization (WHO) has established a maximum contaminant level (MCL) for nitrate in drinking water, setting the safe limit at 50 mg/L[1]. Prolonged exposure to elevated nitrate levels in drinking water has tremendous health effects on human beings and demands research for efficient nitrate removal adsorbents. The remarkable adsorption properties and efficacy of metal oxide nanoparticles have gained considerable interest in their potential for water treatment applications[2]. Our study aimed to examine nitrate ion removal by metal oxide nanoparticles in an aqueous solution. A metal oxide nanoparticle was synthesized by the co-precipitation method, and the morphology, crystal structure,and surface area of the synthesized nanoparticles were characterized by X-ray diffraction (XRD), High- Resolution Transmission Electron Microscopy (HRSEM), and Brunauer-Emmett-Teller (BET). The optimal adsorbent dosage, and the effect of contact time, initial nitrate concentration, and co-existing anionson nitrate adsorption were studied in a batch model. The experimental data were fitted to widely used adsorption kinetic models and adsorption isotherms. Desorption and regeneration studies were carried out to examine the ability to release and recover nitrate ions from the adsorbent. Also, the influence of co-existing ions on the adsorption of nitrate was studied. Our study highlights the potential of metal oxide nanoparticles as a viable and promising adsorbent for nitrate ion removal in water, offering an effective solution for the water treatment process.

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I 120

Characterization, Adsorption and Kinetics studies: Treatment of Textile Dyeing Effluent by novel natural Coagulation cum Adsorption Process

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ABSTRACT

The treatment of textile dyeing effluent is one of the prime requirements for reducing the water pollutant. In this study, Cow Dung Ash (CDA) is used as a natural coagulant for treating the dyeing effluent and used to reduce the physical and chemical characteristics such as pH, Turbidity, COD, Colour, TS present in the effluent. The Coagulant was characterised by FT-IR, XRD, FE-SEM and EDX analysis and its modifications are compared with settled sludge after the treatment. The initial and final characteristics of the dyeing effluent and treated water is analysed, compared and the optimum conditions such as contact time, coagulant dose, pH, dye concentration are obtained. The maximum removal efficiency of colour, turbidity, COD and TS is obtained as 99.7%, 100%, 86.7% and 99.5% at optimum conditions like coagulant dose of 5g, contact time of 20min and optimum pH of 4-6.28 respectively. The CDA is having more surface area due to its fineness and adsorption capacity due to the availability of electrostatic interaction. The adsorption capacity and kinetics study are fitted with Langmuir, Freundlich, Temkin and D-R isotherms and Pseudo-first-order and Pseudo-second-order kinetic models respectively. The experimental data is perfectly fitted with Freundlich non-linear isotherm and Pseudo-second-order kinetic model and obtained the R2 value of 0.95037 and 0.99993 respectively. We hope that, the CDA is technically feasible, efficient and cost effective waste material can be used as natural coagulant and it has the capability to reuse it for multiple times to treat the dyeing effluent.

KEY WORDS: *Colour, Natural Coagulant, Textile dye, Cow Dung Ash, Adsorption, Isotherm, Kinetics*

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A Nano-phytoremediation Approach for Arsenic Pollution Abatement

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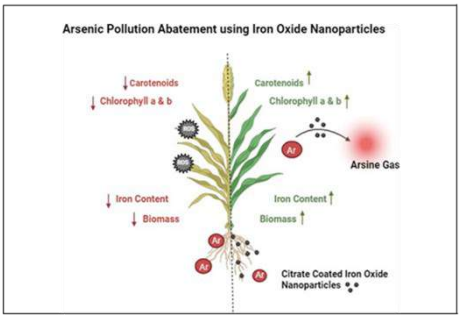
ABSTRACT

Nano-phytoremediation technology is a new, green, and eco-friendly alternative for environmental cleanup and management without harming nature. Nano-phytoremediation using green synthesised nanoparticles harnesses the catalytic activity of the benign nanoparticles as well as the innate ability of plants to degrade and metabolize the pollutants present in the environment. In the present study, arsenic pollution reduction was initiated by nano-phytoremediation using green synthesized Iron oxide nanoparticles (FeNp, Fe_3O_4) along with the plant Setaria italica (common name - Foxtail millet). The Foxtail millets were supplemented with 25 µM/ml of the pollutant -Sodium arsenate. Nano-phytoremediation initiated using FeNp nanoparticles showed enhanced remediation activity. The FeNp nanoparticles (both bare as well as capped nanoparticles) were easily up-taken by the plants. When coated with tri-Sodium citrate, nanoparticles showed better plant uptake than bare Np. The up-taken nanoparticles translocated through roots to aerial parts of the plants further resulting in more photoassimilate production, and thereby overcoming the arsenic stress. Interestingly, FeNp did not show any toxicity in plants. Thus FeNp enabled the plants to overcome the arsenic stress. Another notable feature of the FeNp was that it was capable of catalytically degrading the Sodium arsenate per se into gaseous arsine gas (AsH3), hence making the arsenate less available to the millet plants especially at high FeNp (70-120 mg/L) concentrations. FeNp uptaken by the plants is utilised not only in quenching reactive oxygen species (ROS) such as H_2O_2, but also for the production of carotenoids so as to overcome arsenic stress (As). Hence, we would like to conclude that Nano-phytoremediation approaches could effectively solve arsenic amelioration in Indian farms where arsenic is prevalent in the soil in toxic amounts.



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Ternary Ag-ZnO/g-C_3N_4 nanocomposite photocatalyst for degradation of cationic and anionic dyes

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ABSTRACT

The most significant cause of water contamination is industrial dyes. Because of their persistence, these harmful dyes pose a significant threat to aquatic life and are known carcinogens to humans. In the present study, ZnO-based composite with metal (Ag) has been synthesized through the hydrothermal method. The synthesized samples were analyzed by various characterization techniques. Cationic dye (Methylene Blue) and anionic dye (Methyl Orange) have been used as model pollutants in photocatalytic degradation experiments using homemade photocatalytic apparatus and visible light irradiation. Based on the outcome of the experiments, Ag/ZnO nanocomposite exhibited maximum degradation efficiency within the 40 min exposure of light. The recycling experiments revealed that the Ag coupled ZnO nanoparticles had a greater than 92% degradation efficiency of MB dye, confirming that the stability of ZnO. XPS analysis revealed charge carrier segregation in Ag/ZnO nanocomposite due to the formation of Schottky barriers. Further, melamine was used as a precursor in a chemical precipitation procedure, g-C_3N_4 was modified with silver doped ZnO nanoparticles. Ag nanoparticles are crucial for electronic transition transfer. Ag particles growing on the surface of ZnO and g-C_3N_4 in a ternary heterojunction Ag-ZnO/g-C_3N_4 broaden the photocatalyst's response range to visible light due to the surface plasma-resonance effect. The results showed that the modification of g-C_3N_4 with Ag/ZnO has increased activity under visible light and is suitable for photodegradation when compared to the bare g-C_3N_4.

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Enhanced Photocatalytic Degradation of organic dyes by Cerium oxide nanoparticles synthesized by acrylic amide route

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ABSTRACT

Ploy acrylamide and acrylamide co polymers are used in many industrial processes such as the production of paper, dyes and plastics and also in the waste water treatment. In this work, cerium oxide nanoparticles were prepared by sol gel dip coating route. Acrylamide and N, N-methylene-bis acrylamide monolayer were used as cross linking polymer and Ammonium persulphate acts as gelling agent for the synthesis of cerium oxide nanoparticles. The synthesized powder was characterized by powder X-ray diffraction which indicates all the peaks corresponding to cubic structure and its various parameter such as crystallize size, micro strain, dislocation density were calculated. The morphology, compositional analysis and crystalline nature of the samples were performed by Scanning Electron Microscope, X-ray Photoelectron Spectroscopy and High Resolution Transmission Electron Microscope. The optical absorption and band gap energy of the samples were done by the UV Vis Diffuse Reflectance Spectroscopy studies. To investigate the photocatalytic performances of as-synthesized samples for the degradation of Reactive green (RG19), Reactive orange (RO84), Reactive violet 1 organic dyes were chosen as model pollutants under the visible light irradiation. The enhanced catalytic activity of the samples was noticed towards Reactive violet 1 dye with a higher degradation rate constant compared with other dyes. Further, detailed investigations have made to understand the influence of various photocatalytic reaction parameters such as pH of the dye solution, the concentration of dye and the dosage of photocatalyst over the degradation of organic dye.

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I 124

Synthesis and characterization of TiO_2/MoS_2 nanocomposites for effective removal of organic pollutant in solar light

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ABSTRACT

Heterogeneous photocatalysisis a promising technology to solve environmental problem as it has enormous potential to breakdown organic pollutants into non-toxic byproducts like carbon dioxide (CO_2) and water (H_2O). In the present study, different wt% of MoS_2 adorned with TiO_2 (TiO_2-MoS_2) heterogeneous photocatalyst were synthesized by hydrothermal method. The phoocatalytic properties of synthesized nanocomposites TiO_2-MoS_2 were investigated by various analytic techniques such as XRD, FESEM, TEM, UV-Vis DRS and PL. The altered band gap and large surface area of TiO_2-MoS_2 nanocomposites increases the absorption of visible light as well as separation rate of electron hole pair. The photocatalytic degradation of Rhodamine B (RhB) and Methylene Blue (MB) in a aqueous suspension was employed to evaluate the photocatalytic activity of the synthesized TiO_2-MoS_2 nanocomposite in UV and solar light. The possible electron trapping recombination and photocatalytic degradation mechanism were proposed.Theexperimental results confirm that the most efficient and stable TiO_2-MoS_2 nanocomposites exhibit excellent photocatalytic activity compared to pure TiO_2.

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I 125

Real-time Underwater Garbage Identification and Material Classification using Enhanced YoloV5 Architecture

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ABSTRACT

Marine pollution is an escalating global concern that imperils the health of our oceans and their ecosystems. The impact of underwater garbage poses significant challenges for marine ecosystems and requires effective monitoring and management strategies. Underwater garbage identification and material classification faces problems like poor image quality; distortions obstructing clear visualization; irregular shapes, sizes, and orientation of the garbage; and small objects. To overcome this, an enhanced Yolo V5- based trash identification and classification model is proposed. This model proposes a feature pyramid network-based YoloV5 detector to identify underwater garbage followed by performing color correction, deblurring, and reflection removal. Then a dedicated neural network is tailored for the categorization of biodegradable and non-biodegradable materials associated with underwater trash, providing valuable insights for conservation efforts. Our system contributes to the development of a robust and efficient real- time underwater garbage detection system. The study's outcomes will help environmental agencies to devise effective strategies for mitigating the impact of underwater garbage on marine ecosystems.

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I 126

Nutrient Removal from Municipal Wastewater by Natural Flocculant *Manihot Esculenta* Starch Optimized with Response Surface Methodology

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ABSTRACT

In the second decade of the twentieth century, many aquatic ecosystems worldwide suffered from excessive nutrient loads due to rapid population and urbanization [1]. An overabundance of nutrients discharged directly to water bodies may cause eutrophication issues [2]. Applying chemical coagulants from aluminum sulphate ($Al_2(SO_4)_3$) in wastewater treatment has received many concerns regarding health and environmental impacts. There has been increasing awareness of minimizing the application of chemical coagulants by combining them with plant-based flocculants. Nowadays, many studies focus on modified starch due to higher efficiency and stable floc production without considering the potentially toxic chemicals used during the modification process. If the unmodified starch can function excellently in real wastewater treatment, it could be considered their direct use. This option could reduce the application of hazardous chemicals during the modification process [3]. In this study, an assessment efficiency of unmodified plant-based flocculant from *Manihot Esculenta* (ME) starch and $Al_2(SO_4)_3$ was implemented to remove nutrients such as total phosphorus (TP) and ammoniacal nitrogen (NH_3-N) from municipal wastewater. Response surface methodology by custom design demonstrated that applying ME starch after the coagulation process with $Al_2(SO_4)_3$ improved the treatment performance of TP and NH_3-N removal. The process significantly reduced the chemical dosage and settling times by up to 6 and 4.5 times, respectively. The optimum treatment condition successfully removed TP and NH_3-N up to 85.33% and 59.29%, respectively, at 8 mg/L of $Al_2(SO_4)_3$ dosage, 133 mg/L of starch dosage, pH 9-, and 19 mins settling time. The results revealed that unmodified ME starch could be a potential flocculant in reducing chemical coagulant usage for municipal wastewater treatment.

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I 127

MARINE-GUARDIAN: A Machine Learning-Enabled Application for Real-time Monitoring and Prediction of Marine Pollution

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ABSTRACT

Marine pollution poses a grave threat to the health of our oceans, impacting marine ecosystems, biodiversity, and human well-being. To address this pressing issue, "MARINE-GUARDIAN," an innovative application is designed to track, monitor, and predict marine pollution using advanced machinelearning techniques. The primary objective of MARINE-GUARDIAN is to provide a comprehensive and real-time solution for detecting marine pollutants, analysing their patterns, and predicting potential future incidents. The application utilizes a robust machine learning model trained on a diverse and extensive Marine pollution dataset. This dataset encompasses various parameters such as water quality indicators, pollutant concentrations, weather conditions, and geographical information. The machine learning model employs sophisticated algorithms to recognize patterns, correlations, and anomalies within the data, enabling the accurate identification of pollution sources and trends. MARINE-GUARDIAN offers a user- friendly interface that allows marine scientists, environmentalists, and regulatory authorities to visualize pollution data in real-time. The application provides detailed insights into pollution hotspots, trends over time, and potential risk areas. Users can set up customizable alerts to receive notifications when pollution levels exceed predefined thresholds, facilitating prompt and targeted response measures. Through real-timemonitoring and predictive analytics, MARINE-GUARDIAN contributes to the sustainable management ofmarine ecosystems and supports global initiatives for a cleaner and healthier ocean environment.

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I 128

Water Quality Analysis in the South-Eastern Coastal States of India using Graphical Neural Network

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ABSTRACT

Water pollution is a global issue stemming from the release of dangerous substances into water bodies through human activities, significantly impacting freshwater and marine ecosystems. Major pollutants include sewage discharges, industrial activities, agricultural practices, and urban runoff. This contamination adversely affects water quality, leading to the loss of aquatic life, disruption of ecosystems, loss of coastal habitats, and adverse climate feedback. To address this, we propose conducting a water quality analysis in the southern eastern coastal states of Andhra Pradesh, Tamil Nadu, and Odisha in India. This analysis will encompass a range of physicochemical and biological parameters such as pH, temperature, conductivity, salinity, turbidity, dissolved oxygen, biochemical oxygen demand, and chemical oxygen demand to evaluate coastal water quality. Traditional mathematical models face limitations due to the complexity of representing all physical, chemical, and biological processes, leading to uncertainty and oversimplified data analysis. To overcome these challenges, modified Graph Neural Networks (GNNs) can be employed for predictive modelling. GNNs process data as graphs, making them suitable for analysing complex relational data. By training GNNs on historical water quality data enable forecasting of water quality conditions at specific locations and prediction of environmental impacts on water quality.

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I 129

A comparative study of the adsorption of Congo Red & Eriochrome Black T dyes by *Impatiens Balsam* leaf extract mediated biosynthesized Cerium Oxide nanoparticles

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ABSTRACT

In this work, cerium oxide nanoparticles (CeO_2 NPs) were prepared by an eco-friendly synthesis using *Impatiens Balsam* leaf extract as a reducing and stabilizing agent. The synthesized nanoparticles were thoroughly characterized using various analytical techniques such as XRD, FT-IR, UV-Vis, FESEM, HRTEM, and Raman techniques to understand the morphology, and structural properties. The XRD pattern revealed the cubic phase of CeO_2 NPs, and FESEM and HRTEM images signified the particles to be in the nano scale range. Furthermore, the as synthesized CeO_2 NPs were used for the adsorption of Congo Red (CR) and Eriochrome Black T (EBT) dyes. Batch adsorption experiments were conducted to evaluate the adsorption efficiency of biosynthesized CeO_2 NPs for CR and EBT dyes. Factors influencing the adsorption process like initial dye concentration, pH, contact time, and adsorbent dose, were systematically investigated. The optimum adsorption parameter obtained for highest efficiency were found to be 25 ppm initial dye concentration, 20 mg adsorbent dose, pH 2.0 and 328K temperature. The adsorption mechanism followed a pseudo-second-order kinetics and Freundlich isotherm model indicating multilayer adsorption onto a heterogeneous surface for both the dyes. The negative value of ΔH^o (-30.44 $kJmol^{-1}$) signifies an exothermic nature of adsorption and positive value of ΔS^o (0.155 $Jmol^{-1}K^{-1}$) indicates the increased randomness of dye during adsorption. The above results reveal the potent of CeO_2 NPs, to be an effective adsorbent for the purification of toxic dye contaminated water.

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I 130

Novel rGO – V2O5 – WO3 Ternary Composite for Environmental Applications

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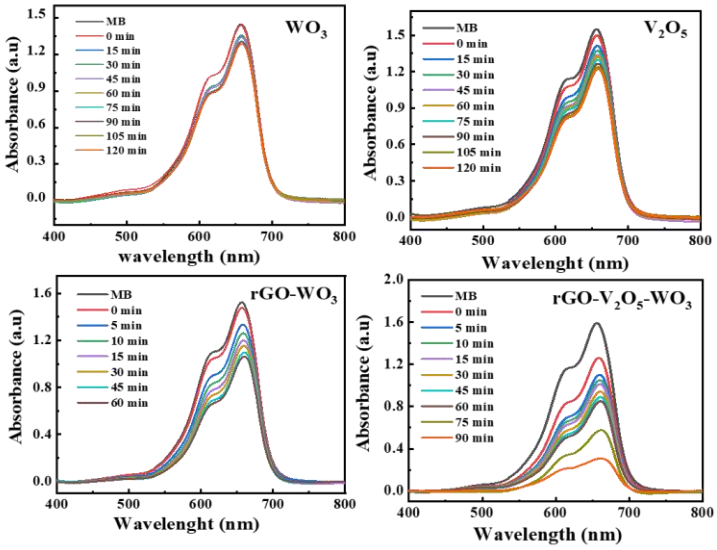
ABSTRACT

Novel rGO-V_2O_5-WO_3 nanocomposites were prepared hydrothermally and implemented the degradation of MB dye. X – ray diffraction confirms the formation of constituent parts of the coposites, rGO, V_2O_5, and WO_3 in single phase and having high phase purity, therein prepared composites were also found to be in single phase. The materials were further studied for the structural details through Raman spectroscopic studies and results suggest the characteristic peaks for the constituent materials and these features were also found in composites. The UV – Visible absorption studies were done to evaluate the band gap of the materails, where the band gaps were of 2.7 eV, 5 eV, 4.9 eV, and 4.8 eV for WO_3, V_2O_5, rGO-WO_3, and rGO-V_2O_5-WO_3, respectively. Photodegradation of methylene blue (MB) dye was manifested in the work with superior degradation efficiency for the ternary composite, rGO-V_2O_5-WO_3 with a rate constant for degradation reaction as 0.0056 Sec^{-1}.



The photodegradation spectrum of the MB solution with catalyst shows the photocatalytic dye degradation for the following compositions WO_3,V_2O_5, rGO-WO_3, rGO-V_2O_5-WO_3

I 131

Graphene Oxide based Plasmonic/Semiconductor SERS Nano-sensor for the Detection, Identification and Visible Light Driven Photocatalytic Degradation of Textile Effluent

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ABSTRACT

SERS is a powerful technique ascribed by the aggregation of electromagnetic and chemical charge transfer mechanisms of electrons that provides the fingerprint information about any molecule even at lowest trace of concentration. This technique offers high sensitivity for the trace level detection of both organic and inorganic containments in water resources. Graphene oxide along with plasmonic metals and a semiconducting metal makes it a dual benefit by enhancing SERS signal and visible light driven photocatalytic degradation of textile effluent (TE). The present study will demonstrate the synthesis and characterizations of graphene oxide and silver (with various silver concentration) nanocomposite by XRD, UV-Visible spectroscopy, Raman spectroscopy and HR-TEM analysis. The efficiency of graphene oxide and silver nanocomposite for the effective detection textile dyes such as Congo red, Crystal violet, Amido Black and real life textile effluent were also tested. The nanocomposite with lower Silver concentration showed photocatalytic degradation on Congo red dye and textile effluent. The selected graphene oxide/silver nanocomposite was doped with TiO_2 nanoparticle to synthesis graphene oxide/silver/TiO_2 (GAT) nanocomposite. The SERS and visible light photocatalytic analysis was done using GAT to study its efficiency.

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I 132

Synthesis and Characterization of Ce-Doped Photoactive Brownmillerite $KBiFe_2O_5$ for Photovoltaic applications

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ABSTRACT

$KBiFe_2O_5$, a fascinating Brownmillerite material, has captured the interest of researchers not only for its multiferroic properties, but also for its potential in the realm of photovoltaics. While $KBiFe_2O_5$ possesses some inherent light-harvesting capabilities, researchers are exploring ways to optimize its performance for solar energy conversion. In this study, we investigated the structural, vibrational, and functional properties of $KBi_{(1-x)}Ce_{(x)}Fe_2O_5$ (x=0,0.05,0.1,0.15) using a combination of X-ray diffraction (XRD), Raman spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy. We synthesized the material via solid state route and Samples were calcined at the temperature range 650 to 800°C. Rietveld refinement shows the material is a monoclinic with space group P2/c at the room temperature. Characteristic phonon modes in FTIR data disappear with increase in Ce doping. The change in bond lengths and angles of the Fe–O tetrahedral structure, as well as changes in reaction to oxygen shortage in KBFO due to Ce doping, can be blamed for the shift in Raman active modes.

Key words: *$KBiFe_2O_5$, Photovoltaic, XRD, Raman spectroscopy, FTIR spectroscopy, Rietveld refinement.*

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J 001

Technological Innovation in Plastic to Biogas Conversion

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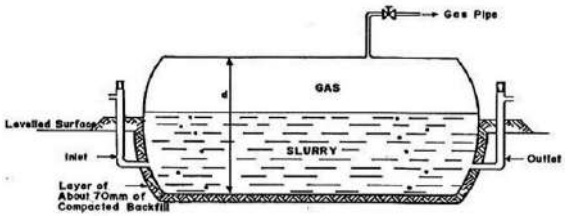
ABSTRACT

Plastic waste has proliferated around the world, posing a serious environmental and financial burden. Traditional ways of disposing of plastic, such incineration and landfilling, increase pollution and greenhouse gas emissions. In this context, the creation of biogas from plastic garbage offers a viable method for managing waste and producing renewable energy, thereby converting waste into wealth. This abstract highlight the key aspects of the plastic-to-biogas process, emphasizing its potential environmental and economic benefits. It discusses the technological advancements and processes involved in transforming non-recyclable plastic waste into valuable biogas through anaerobic digestion. Therefore, the plastic wastes are treated with certain bacterium which completely digests the plastic and converts it into a biodegradable compound. After converting the plastic into a biodegradable compound, then the plastic is processed under anaerobic digestion that yields biogas in a large amount. Additionally, the abstract addresses the environmental advantages of this approach, including reduced greenhouse gas emissions and plastic pollution. Furthermore, it underscores the economic potential of biogas production from plastic waste through revenue generation from the sale of biogas and the creation of jobs in the waste management and renewable energy sectors. The abstract concludes by acknowledging the importance of ongoing research and development to optimize the plastic-to-biogas conversion process, making it a viable and sustainable solution for addressing plastic waste and contributing to the transition to a circular economy.



Keywords: *Plastic waste, Biogas, Waste to Wealth, Anaerobic digestion, Renewable energy.*

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J 002

Impact of Industrial Wastewater Disposal on Surface Water Bodies in Brahmani River Basin, Odisha, India

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ABSTRACT

Agriculture, industry, human and animal needs, and river infrastructure all depend on them. Untreated sewage and other types of pollution have been released into major rivers around the world, including those in the Brahmani Basin, as a result of increased industrial activity and rapid human population in semi-urban and metropolitan cities. Since the dawn of human civilization, anthropogenic and natural processes have continued to contaminate the water supply. Environmental degradation and declining water quality are major world concerns. 13 locations were observed seasonally in this study to determine how monsoonal precipitation affected environmental factors and the Water Quality Index (WQI). Over the course of a year, sampling technique was employed in the pre-monsoon, and post-monsoon phases (2020-2021). Various physicochemical parameters, like TDS, TSS, EC, DO, PH, Turbidity, Alkalinity, SO_4^{2-}, NO_3^-, BOD, TH, HCO_3^-, Ca^{2+}, Mg^{2+}, PO_4^{3-}, Cl^-, Na^+, K^+ and Fe were examined to determine whether water was suitable for a range of applications. The readings for pH, EC, TDS, TH, main cations, and DO were all noticeably under BIS and WHO recommendations. Turbidity, TSS, and in certain cases, BOD values were all above the permissible threshold, implying contaminated waterways. Utilizing the measured values, the Kriging methodology was used to create interpolated maps for each component, and the WQI algorithm was used to estimate the water purity. The findings indicated that the WQI values ranged from 18 to 60 in pre-monsoon phase, from 17.92 to 59 in the monsoon, and from 20 to 78 in the post-monsoon timeframe. The results revealed that the water quality fluctuated between average and good mostly in chosen sites and that pollutants rises from upstream to downstream. Principal component analysis (PCA) and the clustering technique (CA) were also used. These techniques were performed to analyse the state of the water for effective management. The sampling locations are grouped by CA into homogeneous clusters with comparable behaviours. The river's water quality can be described using PCA by identifying key factors that are relevant to each season. PCA was successful in explaining 76%, 74%, and 72% of the overall cumulative variation in water quality over the course of the year. The PCA results showed that the most significant factors affecting water quality were BOD, Fe, turbidity, and TSS. Significant contributors to river water pollution have been highlighted as fertilizers, home and industrial wastewaters, land degradation, soil leaching, organic contaminants, and environmental contamination. The quantifiable benefits, however, varied different seasons. The calculated rates of the criteria and the WQI clearly demonstrate that the Brahmani River water demands a suitable treatment procedure as well as actions to prevent to stop the deteriorating water quality. Appropriateness of methodologies for planning and designing related to sampling sites for regulating water quality management initiatives in river basins. To improve health and protect water resources and the environment, strict rules and regulations must be implemented in order to protect this water resource from pollution.

Keywords: Brahmani Basin, anthropogenic, Water Quality Index, Principal analysis, clustering.

J 003

Facile Green Synthesis of Nonisocyanate Poly(ester urethanes) from Recycled Plastic Waste for Tissue Regeneration

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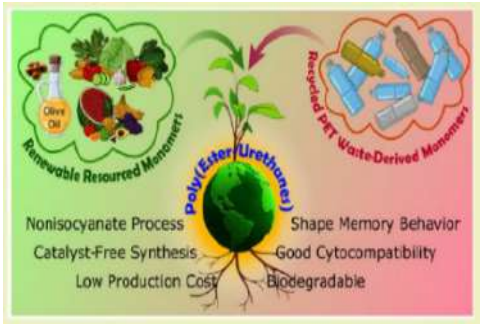
ABSTRACT

Significant progress has been made in synthesis and processing of Polyurethane, expanding their applications across various fields. But, in biomedical application, the utilization of isocyanates and the usage of toxic catalysts for PU synthesis impose a significant challenge. In this study, we present a novel approach where the preparation of a series of poly(ester urethanes) occurs via an isocyanate and catalyst-free melt polycondensation process. To synthesize the poly(ester urethanes), we have employed a combination of poly(ethylene terephthalate) (PET) waste-derived monomers and a diverse range of renewable resources, including oleic acid, ethylene carbonate, citric acid, sebacic acid, and mannitol. The synthesis of the poly(ester urethanes) was confirmed by FTIR spectroscopy and ^{1}H NMR spectroscopy, while the physicochemical properties of the poly(ester urethanes) were investigated using XRD, TGA, DSC, and UTM. The mechanical characteristics of the synthesized poly(ester urethanes) closely resemble those of various soft tissues found in the human body, such as articular cartilage, cervical spinal components, ligaments, aorta, and soft collagenous bone, indicating its promising potential for soft tissue engineering applications. Moreover, the synthesized poly(ester urethanes) exhibited excellent shape memory behavior, along with a good recovery response at ambient temperature. Furthermore, the synthesized poly(ester urethanes) demonstrated certain levels of antimicrobial activity, exceptional in vitro cytocompatibility, and cell proliferation against mouse fibroblast cells (NIH/3T3) as confirmed by alamar blue and live/dead assays suggesting its potential soft tissue engineering applications.



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J 004

Degradation of Waste Synthetic Polymers from Landfills using the Non-Thermal Plasma Technique

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ABSTRACT

Soil pollution from synthetic polymers and insecticides is a growing concern, with 460 million tonne of plastic waste in 2019 compared to 230 million tonne. Only 9% is recycled, 79% ends up in landfills or oceans and 12% is incinerated. Techniques such as biodegradation, catalytic synthetic polymer degradation, and pyrolysis are currently used, but they have limitations like kinetic sluggishness, harmful by-product production and extensive capital investment. Even though these techniques have widespread applications. Thus, we propose the usage of non-thermal plasma (NTP) for the degradation of synthetic polymers. Plasma is considered as the fourth state of matter. Plasma is a partially ionized gas it contains a mixture of electron radicals, ions, photons, etc. based upon temperature, plasma is categorized as thermal plasma, where electron temperature is equal to gas temperature and nonthermal plasma, where gas remains at ambient condition and electron energy can be from 1-10 eV. The NTP is effective as it consumes less energy, and based on plasma operating conditions, the degree of carbonization can be controlled. In this work, we have used NTP working at a fixed output voltage of 7kV and variable plasma operating frequency of 50-12.5kHz. The effect of specific input energy (SIE) and plasma treatment time is evaluated for the carbonization of synthetic polymer. The degradation of synthetic polymer is calculated from weight loss and the concentration and volume of gases evolved during the process. The carbon mass balance is used to evaluate the amount of polymer degraded.

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J 005

Modification of Phyllosilicates Clay using Non-Thermal Plasma for Water Splitting Reactions

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ABSTRACT

The world faces energy issues due to a limited supply of energy resources. The needs of the growing generation can be met by deriving energy from natural resources. Water splitting is one approach that can generate hydrogen, which has exhibited great potential as fuel for future generations. In this context, using the co-condensation method, we have synthesized phyllosilicate clay coordinated with various metal ions such as Mg, Ca, Fe, and Ni. The synthesized clays are characterized using XRD, FTIR and UV-DRS techniques. The synthesized samples are tested for electrochemical application using a 3-electrode setup with Pt, Ag/AgCl and a glassy electrode loaded with material that acts as a counter, reference and working electrode. The study shows that in the absence of phyllosilicate clay, the overpotential lies at -1.1 V, which decreases to -0.8 V for Ni-phyllosilicate clay in a potential window of -1.2 to 1.2 V in 0.2M H_2SO_4. The catalyst sample exhibits good stability and recovery for a minimum of 1000 cycles. The Ni-Phyllosilicate clay was treated using dielectric barrier discharge plasma using a homemade setup. The effect of varying plasma power, treatment time and composition on material properties is evaluated.

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J 006

Isolation of Nanocellulose from *Nelumbo Nucifera* for Waste Water Treatment

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ABSTRACT

Nanocellulose is a member of the carbon family, when mixed with other nanomaterial catalysts forms a novel hybridised nanomaterial known as Nanocellulose supported photocatalyst. To assure the use of biodegradable and sustainable materials, cellulose was employed as a green, sustainable, affordable, and plentiful resource that could be sourced from all over the world to support different semiconductors. Furthermore, cellulose is an appropriate matrix alternative for petrochemical products due to its high hydrophilic nature, flexibility, permeability, transparency, physical and chemical resistance, and thermal stability. Nanocellulose from biogenic waste is produced by organic material derived from plant waste under low-oxygen circumstances. Nanocellulose have been reported for effective dye adsorption in textile wastewater effluent. In the present study, nanocellulose was extracted from the aquatic perennial plant *Nelumbo nucifera* by acid hydrolysis method and assessed for it dye degradation ability. Synthesised nanocellulose was characterised by microscopic and spectroscopic analysis. The mechanism of degradation of malachite green (MG) and methylene blue by nanocellulose were studied at various time intervals under halogen light source. Nanocellulose was assessed for its antibiofilm efficacy against marine pathogens *Vibrio harveyi, Vibrio parahaemolyticus, and Salmonella typhi*. Results demonstrated that synthesised nanocellulose exhibited higher crystalline surface area with wide variety of reactive groups that plays vital role in photocatalytic effectiveness and the presence of oxygen vacancy boost photocatalytic activity even more. Using nanocellulose, the overall removal rate of malachite green and methylene blue was observed to be 95%. Nanocellulose exhibited potent antibiofilm activity against the aquatic pathogens in concentration dependent manner. Over all the results reveal that nanocellulose from biogenic source will act as effective candidate for waste water treatment

Keywords: *Nanocellulose, photocatalytic activity, Nelumba nucifera, Antibioflim activity, Heavy metal adsorption*

J 007

Effect of Hydroxyapatite Nanofertilizer Immobilized with Plant Growth Promoters on Seedling Growth of Fenugreek (Trigonella Foenum-Graecum)

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ABSTRACT

Hydroxyapatite a naturally occurring bio-ceramic material widely used in biomedical applications as source of calcium and phosphorus for bone repair and regeneration in the form of granules, scaffolds, and blocks. The present study focused on the fabrication of hydroxyapatite nanoparticles from bio waste of fish scale *Scarus ghobban*. Hydroxyapatite nanoparticles (HAP) were used as source of calcium (Ca) and Phosphorus (P) the second essential macronutrient for plant growth after nitrogen (N). Vermiwash and Gum Arabic rich in plant growth promoterswere immobilized in hydroxyapatite nanoparticles to develop nanofertilizer. The role of nanofertilizer, is slow and controlled release of the organic fertilizer and pesticide to the plants prolonging the availability of fertilizer for enhanced plant growth. Fenugreek (*Trigonella foenum-graecum)* an edible native herb has been widely reported for its antidiabetic, antioxidant, anti- inflammatory and anticancer properties. Results of the present study showed enhanced growth rate in terms of root length, shoot length and fresh biomass weight in the HAP nanofertilizer treated group when compared to control. Safety evaluation studies revealed that HAP nanofertilizer exhibited neither hemolytic activity in erythrocyte model system nor mortality or morbidity in zebra fish model system indicating its biocompatible nature. To conclude, eco-friendly HAP nanofertilizer improved the productivity of fenugreek *(Trigonella foenum- graecum).*

Keywords: *Trigonella foenum-graecum, Gum Arabic, Vermi wash, Scarus ghobban, Nanofertilizer, Hydroxyapatite nanoparticles*

J 008

Selective Detection of Uric Acid in Presence of Dopamine using Green Carbon Dots (Gcds) - A Turn on Fluorescence Probe from Waste Brachyura Shellsn

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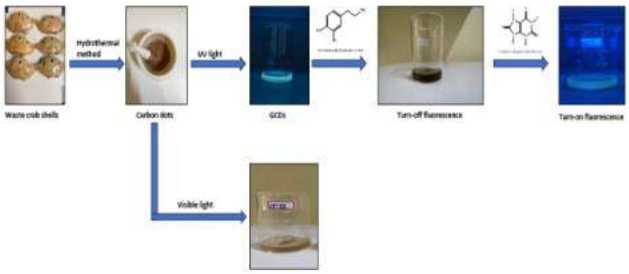
ABSTRACT

Carbon dots a carbon-based nanomaterial because of their diverse physiochemical properties and favourable attributes like good biocompatibility, abundant surface functional groups, high stability, non-toxic nature are of high interest in the sensing of Biomolecules. In this study we report a new, simple, green technique for the synthesis of green carbon dots (GCDs) from waste crab shells and applied the carbon dots for the detection of Uric Acid (UA) in presence of Dopamine (DA). Nano devices made of carbon dots effectively Turns-off or Turn-on their signal in terms of fluorescence in presence of Biomolecules. This property is used to detect UA in presence of DA by using GCDs as a fluorescent probe. The synthesized GCDs are sand coloured under visible light and exhibit green fluorescence under UV-radiation. The GCDs were characterized using UV-Vis, FTIR, SEM-EDAX, HR-TEM, X-ray diffraction and PL spectroscopic technique. The SEM-EDAX data shows a nano fibrous morphology and confirms presence of only Carbon, Nitrogen and Oxygen. The FTIR response confirms the presence of functional groups like −C≡N, –C≡C–, CH, =C-H, O-H on the surface of GCDs. XRD data confirms GCDs to be crystalline in nature and has a particle size of 4.51nm. The quantum yield of the GCDs is also measured. The PL response confirms a continuous decrease in intensity i.e., a Turn Off in green fluorescence with the addition of DA. Whereas with the addition of UA in presence of DA, the fluorescence Turns ON. The minimum detection limit for DA is found to be 1.25×10^{-12}M. The method will be further used for the detection of biomolecules in biological fluids.

Key words: *Green Carbon dots, Fluorescence, Dopamine, Quenching*



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J 009

Synthesis of Ag@Zno Nanoparticles: The Photocatalytic Effects on Rhb Dye Degradation upon Irradiation with Sunlight Light

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ABSTRACT

Due to its efficiency and eco-friendliness, photocatalysis has become a potential technique for the reduction of organic pollutants in water. In present investigation, we looked into the photocatalytic degradation of Rhodamine B, a common dye pollutant, utilizing silver doped zinc oxide (Ag@ZnO) as the photocatalyst. The Ag@ZnO nanoparticles was synthesized by using a simple and cost-effective hydrothermal procedure and characterized with various techniques, like X-ray diffraction (XRD), FT-IR, DRS-UV, Raman, field emission scanning electron microscopy (FE-SEM) with energy-dispersive X-ray spectroscopy (EDS), High resolution Transmission electron microscope (HR-TEM). Rhodamine B degradation under UV light irradiation was used to gauge Ag@ZnO photocatalytic activity. The outcomes showed that Ag@ZnO had excellent photocatalytic activity, resulting in the considerable breakdown of Rhodamine B in a short time. With a high degradation rate and efficiency, the improved reaction conditions improved photocatalytic performance. The study also shed light on the intermediate products created during the degradation process and the photocatalytic mechanism, which may help in understanding the reaction pathway.

Keywords: *Ag@ZnO, photocatalysis, semiconducting*.

J 010

Sonifier-Assisted Acid Leaching Process for Removal of Metal Impurities from Diamond Wire-Sawing Silicon Kerf Loss

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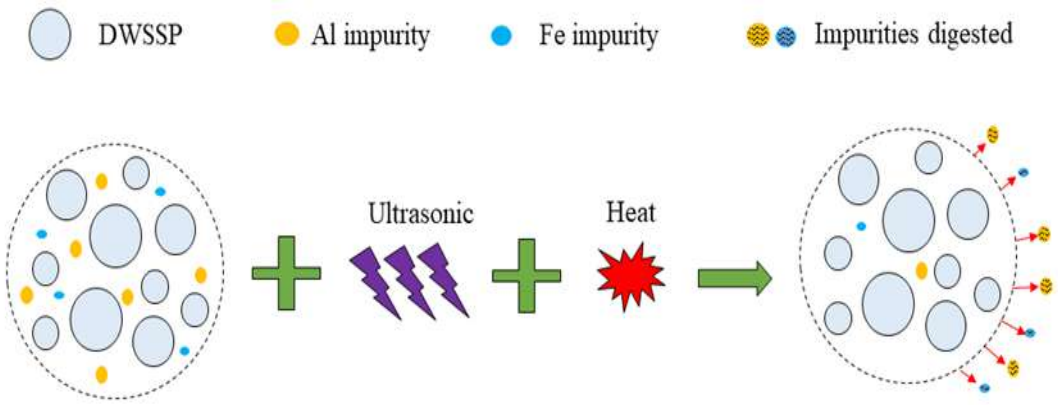
ABSTRACT

The diamond wire-saw silicon powder (DWSSP) or kerf is obtained from a diamond wire saw machine. The DWSSP contains metallic impurities originating from the growth and cutting processes. Initially, the DWSSP was analyzed to determine its average particle size, which was found to be 1.8 µm. Elemental analysis revealed the presence of silicon (Si) at a weight percentage of 52.05%, oxygen (O) at 42.24%, and carbon (C) at 4.72%. The metal impurities aluminium (Al) and iron (Fe) were identified in the prepared sample at a concentration of 9.45 parts per million (ppm) and 18.35 ppm, respectively. To purify the DWSSP, an acid-leaching procedure was employed to get a high yield of Si. The many leaching conditions have been optimized, considering a temperature of 80°C, a leaching duration of 60 min, an acid concentration of 15%, a liquid-to-solid ratio of 100ml/5g exposed to sonifier with 40KHz frequency, and 150W power. Under this optimized condition, the metal impurities are removed by 99.98%, resulting in a DWSSP purity of 99.62%. The leaching process was regulated using the homogeneous reaction model, and the activation energy for Al and Fe was determined to be 24.24 kJ/mol and 15.99 kJ/mol, respectively.



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J 011

Optically Tuned Biomass-Derived Nanocarbon for Multifarious Applications

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ABSTRACT

The distinctive optical properties exhibited by the carbon nanomaterials give promising leads for diversified applications. Tunability of these optical characteristics through simple and feasible techniques adds to the purview of nanocarbon materials towards future technologies. Here, we report the synthesis of fluorescent down-converting nanocarbon from biomass using a simple microwave-assisted solvothermal method. The absorption and emission properties of the obtained samples are contingent on the solvents used for synthesis. Therefore, the solvent engineering strategy was effectively used for tuning the emission and absorption spectra of the biomass-derived nanocarbon materials. The possibility of using these optically tuned nanocarbon samples for various applications is also examined in the present work.

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J 012

Refractories Fabricated from Oxides of Al and Mg Derived from Beneficiation of Aluminum Dross

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ABSTRACT

Black aluminium dross (Al Dross), the slag produced during molten aluminium processing contains composite oxides of aluminium (α-Al_2O_3, corundum phase) and magnesium ($MgAl_2O_4$) as its major phase. It also contains nitrides and chlorides of aluminium and few other compounds (minor). The oxides possess high thermal and structural stability (~1000°C) with excellent scope to be produced as ceramics and refractories for use in engineering industries. However, the major deterrent to use black Al dross as an engineering product is the presence (~5%) of aluminium nitride (AlN) which due to its high thermal conductivity cannot be used as a refractory. In this work, α-Al_2O_3 and $MgAl_2O_4$ were beneficiated from black Al-dross in a cost effective and environmental friendly manner (neutralization of the emanating pungent ammonia fumes) to obtain > 98% oxides of Al and Mg. The beneficiation was carried out by leaching 2kgs of raw dross (sourced from Belgaum, Karnataka aluminium foundry cluster) with equal volume of carbonated water. The chlorides and nitrides were removed during the leaching process. The treated mass was oven dried followed by calcination of the residue at ~1000°C (or higher temperature) in air atmosphere in a muffle furnace or gas fired furnaces available in the foundries. The resultant white crystalline powder, analysed by XRD, was a composite of only α-Al_2O_3 and $MgAl_2O_4$ (AlN and chlorides were completely removed). The beneficiated ceramic powder (~ 1kg) was ball milled, compacted into solid cylinder blocks (50mm ϕ x 25 mm height, sintered at 1500°C/4 hours in ambient air. The defect free sintered blocks were neither cracked or warped. They were subjected to thermal fatigue test by following the guidelines of IS 1528 (Part 3): 2010 (Methods of sampling and physical tests for refractory materials, determination of spalling resistance, air quenching test). The blocks withstood more than 100 thermal fatigue cycles before the first crack appeared. Fracture surfaces were examined by using SEM and other details are presented in the paper.

Photographs of Al dross beneficiated α-Al_2O_3 + $MgAl_2O_4$ composite powder and thermal fatigue test

J 013

Reclaiming Waste: Sustainable Photocatalytic Tetracycline Abatement using Exhausted Desiccant Supported Zinc Indium Sulphide

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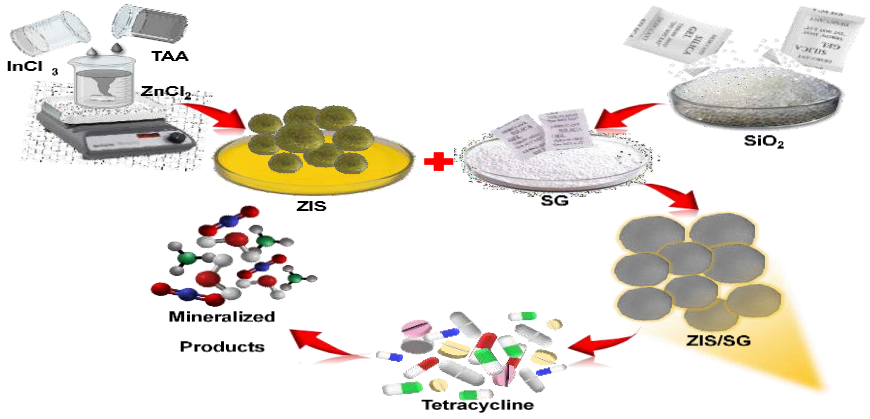
ABSTRACT

Employing an affordable and sustainable visible-light-driven system is pivotal for tackling organic pollutants in the field of photocatalysis. This study introduces a novel approach where a pioneering photocatalyst, zinc indium sulfide (ZIS), was synthesized and supported on a silica gel matrix (SG), a residual material from multiple dehumidification processes. This heterojunction fabrication significantly improved light absorption and charge separation efficiency. The photocatalytic efficacy was assessed by degrading tetracycline (TC) under light exposure. Detailed analysis using spectroscopic and microscopic methods was performed on the nano- photocatalyst. The ZIS/SG catalyst displayed exceptional efficiency, achieving nearly 98% degradation of TC under visible light—outperforming the pristine ZIS and SG catalysts by 6.9 and 13.5 times, respectively. Moreover, this catalyst effectively managed TC levels in real-time within pharmaceutical plant effluent, exhibiting a degradation efficiency of 78.2%. With cost-effectiveness, improved TC mineralization, and the ability to be reused up to six times (with an efficiency of around 85%), the ZIS/SG photocatalyst showcases the essential attributes of an ideal catalyst. This innovative nano-photocatalyst opens up new possibilities for advancing the process of photocatalytic decontamination of persistent emerging pollutants by providing satisfactory reusability and stability.



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J 014

Harnessing Waste for Sustainable Energy: A Self-Powered Anemometer and Wind Energy Harvester from Recycled Diaper Wastes

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ABSTRACT

The escalating concerns surrounding global waste management and the pressing need for sustainable energy sources have prompted innovative solutions at the nexus of resource recycling and energy generation. Disposable diapers, ubiquitous in modern society, and oven cook sheets, disposed of in landfills, contribute significantly to environmental challenges due to their non-biodegradable nature when disposed of conventionally. This manuscript presents a groundbreaking approach to simultaneously address waste reduction and renewable energy generation by recycling discarded materials like diapers and oven cook sheets for anemometer functionality and wind energy harvesting by fabricating a rotating triboelectric nanogenerator (TENG) in freestanding mode operation. The fabricated self-powered anemometer could generate maximum open circuit voltage and short circuit current of 110 V and 9 µA, respectively, and measured windspeed of the range 0.5 – 20 m/s. A capacitor charging test demonstrated the anemometer's exceptional electrical performance, showcasing its ability to charge a 0.1 µF capacitor to 8 volts in just 3 seconds. Apart from wind speed monitoring, the anemometer was exemplified by its capacity to power electronic gadgets like digital thermometers, clocks, calculators, and LEDs, offering a practical solution for self-sufficient energy utilization. As outlined in this study, the journey from waste to energy represents a promising stride toward a circular and sustainable approach to energy generation.

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Exploring the Feasibility of Utilizing Dye-Contaminated Effluent Wastewater for Plant Growth: Win-Win Situation of Non-Thermal Plasma Assisted Dye Mineralization and Nitrogen Fixation

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ABSTRACT

Win-win situation of dye mineralization and nitrogen fixation (nitrate and nitrites) in wastewater have been explored using non-thermal plasma dielectric barrier discharge bubbler reactor (NTP-DBD). The Crystal violet (CV) and Rhodamine B (RhB) dyes were used as a model pollutants. The feasibility of utilizing NTP treated water, dyes contaminated wastewater, for sorghum bicolor (great millet) seed germination and plant growth has been investigated. The degradation mechanism of CV and RhB under NTP discharge has also been studied.

It was found that the dye degradation efficiency increased with increasing treatment time and plasma input power. Within 16 min of plasma treatment both CV and RhB were removed to 99%. The results showed that the degradation of CV and RhB by NTP was mainly initiated and controlled by the reactive oxygen species (ROS) generated in the plasma discharge. The plasma treated wastewater was utilized for sorghum seed germination and evidenced the enhanced rate of germination and plant growth as compared to tap water. After three days of sowing about 65% germination reached which is 20% higher than the germination obtained with untreated wastewater. Although seeds were germinated, the plant growth was stopped and died after 7 days of sowing. Notably, plants were growing longer and healthier when seeds sowed with plasma treated water as compared to tap water. These findings suggest that non-thermal plasma treatment can be a promising and sustainable approach for treating textile industry effluents and utilizing the plasma treated solution for enhancing the crop productivity.

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J 016

The Comparative Study of Chemically Modified Lubricants Prepared using Activated Charcoal and Sulphuric Acid

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ABSTRACT

Lubricants are substances used to reduce friction and wear in manufacturing industries. Mineral-based lubricants are commonly used which are not environment friendly and due to this vegetable-based lubricant are being in focus by researchers. At present research is being carried out on waste cooking oils-based lubricants considering the economic feasibility of pure vegetable oils. Waste cooking oil can pose significant challenges when used as a lubricant in engines due to the presence of solid particles or contaminants. These particles can clog filters, causing abrasive wear, promote corrosion, reduce lubricity, and contribute to engine deposits. So, in this study, a comparison of the lubricant properties of waste cooking oil treated with sulfuric acid (H_2SO_4) and activated charcoal for the chemical modification of waste oil is being done. The results show that the tribological and physiochemical properties of Activated charcoal esterified lubricant showed better properties than H_2SO_4 esterified lubricant.

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Unravelling the Affinity of Iron Rich Ladle Slag in Alkali Medium Towards Inorganic Cementitious Binder for Field Applicability

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ABSTRACT

Upcycling of industrial waste for innovative construction materials is a potential approach to thrust out the sustainable development and has a threefold environmental impact. Firstly, the reduction of disposal of waste slag, secondly land resources which are unfit for use can be accessed; thirdly, new construction material with low carbon footprint. Ladle slag (LD) a waste from metallurgical industry, is commonly regarded as limited reaction with alkali and in previous studies, it has not been used as sole binder for alkalination. In view of this this study aims to utilise Ladle slag, for the production inorganic binding material after assessing their chemical and mineralogical variability. The reaction between LS and alkali silicate tested by varying the silica modulus (SiO_2/Na_2O) from 0.67 to 3.9 and the consolidated solid tested for the compressive strengths. The unconfined compressive strength of optimized alkali activated slag paste increased from 5.7 N/mm2 to 21. 4 N/mm2 while Ms increased from 0.8 to 1.4. The precipitation of calcium as calcium silicate hydrate increased by accelerated kinetics of higher silica content of activator solution, thereby improving the dense microstructure as seen from the SEM micrograph. The phase analysis by Rietveld X ray diffraction of LD reveal that major constituent present are Calcium silicate (Ca_3SiO_5), Hematite (Fe_2O_3) and after alkali attack, the major reaction product is C-S-H, basic binding gel with C-A-S-H. The functional group analysis by FTIR yield the shifting of Si-O bond frequency observed at 854 cm^1 to higher frequency number at 906 cm^1 conforming the polymerised Si-O network. Thus, utilisation of the highly crystalline, iron rich ladle slag as a sole precursor in alkali activation is promising. Further analysis of the durability and the effect of aggregate on the properties of composites are the subject areas for future study.

Keywords: *Ladle slag, Waste utilization, Alkali activated materials (AAMs), C-S-H gel, Compressive strength.*

J 018

Waste to Electricity Towards Sustainable Energy Harvesting and Self-Powered Triboelectric Nanogenerator from Ferrum (Fe) metals

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ABSTRACT

Sensor devices in today's rapidly automated world must be highly reliable energy harvesters and self-powered sensor devices. Several industries utilize sensor devices that operate on solar power and power batteries. The sensor device as an energy harvester as well as self-powered is necessary to promote wearable and portable electronics. Here a self-powered and energy-harvesting system is developed with cost-efficient and flexible nanotechnology called triboelectric nanogenerator. The materials are composed of waste ferrous metals from the earth, ecoflex, Al, and Kapton. The surface morphology created ecoflex film with Fe as a negative layer, aluminum as an electrode, and a positive layer. The charge accumulation happens on a Kapton film that is kept below an ecoflex film. The electricity was obtained at the mechanical motion as the contact and separation initiated on the device. Due to the metal materials associated with the ecoflex film the Metal-TENG device provided a high output voltage and a current. The proposed device with recyclable material, and stable output can provide power to light up the low power electronic devices like LEDs, and LCDs. The device can provide a security alarm with the help of WiFi modules. The studies and results confirm that the Metal-TENG device can approach energy harvesting and security applications.

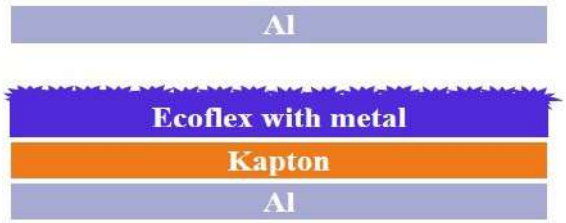

Fig. 1. Schematic structure of the device

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J 019

Upcycling of Waste Floral Foam into Nanoporous Activated Carbon for Significant CO_2 Capture and Supercapacitor Applications

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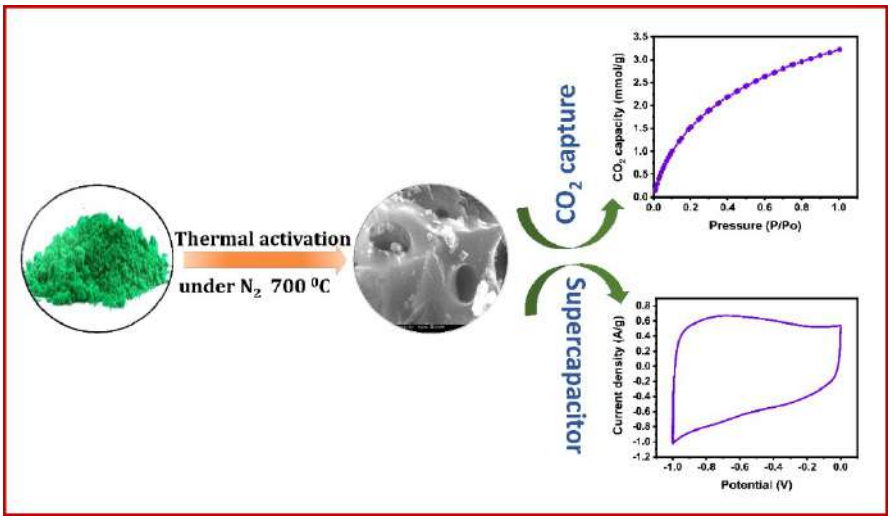
ABSTRACT

Floral foams are widely used worldwide, especially in floral arrangements, and have the potential to release hazardous microplastics into the environment. So herein we propose a twofold strategy to address the issue of floral foam waste. As activated carbon holds great potential for CO_2 capture and supercapacitor, conversion of waste floral foams into value added activated carbon could be a viable means to reduce the load of floral foam waste while also capturing CO_2 for a clean environment and as cost-effective electrode material for energy storage. For production of nanoporous activated carbon, the waste floral foam was initially acid-pickled and subsequently activated thermally at different temperatures ranging from 500 to 800 ºC under N_2 atmosphere. The resulting optimal sample NAC700 exhibits a high surface area of 732 m^2/g, abundant ultramicropores (≤ 0.8 nm), and rich surface oxygen functionality. Owing to combined effect of surface functionality and ultramicroporosity, the optimal sample NAC700 demonstrates an excellent CO_2 capture capacity of 3.22 mmol/g at 15 ºC and 1 bar. In addition, NAC700 also provided a good specific capacitance of 187 F/g at 0.2 A/g and 116 F/g at 5 mV/s. The strategy proposed here offers a sustainable approach for neutralizing waste floral foam by upcycling it into nanoporous activated carbon that holds substantial potential for CO_2 capture and energy storage.



J 020

Closed-loop Circularity in Polyolefin Vitrimers through Covalent Adaptive Network

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ABSTRACT

Globally, approximately 400 mega tons of plastic waste have been generated, with around 16% of this total being recycled. Dealing with such a massive amount of plastic pollution it is crucial to implement a closed-loop circular economy for plastics. However, one of the major challenges in achieving this circularity lies in the collection, sorting, and processing of post-consumer recycled (PCR) plastics. In this context we have successfully prepared vitrimers of PCR-Polypropylene (PCR-PP) which possesses abundant functionality and enabled the design of a single and dual covalent adaptable network (CAN). This addresses a long-standing challenge of retaining properties after grafting, as chain scission in the melt can often lead to property degradation. The consequences of these networks the structure-property correlation was evaluated. The PCR-PP Vitrimers demonstrate re-processability with over 90% recovery in mechanical properties even after the 5th sequence of recycling. Through dynamic exchange, the varying reactivity influences both the stress relaxation rates and the flow activation energy, making it an additional design parameter to consider. This study not only opens new avenues for recycling PCR-PP but also provides valuable guidance for researchers working in this field, both in academia and industry.

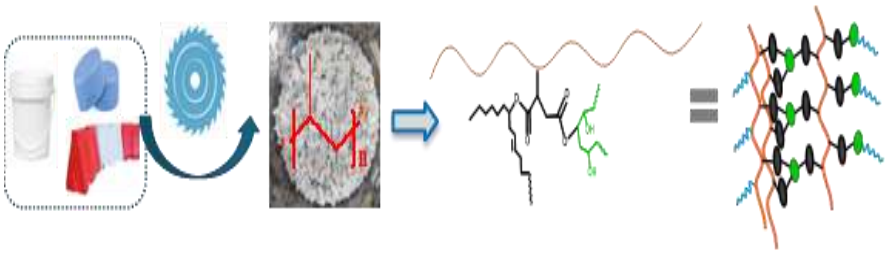

Figure: Schematic presentation of formation of PCR-PP based Vitrimers.

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J 021

Conversion of Waste LCD Monitors/Screens into Electrochemical Sensors

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ABSTRACT

A novel sensing platform for electrochemical sensing applications utilising liquid crystal display (LCD) as the working electrode was developed. This facilitates the establishment of a sustainable electronic refuse recycling system and an economically viable methodology for electrode modification. In this investigation, a discarded LCD screen modified with Ti3C2Tx MXene was employed as a dopamine (DA) detection platform. The sensor response of the Ti3C2Tx modified LCD considerably improved when compared to bare LCD in the cyclic voltammetric studies. The developed sensor was able to detect DA from 10 nM to 100 µM with a limit of detection of about 4.5 nM with very high selectivity, stability, and repeatability. Our testing involved a variety of LCD panels obtained from different manufacturers. We discovered that all the LCDs we utilized can detect DA with minimal adjustments to the current response. Additionally, the sensor's practical applicability is assessed through the detection of DA in human serum samples. Incorporating e-waste materials into electrochemical sensing applications would constitute an environmentally conscious and economically viable strategy (Fig 1). To the best of our knowledge, the possibility of using scrap LCD screens for electrochemical sensing applications has not been reported to date. Moreover, the current innovation offers a cost-effective solution for addressing or minimizing the escalating volume of e-waste produced in the environment. Therefore, repurposing discarded LCDs as electrodes in electrochemical sensing applications and sustainable approaches to upcycle hazardous e-waste.

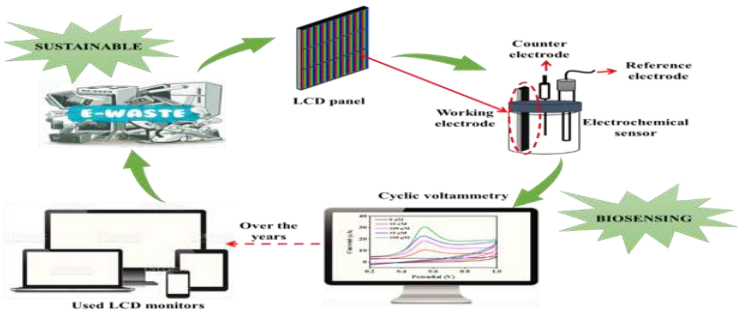

Fig 1. Graphical representation of conversion of E-waste to electrochemical sensor

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J 022

In-situ Synthesis of Metal Nanoparticles Decorated in Biomass Derived Carbon and its Application in EMI Shielding

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ABSTRACT

India produces 350 million tonnes of agricultural waste annually out of which maximum ends up in landfills. Agricultural biomass contains mostly cellulose, hemi-cellulose and lignin, which can be used for useful products.[1] The present work involves the synthesis of porous carbon from an agricultural waste through one-step pyrolysis and carbonization method. Further, metal nanoparticles decorated with carbon composites were synthesized through one step thermal reduction and carbonization method. Advanced characterization methods such as XRD and Raman spectra showed the presence of carbon and metal nanoparticles. FESEM and HRTEM exhibited the porous structures of carbon with metal nanoparticles decorated on the top of it. The synthesized powders were used to make composites by taking PVDF matrix through a facile solvent-casting method. The fabricated flexible film investigated for EMI shielding applications in the X-band frequency region (8-12 GHz). The composites made with metal decorated carbon showed better EMI shielding effectiveness (SE) than the pristine carbon composites. The 20 wt.% metal nanoparticles decorated carbon -PVDF composite showed an excellent EMI SE of more than 20 dB (> 99% EM attenuation) with a thickness of 0.5 mm, which meets the standard industrial value.[2] The one-step synthesized metal nanoparticles decorated carbon from biomass can be an ideal candidate for conductive paints and microwave absorption applications.

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J 023

A Novel Eco-Friendly Treatment: Removal of Colour from Cottage Dyeing Effluent by Natural Coagulation cum Adsorption Process

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ABSTRACT

A lab-scale experiment was conducted to treat the textile dyeing effluent with the naturally available indigenous plant-based material such as Mahua Longifolia (Iluppai) oil cake powder (MCP) as a coagulant. The coagulant dosage, pH and dye concentration are varied, evaluated and optimized in the lab scale batch coagulation process and its characterization was performed by FTIR, UV-Visible spectrophotometer, XRD, FESEM, EDX and also zeta potential. These MCP was added at various dosages and the initial and final characteristics of textile dyeing effluent like pH, turbidity, Chemical Oxygen Demand (COD), and colour are tested and compared for the coagulation process. For MCP dosage, the maximum removal efficiency of turbidity, COD and colour is 96%, 74.8% and 94.8% respectively at the coagulant dose of 2.7g. The removal efficiency of turbidity, COD and colour is increased when the pH level is varied in the acidic range such as pH 4. The coagulant dose of 2.7g of MCP has given the maximum turbidity, COD and colour removal efficiency of 97.6%, 75.6% and 95.8% respectively at acidic state of pH 4. The equilibrium adsorption capacity (qe) of the MCP coagulant material is studied and the results are fitted with isotherms like Langmuir and Freundlich isotherms and, kinetics models such as Pseudo-first-order and Pseudo-second-order kinetic models respectively. The indigenous plant-based coagulant (MCP) is locally available novel by-product material and cheaper in rate, which can be used as a coagulant for treating the industrial effluent and it has given better efficiency compared to chemical-based coagulants.

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J 024

Chicken-eggshell-derived CaO nanoparticles as green catalytic material for environmental applications

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ABSTRACT

Amongst various food wastes, eggshells contain various minerals and bioactive materials, and they can become hazardous if not properly disposed. However, they can be made useful for the environment and people by converting them to environmentally friendly catalytic materials or environmental purification agents. Simple calcination can enhance their properties and thereby render them suitable for catalytic and environmental applications. This work aimed to prepare CaO from waste eggshells and examine its effectiveness in photocatalytic pollution remediation and its antibacterial activities. Calcium oxide nanoparticles were prepared by subjecting waste eggshells (ES) to high-temperature calcination, and the synthesized CaO nanoparticles were characterized for their structural, morphological, chemical, and other properties. Furthermore, their photocatalytic degradation of methylene blue dye and antibacterial efficiency against *Escherichia coli* and *Staphylococcus aureus* were investigated. It is found that the green-converted CaO can be efficiently used in environmental applications

J 025

Ecofriendly synthesis of ternary nanocomposite ($Fe_3O_4/SiO_2/Ag$) from *Nerium oleander* leaves for catalytic degradation of environmental pollutants

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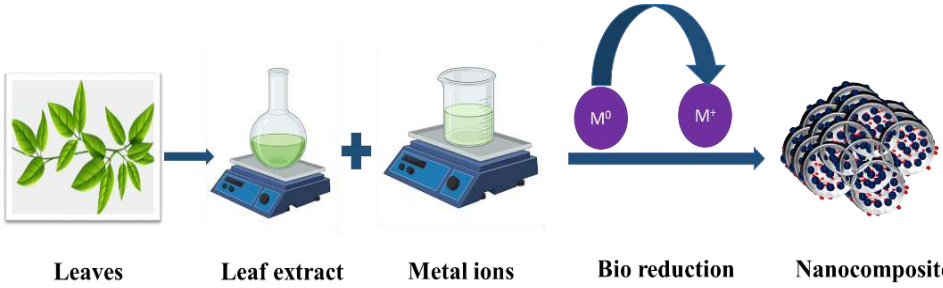
ABSTRACT

Synthesis of ternary nanocomposites using green and environmentally friendly methods, poses some challenges. In this study, we successfully employed green techniques to produce the ternary nanocomposite Fe3O4/SiO2/Ag (FSA). The analytical characterization of this nanocomposite included examinations of crystallinity, structure, morphology, and optical properties. X-ray diffraction (XRD) studies confirmed the presence of individual nanomaterials in the FSA nanocomposite through well-defined diffraction peaks. Transmission electron microscopy (TEM) revealed the specific characteristics of SiO2 in its microspheres shape as well AgNPs in spherical shape. Fourier transform infrared spectroscopy demonstrated the chemical bonds of Si-O-Si and Fe-O in the FSA nanocomposite. Optical analysis of nanocomposite revealed a broad absorption peak ranging from UV to visible region. The FSA nanocomposite exhibited catalytic activity in the degradation of both individual dyes and dye mixtures for water treatment applications. Notably, the FSA nanocomposite demonstrated efficient degradation in a short time span by their synergistic effect.

Keywords: *Green synthesis, nanocomposite, ternary, catalytic activity, dyes.*



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J 026

Catalytic cleaning of textile dye effluents with antibacterial deactivation of SnO_2 / ZnO nanocomposite

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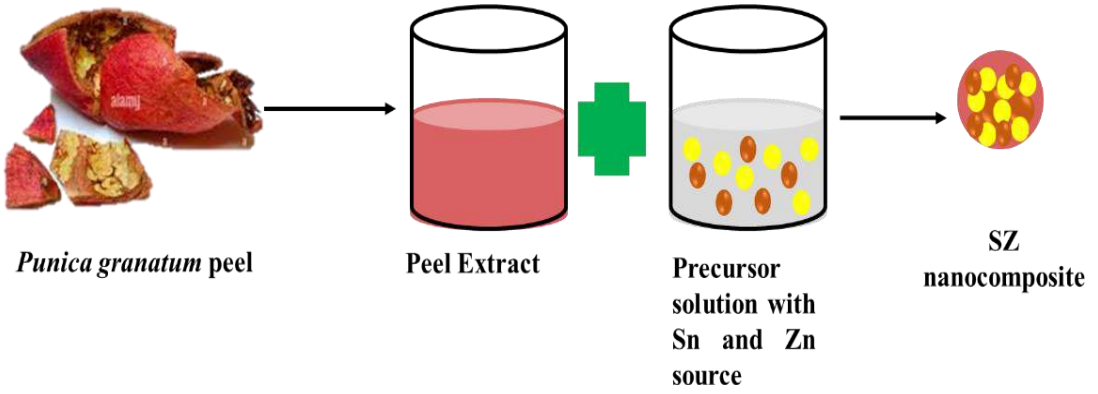
ABSTRACT

Synthesizing nanocomposites through green and environmentally friendly methods presents several intricate challenges. In this study, we have effectively utilized green techniques to fabricate the semiconductor nanocomposite SnO_2/ZnO (SZ) with peel extract of *Punica granatum*. The SZ nanocomposite is studied for their structural, morphological and optical properties. Structural properties elucidated the sharp crystalline planes of tin oxide in conjugation with ZnO crystal system. The morphological properties portrayed their quantum confinement. Optical properties imprinted broad absorption band covering from 250 nm to 400 nm. Green fabricated SZ nanocomposite is employed in the study of antimicrobial activity against gram-positive and gram-negative pathogens. In parallel, the degradation efficiency of SZ nanocomposite is evaluated for textile dyes via catalytic process.

Keywords: *Green synthesis, nanocomposite, catalytic activity, dyes, Punica granatum.*



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J 027

Sustainable E-Waste Management: Quantifying Precious Metal Values in Electronic Devices for Incentivized Recycling

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ABSTRACT

The rapid proliferation of electronic devices has led to a significant increase in electronic waste (e-waste),posing profound environmental and societal challenges [1]. In response, this research aims to develop a comprehensive approach to incentivize e-waste recycling by quantifying the precious metal values embedded within various electronic devices. Leveraging advanced machine learning techniques, including regression analysis and random forest algorithms, we seek to provide accurate estimations of precious metal content [3] across a diverse array of electronic devices based on intrinsic characteristics such as type, size, weight, and age [2]. To achieve this, we will collect a comprehensive dataset containing information about the aforementioned characteristics of electronic devices and the corresponding amounts of precious metals contained within. This dataset will serve as the foundation for our analysis and model development. Additionally, we will develop an online portal to facilitate user engagement and promote responsible e-waste disposal. Through this portal, users can input details about their electronic devices to determine the estimated value of precious metals contained within. By offering incentives tied to the estimated value, users will be motivated to responsibly dispose of their e -waste through authorized e-waste management teams. We anticipate that the implementation of this approach will yield several significant results. We aim to provide accurate estimations of precious metal content in electronic devices, enabling informed decision-making in e-waste recycling, and hope to significantly increase participation rates in recycling initiatives by incentivizing e-waste recycling through the online portal. Ultimately, the impacts of this research extend beyond e-waste management. By promoting sustainable practices and resource conservation, we aim to contribute to the development of a more environmentally conscious and circular economy. Through interdisciplinary collaboration and stakeholderengagement, we aspire to pave the way for scalable and impactful solutions to the global e-waste crisis.

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J 028

Wealth out of Waste - A novel modified GIC

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ABSTRACT

Conventional Glass Ionomer cement (GIC) is one of the most prevalent dental restorative materials. Despiteits several favorable properties, GIC exhibits poor physical properties such as low compressive strength, poor wear resistance, difficulty in handling characteristics, and water sorption. Various modifications of GIC have been extensively explored in the literature to improve its properties namely, fibre-reinforced GIC,zirconia containing GIC, Nano chitosan modified GIC, etc. Fly ash (FA) is a by-product of burning pulverized coal in an electrical generating station which is an unburnt residue collected by electrostatic separators. It is a finely divided amorphous aluminosilicate with varying amounts of calcium, which whenmixed with Portland cement produces various calcium silicate hydrates(C-S-H) and calcium aluminate hydrates. These pozzolanic reactions are usually beneficial to the concrete in the field of engineering in that they increase the quantity of the cementitious binder phase (C-S-H) improving the long-term strength, durability, and other desirable mechanical properties. Numerous studies have focused on addressing industrial wastes like FA, aiming to foster a sustainable and eco-friendly environment by transforming waste into valuable resources. Recently, researchers have integrated FA into mineral trioxide aggregate (MTA), a biomaterial used in dental pulp capping, demonstrating notable enhancements in both the physicochemical and biological characteristics of FA-modified MTA. Likewise, FA can be integrated intoC-GIC to achieve enhanced and desirable properties. Hence, the present preliminary study is aimed to synthesize FA-modified GIC (FA-GIC) in different proportions (0.1, 0.25, 0.5 and 1% w/w) and optimize them using different physicochemical characterization studies namely, surface topography assessment, phase analysis and functional group assessment and pH analysis using SEM-EDX, XRD, FTIR and digitalpH meter respectively. The current poster will highlight the results of the same.

K 001

Theoretical Study of SDS Influence on the Hydrogen Bond Network and the Kinetics of Methane Hydrate Formation from Metastable Gas Solution

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ABSTRACT

Classic gas hydrates are inclusion compounds with a crystalline structure formed by the hydrophobic molecules trapped in the cavities formed by water molecules. Light hydrocarbons, CO_2, N_2, H_2S and their mixtures are the most common gases that form hydrates. A distinctive feature of these compounds is the high specific gas content in the structure, which can be used for storing and transporting hydrogen and natural gas, for separation and further burial of greenhouse gases mixtures, for desalination of sea water, etc. However, the slow formation kinetics is a problem: the rate of hydrate formation strongly depends on the supercooling, excess pressure, mixture compound and usage of promoters or inhibitors. The use of surfactants is an effective way to increase the hydrate formation efficiency. It was found that sodium dodecyl sulfate (SDS) is the most effective compound accelerating the hydrate growth process. We investigated the influence of SDS molecules on the methane hydrate formation kinetics and on the water hydrogen bond network using molecular dynamics (LAMMPS package). The systems containing 3000 H_2O molecules (TIP4P/Ice model), 0-20 SDS molecules and 0-313 CH_4 molecules (OPLS-UA forcefield) were constructed by random distribution, equilibrated (500 ps, NVT ensemble) and simulated for 100 ns at 270 K (NPT ensemble). Via the calculation of water F_3 and F_4 order parameters we observed the slight disordering effect of SDS and notable ordering effect of ideally stirred gas molecules on the water short-range order. The repeatable hydrate growth was observed for systems containing 0-2 SDS molecules. At lower gas concentration the presence of SDS molecules significantly enhanced the hydrate formation. At all gas concentrations the presence of SDS molecules made hydrate structure more crystalline in contrast to rather amorphous-like which is usually forming without surfactants.

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K 002

Nanoparticle Influence on Methane and Carbon Dioxide Hydrate Formation: A Molecular Dynamics Study

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ABSTRACT

As the urgency for greenhouse gas mitigation rises, there's a growing interest in the technology of gas hydrates for the transportation and storage of greenhouse gases. Rapid formation of these hydrates, however, remains a challenge. Several nanoparticles, including SiO_2, Al_2O_3, Ag, AgO, and surfactants like SDS, have shown the capability to hasten the hydrate phase creation, a finding backed by both theoretical and practical research. The study of how these nanoparticles influence the kinetics and thermodynamic variables during methane and CO_2 hydrate formation could pave the way for improved greenhouse gas management using hydrate technologies. For this investigation, the Gromacs [1] software package was employed, utilizing molecular dynamics methods to simulate hydrate formation in systems containing methane/CO_2, water, and varied nanoparticles. Different thermostats and barostats were used to study these systems under multiple ***p, T*** conditions. The modeling of nanoparticles, methane, CO_2, and water molecules took into account the Lennard-Jones potentials, while the TIP4P/Ice model [2] was designated for water. All systems maintained a significant water phase with the inclusion of nanoparticles and gas molecules, abiding by three-dimensional periodic boundary conditions set for a designated molecular count. Post initial system equilibration, temperatures were elevated within the range typically witnessed during gas hydrate formation at specified pressures. This paper offers a thorough molecular dynamics assessment on how nanoparticles influence the methane and CO_2 hydrate formation. It was deduced that nanoparticles enhance the speed of hydrate creation, a result that aligns with experimental findings. The paper also reviews the dependency of structural order over time, while meticulously studying variations in induction periods and the volume of gas trapped in the hydrate under assorted conditions. This research was generously supported by the Russian Science Foundation (project 22-19- 00428).

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K 003

Vortices as Probe to Disorder Tuned BCS-BEC Cross-Over in Superconductors

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ABSTRACT

Amongst the most significant discoveries of the nineteenth century which reshaped our knowledge and understanding of quantum phase transition, is the discovery of "superconductivity" by Heike Kamerlingh Onnes in 1911. Characterized by the complete absence of resistivity and perfect diamagnetism in materials, the phenomenon of superconductivity was fascinating and intriguing but at the same time defied the set notions of classical physics. A couple of decades down the line, Pyotr Kapitsa, John F. Allen and Don Misener, in 1937 discovered the phenomenon of "superfluidity", wherein matter behaves as fluid and is characterized by zero viscosity. These two seemingly disconnected phenomena apparently belonged to the different schools of quantum statistics and were pursued based on different set of theories and experiments with spectacular success until the dramatic turn of events at the beginning of this millennium, with the advent of ultra-cold atomic gases and Feshbach resonance. It was demonstrated that the paradigms of these two "super" properties of the quantum gases, describable by fermionic and bosonic pictures are in fact, connected. This smooth connection between the two paradigms viz. Bardeen-Cooper-Schrieffer (BCS) and Bose-Einstein Condensation (BEC), traditionally used for superconductors and superfluids, respectively and experimentally observed in ultra-cold atomic gases in now well known as the "BCS-BEC crossover". Experimental realization of BCS-BEC crossover in 2004-2005, in ultracold atomic gases via Feshbach resonance established that the BCS and BEC regimes, typified by weakly bound Cooper pairs and tightly bound molecules, respectively, are basically the two extremes of a continuum. Subsequently, this cross-over regime turned out to be the host of one of the most fascinating and complex quantum phases, namely, the pseudogap, wherein neither a completely fermionic nor a bosonic description holds good.

Interestingly, it took another almost twenty years to experimentally realize the BCS-BEC crossover in a solid-state superconductor and it is only recently that this phenomenon could be experimentally realized in iron chalcogenide superconductor FeSe, via chemical doping. The observation gave the required impetus to the search for possible candidate materials to observe the crossover phenomenon. The theoretical understanding of the underlying physics however, remains far from being settled. In this work, we propose a novel protocol to capture and understand the physics of doping/disorder tuned BCS-BEC crossover, experimentally observed in FeSe. Within the framework of the microscopic Bogoliubov-de-Gennes (BdG) theory we use the superconducting vortices as a probe to track the disorder induced BCS-BEC crossover. Based on the thermodynamic and spectroscopic signatures viz. (i) the vortex number and (ii) the local single particle density of states in the vortex core, we demonstrate that an engineered disorder potential can serve as a suitable tuning knob to control the BCS-BEC crossover. The "quantum limit" vortices as ascertained via the spectroscopic signatures of the vortex core structure observed in our work unambiguously attests the crossover phenomenon, in agreement with the experimental observations in doped FeSe. From the theoretical point of view, our results as obtained from a relatively simple model Hamiltonian provides an entry point to understand the physics of disorder induced and/or orbital selective BCS-BEC crossover in multi-band superconductors. The protocol of realizing the BCS-BEC crossover in solid state superconductors presented in our work is expected to pave way to the future design and experimental realization of candidate materials.

K 004

First Principle Investigation of Thermoelectric and Optical Properties of $CuSbSe_2$ and $CuBiSe_2$ Compounds

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ABSTRACT

Theoretical investigation of $CuSbSe_2$ and $CuBiSe_2$ have been performed using FP-LAPW implemented by WIEN2K code based on the Density functional theory (DFT) within the Generalized Gradient approximation (GGA). The volume optimization is performed using the Birch Murnaghan equation of states. The optimization is also done for c/a ratio and b/a ratio since $CuSbSe_2$ and $CuBiSe_2$ compounds belong to the orthorhombic structure with space group 62. The Thermoelectric properties of the compounds are analyzed by evaluating the seebeck coefficient, power factor, thermoelectric figure of merit, electrical and thermal Conductivity. The optical properties of the compounds are investigated by evaluating the optical spectra and the changes in the properties such as complex dielectric function, absorption, energy loss function, refractive index and refractivity. $CuSbSe_2$ and $CuBiSe_2$ plays a vital role as a potential absorber material for thin-film solar cells, since it exhibits a high absorption coefficient. It also contributes to the low-cost, nontoxic and earth- abundant materials.

Keywords: *Orthorhombic; Thermoelectric properties; Thermoelectric figure of merit; Dielectric function; Energy loss function*

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K 005

DFT Study of Structural, Electronic, and Optical Properties of Double Perovskite Cs_2LiInF_6 for Optoelectronic Device Applications

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ABSTRACT

The structural, electronic, optical, and elastic characteristics of Cs-based double perovskite Cs_2LiInF_6 are explored under the concept of density functional theory (DFT) [1] using the full potential linearized augmented plane wave (FP-LAPW) method [2] with the generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE-GGA) as the exchange-correlation functional [3]. The optimized lattice constant is obtained by fitting the Birch-Murnaghan equation of state [4] for total energies as a function of volumes. The compound is found to be stable in the cubic phase with the values of Goldschmidt's tolerance factor and octahedral factor [5] calculated to be 1.005 and 0.586. An electronic bandgap of 4.74 eV was found from the band structure plot respectively. The optical parameters, such as reflectivity R, optical conductivity σ, refractive index n, and absorption coefficient α are calculated in the energy range of 0-12 eV. The results show good absorption of incident electromagnetic radiations in the ultraviolet region and thus appear as a good candidate for optoelectronic devices that operate in the ultraviolet range of the spectrum.

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K 006

First Principles Study of Thermoelectric Properties of $CsPb_{1-x}Sb_xBr_3$ (X = 0, 0.125, 0.25, 0.75,0.875)

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ABSTRACT

The study is carried out to design and develop novel perovskite materials for thermoelectric applications. Perovskite compound have advantage of low toxicity, eco-friendliness, and high element abundance. Thermoelectric properties of perovskite materials can be enhanced by doping. The effects of ternary addition of Sb in phase transition, structural, electronic and thermoelectric properties of $CsPb_{X-1}Sb_XBr_3$(x=0, 0.5) compounds are carried out. Band structure calculations are made on cubic parent $CsPbBr_3$ and Sb doped $CsPbBr_3$ compounds. The replacement of four Antimony atoms in parent $CsPbBr_3$, leads to the phase transition of $CsPbBr_3$ compound. In order to analyze the structural, electronic and thermoelectric properties of $CsPb_{1-X}Sb_XBr_3$(X=0, 0.125, 0.25, 0.75, 0.875) compounds, the Full Potential Linearized Augmented Planewave (FP-LAPW) method is implemented in the WIEN2k code using Density functional theory. Density functional theory calculations had been done to calculate the electronic structure and thermoelectric properties of host and Sb doped $CsPbBr_3$ Perovskite materials. All the calculations were performed by using GGA to predict the band gap and the thermoelectric behavior of the Perovskite materials. The thermoelectric properties of the compounds have been calculated in a temperature range of 100K-1000K.

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K 007

The Effect of co-doping using C & Si atom on the Boron Phosphide (BP) Nanosheets: A DFT Study

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ABSTRACT

Using Density functional theory (DFT), we have studied the effect of co-doping using group IV elements such as carbon and silicon on the boron phosphide (BP) nanosheets through the structural stability and electronic properties. The structural stability and the electronic properties of the pure boron phosphide nanosheet and co-doped boron phosphide nanosheet were assessed by the band structure, the density of states (DOS) and the projected density of states (PDOS), charge transfer, electron localization function (ELF), and electron difference density (EDD). The stability of the material is completely studied using the perturbation method and the formation energy. Our results show that the co-doped system shows a more semiconducting nature than the pure BP nanosheet. Also, the band gap of BP material shifted from direct to indirect as a result of co-doping by group IV elements. The co-doped system possesses redshift and major changes in the conduction band due to the chemical shift 0.47 eV and 0.06 eV. This concludes that the co-doped system possesses an n-type nature and is visualized clearly using DOS and PDOS analysis. These findings could lead to the development of nanoelectronics and gas-sensing devices.

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K 008

Enhancing Photocatalytic Activity of Copper Oxide through Introducing Ti, Zn, and Sn: A Density Functional Theory Study

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ABSTRACT

Copper oxide (CuO) exhibits promise as a photocatalytic material; however, it shows certain optical and electronic constraints. In contrast to binary materials, ternary compounds present a broader spectrum of properties that can be tailored for specific applications. This investigation employed Density Functional Theory (DFT) calculations to explore the impact of introducing additional metal cations into copper oxide, focusing on M-CuOx compounds (M= Ti, Zn, or Sn). The new compounds exhibited interesting features, including reduced band gaps, describing them potentially more efficient in utilizing visible light for chemical reactions compared to pure CuO. Furthermore, some of these compounds displayed more negative energy levels, suggesting a potential capability for water splitting, impossible for single CuO. These changes in electronic properties and band gaps were attributed to the introduction of the secondary metal element and structural alterations, notably an increased interlayer spacing within the CuO structure. These materials demonstrated relatively high static dielectric constants, facilitating exciton dissociation, and favourable electron mobility along at least one direction. However, the mobility of positively charged particles (holes) was constrained. This comparative analysis reveals significant trends in material properties as a function of composition, offering valuable insights for the selection and customization of materials for specific scientific and technological applications.

Keywords: *Copper oxide; Photocatalysis; Density Functional Theory; Electronic properties*

K 009

DFT Study on Electronic Properties of Black Phosphorene and Au-Decorated Black Phosphorene

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ABSTRACT

Recently, 2-D materials have become more popular in the sensors manufacturing sector. In this work, we studied the potential of Black phosphorene, a two-dimensional allotrope of phosphorus. It has recently gained significant attention due to its exceptional electronic, structural, and chemical properties. Its high surface area, semiconducting nature, high carrier mobility, direct band gap, tunable anisotropic properties, and oxidative stability make it an attractive platform for biosensor design. The electronic properties of black phosphorene and Au-decorated black phosphorene were investigated using density functional theory (DFT) (1). The band structure, the density of state, charge transfer, chemical potential, and total energy of the system are used to analyze the electronic properties. We observed reasonable changes in the band structure and density of states of Au-decorated black phosphorene, which shows high electrical conductivity, and chemical stability. Our result concluded that Black phosphorene with Au-decorated phosphorene is a promising material for biosensing applications as well as for nanoelectronic devices (2, 3).

Keywords: *Black phosphorene, DFT, Au-decorated*

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K 010

Comparative Analysis of Pristine $MoSe_2$ and Rh-$MoSe_2$ Monolayer: DFT Study

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ABSTRACT

Transition Metal Dichalcogenides (TMDCs) are a group of 2D materials, which has become a hot topic in recent years due to their promising physical, electrical, chemical, and optical properties at the monolayer level. $MoSe_2$ monolayer with high surface-to-volume ratio, high electrical conductivity and tunable semiconducting nature are used in transistors, photo-detectors, energy storage and sensors. As a noble metal with strong catalytic behaviour and electron mobility, Rhodium (Rh) is frequently applied in carbon nanotube, graphene, and MoS_2 systems as dopant to enhance the properties of the system. We have analysed the geometry, stability and electronic properties of pristine $MoSe_2$ and Rh-$MoSe_2$ using Density Functional Theory (DFT). The stability of the system has been studied by the formation energy and total energy of the systems. The electronic properties are analysed by band structure, the density of states, projected density of states, charge transfer and chemical potential. Rh-$MoSe_2$ shows better stability than pristine $MoSe_2$ which is calculated and confirmed from the formation energy values. From the comparative findings, we have observed that the Rh dopant enhances the conductivity and the charge transfer of $MoSe_2$ monolayer. Our analysis will contribute certain guidance for experimentalists to explore the potential application of Rh-$MoSe_2$ monolayer for gas sensing applications.

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K 011

DFT Analysis of the Mechanical Stability, Electronic and Optical Properties in Actinium based Perovskite.

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ABSTRACT

Ultra-wide band gap semiconductors (UBWG) with good absorption in UV-C spectrum are good candidates for deep-UV optoelectronics [1,2]. Using density functional theory (DFT), a new actinium-based perovskite ($AcAlO_3$) with wide band gap is examined. The tolerance factor, octahedral factor, volume optimization and phonon dispersion curves substantiate its dynamical stability against small homogenous distortions. For deeper insight, the electronic properties are compared in Generalized gradient approximation (GGA-PBE) and modified Becke-Johnson (mBJ) exchange-correlation potential with the inclusion of spin-orbit effects [3]. A direct band gap (Γ-Γ) of 5.5 eV is observed in the mBJ band structure. The upper valence bands are comprised of dispersion less oxygen-2p bands and lower conduction bands of parabolic Ac-4f bands. The optical properties such as absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric tensor are computed. The electromagnetic absorption of the compound is predominantly in UV-C region. Such detailed computational studies suggest that the material may find a prospective place in deep-UV optoelectronics devices.

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K 012

"Quantum Analysis of Graphene-based Architectures for Optimizing Artificial Intelligence: A Comprehensive Study"

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ABSTRACT

This comprehensive study investigates the synergistic potential of quantum computing and graphene-based architectures in optimizing artificial intelligence (AI) systems. Through a thorough examination of the unique properties and behaviors of graphene at the quantum level, this research delves into the intricate interplay between quantum phenomena and the enhanced performance of AI hardware and algorithms. Utilizing advanced quantum simulation techniques, the study showcases the profound impact of graphene on accelerating AI training processes, improving computational efficiency, and enabling the development of robust and energy-efficient AI systems. Furthermore, this paper discusses the challenges and opportunities associated with integrating graphene into AI frameworks, emphasizing the importance of quantum analysis in understanding the fundamental mechanisms underlying the optimization of AI functionalities. The findings presented in this research offer valuable insights into the promising applications of graphene in revolutionizing the landscape of artificial intelligence.

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K 013

Design and Develop Magnesium Chalcogenide Thermoelectric Materials

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ABSTRACT

In this paper, the study is going to be carried out to design and develop magnesium chalcogenide thermoelectric materials. Structural, phase transition, electronic and thermoelectric properties of Magnesium Chalcogenide materials is studied. By means of Full Potential Linearized Augmented Plane wave (FP-LAPW) method as implemented in the WIEN2k code is used to analyse the structural, electronic and thermoelectric properties. Thermoelectric materials convert heat energy to electrical energy based on Seebeck and Peltier effect. This leads to utilize hardly usable in thermoelectric systems for cooling or heating in niche applications and are being studied as a way to regenerate electricity from waste heat. Almost lost thermal energy into productive applications as efficient as possible. They are very useful for heat energy harvesting and cooling applications as green and sustainable energy resources. The ground state properties such as equilibrium lattice parameter, bulk modulus and total energy of the compounds are obtained by generating a supercell and by fitting the volume optimization data in Birch-Murnaghan equation of state. Density functional theory calculations have been carried out to calculate the electronic structure and thermoelectric properties. All the calculations were performed by using various exchange correlation methods to predict the band gap and the thermoelectric behaviour of the materials.

Keywords:

Structural properties, electronic properties, thermoelectric properties, electrical conductivity, Power factor, Seebeck coefficient

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K 014

Computational Insights on Tuning TADF Properties via Multi-Donor-Acceptor Linkages

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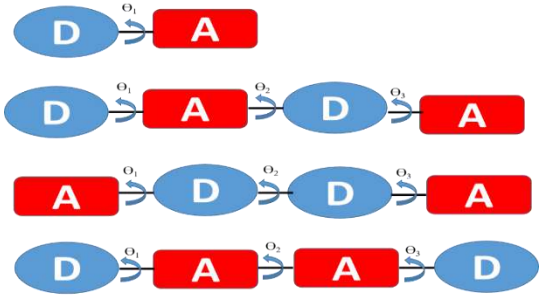
ABSTRACT

Thermally activated delayed fluorescence (TADF) is an exciting mechanism in the field of organic optoelectronics, offering the potential for efficiently converting triplet excitons into emissive singlet excitons. This property has significant implications for enhancing the quantum efficiency of applications such as organic light-emitting diodes (OLEDs). This work is assigned to explore the design and development of efficient TADF molecules by investigating different arrangements of donor (D) and acceptor (A) connections. Specifically, this study will examine the D-A, D-A-D-A, A-D-D-A, and D-A-A-D connection arrangements and their effects on the ground and excited state properties of TADF molecules. Through this study, we aim to establish a connection between donor-acceptor architecture and TADF properties by evaluating both ground and excited state characteristics of the newly designed molecules with the donor of 5,10 dihydrophenazine and acceptor of diphenylsulfone and benzophenone.



Molecular design strategy adopted in this work.

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K 015

Examining the Interaction of Collagen like Peptides with Copper Nanosurfaces: A Theoretical Approach

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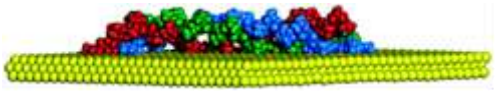
ABSTRACT

Collagen is an important structural protein that provides a crucial mechanical framework which becomes vital to many structural and functional roles of tissues including the extracellular matrix. It forms a triple helical structure consisting of three polypeptide chains, rich in glycine, proline and hydroxyproline residues which are essential for its stability and function.

Copper is an essential trace element required for various biological processes including enzyme catalysis, redox reactions, and connective tissue formation. In the context of collagen, copper is particularly significant due to its involvement in post-translational modifications in collagen protein. This modification, known as hydroxylation, is essential for collagen's stability and functionality. Interaction of collagen like peptides (CPs) with copper nanosurfaces (CuNs) is a fascinating and a biologically significant phenomenon that plays a crucial role in maintaining the structural integrity and functionality of various tissues in the human body. Understanding these interactions of collagen-like peptides with copper nanosurfaces/nanoparticles is of significant interest due to its potential application in biomaterials, tissue engineering, nanotechnology, nanomedicine and cancer treatment. In this work, we are planning examine such interactions via in-silico approach using the following objectives.

- To understand the adsorption pattern of fibrillar proteins and to predict the associated conformational changes in CPs.
- To assess the binding affinity and to elucidate the interaction between model triple helical peptides with CuNs.
- To investigate the effect of peptide sequence and composition of CPs on its interaction with the copper surface.



Expected CPs-CuNs interaction from the MD simulation.

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K 016

Finite Element Simulation of Solid-State Sintering of Micro Ceramic Injection Molded Alumina based on Phenomenological Constitutive Law

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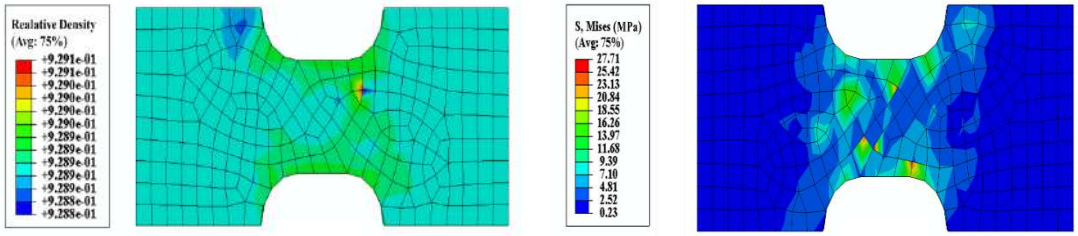
ABSTRACT

This study speaks of finite element simulation of sintering densification behavior of Micro Ceramic Injection molded (μ-CIM) alumina sample adopting a thermo-elasto-viscoplastic constitutive model. The applicability of the developed numerical model lies in designing/optimising sintering process parameters such as heating cycle which includes heating rate, isothermal holding time and cooling rate, sintering temperature, initial relative density in a way that it can predict the optimum final relative density distribution, shrinkage, stress distribution etc. The simulation studies have been performed using finite element code ABAQUS, with the incorporation of user subroutine i.e., UMAT. The constitutive parameters such as free sintering strain rate and uniaxial viscosity (as functions of relative density and temperature) have been modelled using the phenomenological equations derived by Kim and co-workers, to define sintering behavior of alumina powder. The simulation results show that the final relative density distribution of the sintered sample depends on cooling rate as well, along with the heating rate and isothermal holding time. In this study, the phenomenological free sintering rate equation is applied to a micro injection molded body (tensile sample) for the first time to simulate the sintering densification, and the close agreement between the model predictions of relative density and shrinkage to that of experimental observations confirms its accuracy.



(a) (b)

Fig. 1. (a) Simulated relative density contours of sintered tensile sample after heating at 1873K with a heating rate of 6K/min according to stairway circle and holding at 1873K for 1hr and cooling to room temperature at 10K/min and (b) distribution of Mises equivalent stress in the sintered specimen.

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K 017

Early COPD Prediction using Machine Learning and Blood Lipid Biomarkers

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ABSTRACT

Chronic Obstructive Pulmonary Disease (COPD) is a prevalent and debilitating respiratory condition that often remains undetected until it reaches an advanced stage, leading to significant challenges in effective management. Early diagnosis of COPD is paramount for improved patient outcomes, as delayed intervention can result in irreversible lung damage. This abstract presents a novel approach to predicting the onset of COPD using machine learning, specifically the XGBoost algorithm, and blood lipid levels as biomarkers. The research proposes a groundbreaking methodology that harnesses readily accessible and cost-effective blood lipid data to facilitate early COPD detection. COPD is characterized by chronic inflammation in the airways and lungs, leading to restricted airflow and reduced lung function. The disease is associated with a multitude of risk factors, including smoking, environmental exposures, and genetic predisposition. Unfortunately, the nonspecific nature of early symptoms often leads to underdiagnosis, making innovative diagnostic tools essential. Machine learning, with its ability to extract valuable insights from complex datasets, has emerged as a promising avenue for early disease prediction. The XGBoost algorithm, known for its robust classification capabilities, is employed in this study to develop a predictive model. This model leverages blood lipid profiles, including cholesterol and triglyceride levels, as potential indicators of COPD risk. One significant advantage of this approach is the accessibility of blood lipid data through routine blood tests, rendering it a convenient and cost-effective alternative to more invasive and time-consuming tests, such as Arterial Blood Gases (ABG). This accessibility and ease of data collection make it an attractive avenue for early COPD prediction.

The overarching goal of this study is to enhance timely diagnosis and intervention for COPD. By identifying individuals at risk of COPD before symptoms become pronounced, healthcare providers can offer early interventions, including smoking cessation support, lifestyle modifications, and appropriate medications. These proactive measures can potentially slow the progression of the disease and improve overall patient outcomes. While the promise of this approach is evident, further research, validation, and clinical trials are necessary to establish its reliability and effectiveness in real-world clinical settings. If successful, this innovative methodology could revolutionize the early diagnosis and management of COPD, offering a lifeline to those at risk of this debilitating respiratory condition.

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K 018

Single Atom Decorated V_2CO_2 for CO_2 Hydrogenation using Ab-initio Calculations

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ABSTRACT

CO_2, a notorious greenhouse gas, is a global concern in recent times, whose concentration in the atmosphere is increasing abruptly. In order to mitigate the negative effects of CO_2 and make use of it in a sustainable manner, we are trying to convert CO_2 into useful green fuels such as methanol, ethanol and chemicals such as formic acid, formate, etc. Seeking for a good catalyst towards the reduction of CO_2, we observed an intriguing family of non-noble 2D layered materials, Mxenes. It shows excellent performance as an electrocatalyst for heterogenous catalysis such as hydrogen evolution reaction (HER), carbon dioxide reduction reaction (CO_2RR) and so on. Here, in this work, the mechanistic reaction pathway towards the formation of formate by Electrochemical Reduction (ECR) of CO_2 is being carried out on different active sites of vanadium carbide with fully oxygen terminated surface (V_2CO_2), decorated with different transition metal single atoms[1]. This is achieved using Density Functional Theory with BEEF-vdW functional for accurate forecast. The enhancement in the CO_2RR activity of the single atom decorated system is due to the presence of large number of electrons in the single atom, which acts as an electron donor. To achieve high performing electrocatalyst for CO_2 reduction, we determined the limiting potential of corresponding hydrogenated derivatives of various single atom decorated V_2CO_2. This work predicts new opportunities for cost effective catalytic materials for CO_2 reduction.

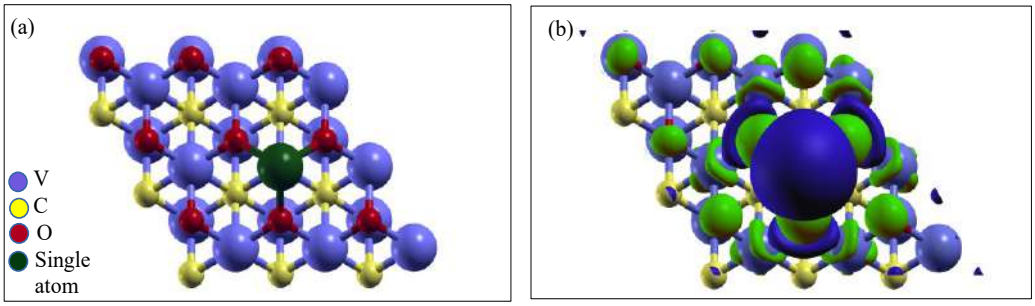

Figure 1: Top view of the (a) optimised single atom decorated V_2CO_2 (b) Charge density difference of the single atom decorated V_2CO_2

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K 019

Functionalization of Single Walled Aluminum Nitride Nanotube with Amino Acids using First Principles Study

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ABSTRACT

In this study, we investigate the functionalization of Aluminum Nitride Nanotube (AlNNT) with amino acids (Glutamine, Arginine, and Phenylalanine) using first-principle's density functional theory (DFT) calculations. We employ DFT techniques to model the interactions between amino acids and AlNNT, examining the structural and electronic properties of the functionalized systems. We examined various aspects of the structures, including their geometry and electronic properties, such as bond lengths, bond angles, total energy, formation energy, band structure, chemical potential, density of states (DOS), projected density of states (PDOS), charge transfer, electron difference density, and exchange-correlation potential. The (5, 5) AlNNT exhibits a energy bandgap value of 3.31 eV, implying its semiconducting nature. Furthermore, the chemical potential of the pristine system is determined to be -4.12 eV. From the DOS analysis, it can be seen that the band structure profile and the energy states of the pristine system matches well. Notably, the valence band displays a more pronounced level of energy hybridization compared to the conduction band, that is clearly reflected in the band structure. Overall, the findings from this research offer a foundation for the development of novel drug delivery systems based on amino acid-functionalized AlNNT, potentially leading to more efficient and precise drug administration in biomedical applications.

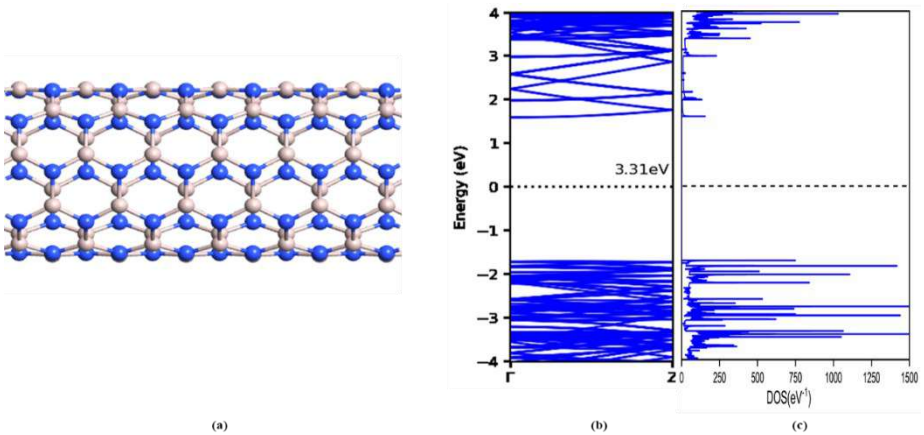

Fig.1. Optimized structure (b) Band Structure (c) DOS of AlNNT.

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K 020

DFT Study on Functionalization of Boron Nitride Nanotubes (Bnnt) with Various Functional Groups

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ABSTRACT

In this study, first-principles calculations were carried out to examine the structural and electronic properties of single-walled Boron Nitride Nanotube (BNNT), which have been functionalized with a various functional group, such as hydroxyl, amine, and amide. The optimization and perturbation of individual BNNT as well as functionalised BNNT with functional groups were performed using quantumATK software. The assessment of structural stability involved the repeated random perturbations to identify the minimum total energy difference. Our findings reveal that the (5, 5) BNNT exhibits a wide-bandgap semiconducting behaviour, with an energy bandgap of 4.46 eV. The pristine BNNT demonstrates a chemical potential of -3.81 eV. The electronic properties of BNNT were assessed by analyzing total energy, formation energy, bandgap, density of states (DOS), projected density of states (PDOS), chemical potential, exchange-correlation potential, electron difference density, dipole moment, percentage ionic character and charge transfer. Furthermore, the structural properties of BNNT, such as bond length and bond angle, were comprehensively elucidated. Covalent modification of BNNT with functional groups leads to an increase in negative solvation energy, signifying enhanced solubility of the system. This enhanced solubility suggests a reduction in toxicity, thereby creating an opportunity for their use as carriers in drug delivery applications.

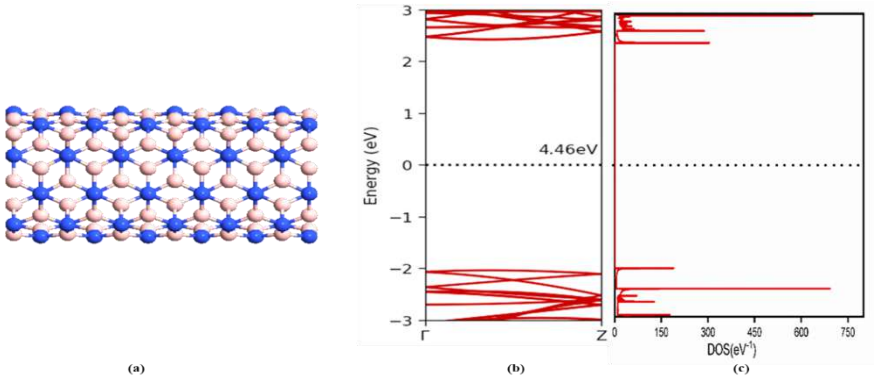

Fig.1. Optimized structure (b) Band Structure (c) DOS of BNNT.

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K 021

Effect of Metal Cluster on Niobium based Mxene for Hydrogen Evolution Reaction (HER)

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ABSTRACT

Green Hydrogen has the potential to solve the energy crises and environmental problems, its production via electrochemical water splitting has been widely studied. Expensive noble metals like platinum is used a catalysts for Hydrogen Evolution Reaction (HER). Two dimensional layered materials, namely "MXenes" have attracted immense attention as catalyst for electrochemical water splitting due to its unique properties. In this work density functional theory is used to get an insight into the catalytic activity of Nb_2CO_2 MXene decorated with Cu_3 cluster for Hydrogen Evolution Reaction. We found an enhancement in the catalytic activity of Nb_2CO_2 when decorated with Cu_3 cluster. Our results show that the clusters centre is the most active catalytic site for HER, with a Gibbs free energy of -0.10 eV for hydrogen adsorption. Stability of the designed catalysts was confirmed through binding and cohesive energy analysis. Charge density difference and Bader charge analysis indicates that the increase in catalytic activity is due to the accumulation of charge at the centre of the Cu_3 cluster. We also studied the electronic properties of the system, and observed that the catalysts remained metallic after Cu_3 adsorption on the MXene surface. Our findings may provide insights to fabricate cheap MXene-based catalyst material by depositing small clusters of copper which is slightly superior to platinum and a potentially cost-effective HER catalyst.

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K 022

Structure, Synthesis and Molecular Docking Studies of N, N'-Pyridine-2,6-Diylbis-[3-(Pentaflurophenyl) Urea] Crystals

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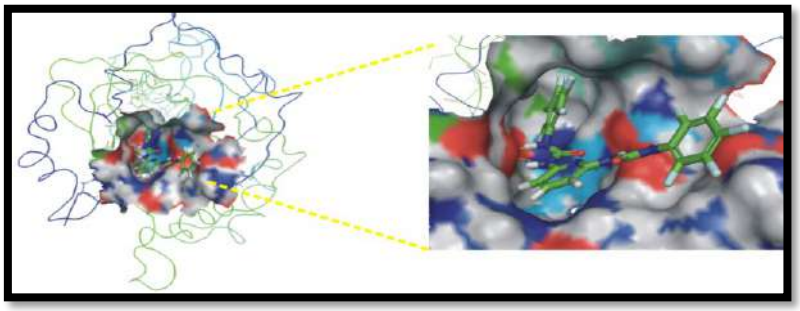
ABSTRACT

The chemical N,N'-Pyridine-2,6-diylbis-[3-(pentaflurophenyl)urea] was synthesized by using diamino pyridine and pentafluorophenylisocyanate, the synthesized crystal crystallizes in Triclinic system with P^{-}_{1} Space group, with parameters as a = 7.5939(5) Å, b = 12.4169(9) Å, c = 13.5494(9) Å, α = 100.927^{O} (2), β = 104.223(2)^{O} , γ = 96.779^{O}(2) and volume 1197.67 (14) Å^{3}. Single crystal XRD reveals that the versatile sensor having N-H ... O and N ... O interactions which imparts more stabilization to the molecule, which was proved by FT-IR, Raman, NMR and mass spectral studies. The optimized molecular structure, vibrational analysis, electronic properties of title compound was calculated by using density functional theory (DFT) Method. The structure of the synthesized compound resembles active NAMPT (Nicotinamide Phosphoribosyl transferase) protein to investigate the bio molecular interactions. This resemblance is helpful in calculating the activities of newly designed inhibitors on the basis of docking scores through Molecular docking studies.



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K 023

Enhancement of Visible Light-Driven Water Splitting and CO_2 Conversion Activities of $SrTiO_3$ by Doping Engineering

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ABSTRACT

Efforts to enhance the photocatalytic efficiency of $SrTiO_3$ for overall water splitting and CO_2 conversion under visible light irradiation have proven to be a crucial strategy in meeting global energy demands.[1,2] One of the widely employed methods in this endeavor has been doping transition metals. However, recent experimental investigations have revealed that co-doping is a more promising technique compared to single-element doping. A comprehensive review of the existing literature on this subject has inspired us to explore the key criteria for selecting co-dopants through theoretical calculations, which eventually facilitate the design of efficient catalysts.[3,4] The results of this investigation showed that doping $SrTiO_3$ with only Ni is insufficient to provide the requisite levels of photoactivities for H2 production and CO2 reduction. Additionally, it has been investigated that Ni^{4+} state, which exists in the Ni-$SrTiO_3$ without any defect, is not preferred for achieving significant photo conversion efficiency. Interestingly, the Ni^{2+} state is found to be the preferred charge state. Therefore, in our current study, we have selected rare earth element (La), transition metals (Cr, W, Mo), and non-metal (F) as co-dopants to stabilize the Ni^{2+} state of Ni. Our approach employs density functional theory (DFT) to investigate the inherent changes resulting from co-doping. We have calculated the defect formation energy to assess the doping process's viability. Additionally, we have estimated the band edges alignment concerning the redox levels of water and CO_2, with the aim of evaluating the performance of these materials in water splitting and CO_2 reduction processes.

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K 024

Theoretical Investigation of the Structural, Electronic and Thermoelectric Properties of Janus R-MoXY Heterostructure

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ABSTRACT

The heterostructures is a stack of materials with different bandgaps that enable exact control and manipulation of electronic and Thermoelectric properties. This makes it possible to create devices with unique properties that are impossible to achieve with a single material. In this work, we calculate the structural, electronic and thermoelectric properties of MoXY (X,Y = S, Se, Te) Janus Material using Density Functional Theory (DFT) in combination with Non-Equilibrium Green's Function(NEGF). We use the Perdew–Burke–Ernzerhof (PBE) function of the generalized gradient approximation (GGA) as an exchange-correlation potential, implemented by the Quantum ATK package [1] to calculate ground state properties. The band gap of the Janus MoXY material was calculated, and it is inconsistent with published results [2]. The studies on band structure reveals it has a direct band gap. The DOS studies indicates that the distribution of energy levels is influenced by the presence of Mo atom [3]. Further we constructed a Janus MoXY based heterostructure by stacking technique. Our studies indicate when Group 'VA' material is used to construct the heterostructure with R-MoXY, the charge separation [4] takes place that results in the increase in the flow of electricity. In addition, the thermoelectric parameters such as the Seebeck coefficient, Thermal conductivity, and the Thermoelectric figure of merit (ZT) function were analysed. Our results confirm that the Janus Material based Heterostructure is a promising material for thermoelectric applications.

Key Words: *Density Functional Theory (DFT), Janus Material, Thermoelectric Properties, Figure of merit.*

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K 025

A First-Principles Study of the Topological Phase in Zintl Compound KCd_4As_3

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ABSTRACT

Topological materials (TMs) are exotic materials which are insulating in bulk but have exotic metallic states present at their surfaces attracting significant research efforts in condensed matter physics [1-3]. These materials have potential applications in Spintronics [4], Quantum computing [5], Chemical catalysts [6], and thermoelectric energy harvesting [7]. TMs can be divided into several categories e.g., topological Insulators (TI), topological semimetals (TSM), topological crystalline insulators (TCI) and many more. Time reversal symmetry (TRS) and spin-orbit coupling (SOC) play an important role in TIs. Consequently, inversion in bulk bands is observed at high symmetric points in the bulk Brillion zone which are protected by TRS and inversion symmetry. The calculation of Z_2 topological invariants and surface Dirac cone are used to identify the topological nature of materials. These surface states are doubly protected and do not allow the backscattering in absence of a magnetic field.

In this work, we report the topological phase in the centrosymmetric layered arsenide KCd_4As_3 using *first-principles* calculations. It was reported that KCd_4As_3 exists in a rhombohedral structure with space group $R\bar{3}m$ (166). This material has a similar crystal structure to experimentally synthesized $RbCd_4As_3$ [8] which shows topological character at ambient conditions [9]. We investigated the topological nature of KCd_4As_3 and identified that this material exhibits a topological non-trivial nature. The Z_2 topological invariants are calculated with the help of product of parities at time reversal invariant momenta (TRIM) points and found of non-zero value. The Surface density of states (SDOS) is also calculated where a Dirac cone is observed near the Fermi level. The existence of topological band inversion and the Dirac cone confirms that KCd_4As_3 is topologically non-trivial.

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K 026

An ab-initio Study of Topological Phase Tuning in Zintl Compound $RbZn_4P_3$

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ABSTRACT

Topological phase of matter [1-2] is becoming increasingly popular after the discovery of topological insulators (TIs). Exploring a topologically trivial material that can be made topologically non-trivial by strengthening spin-orbit coupling (SOC) is quite interesting. The external pressure [3] is a particularly advantageous tool because it has no effect on the system's charge neutrality. Both theoretically and experimentally, numerous types of Zintl compounds including binary, ternary, and quaternary have been investigated. According to first-principles calculations, the structural phase transition leads the topological phase transition in $NaCd_4As_3$ [4], which changes it from a topological crystalline insulator (TCI) to a topological insulator (TI). The topological phase transition has been attributed to the breaking of mirror symmetry. $RbZn_4P_3$ have isoelectronic structure with $NaCd_4As_3$ but with different space group. Presently, using first-principles calculations, we examined the topological phase characteristics of the ternary Zintl compound $RbZn_4P_3$ under the influence of hydrostatic pressure and epitaxial strain. RbZn4P3 shows topological phase transition under hydrostatic pressure of 10.5 GPa and under axial strain of 2% topologically non-trivial phase can be seen. Further, non-trivial phase can be verified with the help of parity table and observed surface states.

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K 027

Exploring the Thermoelectric Potential of $CsGaSb_2$ Zintl Phase Compound: A Computational Study

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ABSTRACT

Thermoelectric (TE) materials have attracted significant attention for their potential in converting waste heat into useful electrical energy, holding promise for various energy harvesting applications. Achieving high TE performance of a material requires a high power factor and a low thermal conductivity. The recent discovery of antimonide based Zintl phase compounds has prompted exploration in the search of high-performance TE materials, as they exhibit phonon-glass electron-crystal behaviour. Thus, the present study systematically examines the transport properties of a ternary antimonide Zintl phase $CsGaSb_2$, which crystalizes in the tetragonal structure, using first-principles calculations in conjunction with Boltzmann transport theory. Our computed structural parameters, agree well with the available experimental reports, authenticating the robustness of our theoretical framework. This compound is found to be thermodynamically and mechanically stable. $CsGaSb_2$ is found to be direct band gap semiconductor employing Tran Blaha modified Becke Johnson functional. We propose a strategy to improve the power factor and TE performance by optimizing carrier concentration. The high power factor and low thermal conductivity, resulting in high figure of merit of the investigated compound. Thus, the present study may provide valuable insights in exploring the effect of carrier concentration on transport properties of Zintl phases and their prospective energy harvesting applications.

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K 028

To Uncover the Potent Inhibitor for Parkinson's Disease by Overexpression of HDAC4 and Atomistic Revelations from Molecular Dynamics Simulations

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ABSTRACT

HDAC (histone deacetylase) enzyme overexpression is associated with a wide range of diseases, including cancer and neurological problems, making HDAC inhibitors potentially therapeutic. Most people have Parkinson's disease (PD), which is a movement disorder. PD development involves -syn aggregation and uneven protein homeostasis. Over 1% of those over the age of 60 have Parkinson's disease, the second most prevalent neurodegenerative condition. According to estimates, 1.04 million people were diagnosed with PD in 2017, and by 2040, that figure is anticipated to quadruple. People of all ages, colors, and ethnicities are affected by PD. HDACs have the ability to control autophagy, which is linked to the onset and progression of PD. In vitro and in vivo PD models show the neuroprotective benefits of many HDAC inhibitors. HDAC4 is highly expressed in brain tissue and is crucial for brain development, proper brain function, neurodegeneration, and the death of neuronal cells. Screening will be carried out for the inhibitors obtained from available databases of FDA-approved drugs. Molecular docking and molecular dynamics will be performed to understand the molecular interaction of drug molecules in the targeted protein. Force field parameters for the zinc active site will be developed. Free energy calculations will be carried out for the protein-ligand complexes. The most potent HDAC4 inhibitor will be reported and this study will provide valuable information to in vitro studies related with Parkinson's disease.

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K 029

Theoretical Evaluation of $Li_xMg_{(1-x)}Fe_2O_4$ as an Electrocatalyst for Enhanced Hydrogen Evolution

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ABSTRACT

The theoretical investigation to describe the electrocatalytic potential of $Li_xMg_{(1-x)}Fe_2O_4$ as an alternative material for hydrogen evolution reactions (HER) is studied. The rising cost of noble metals like platinum (Pt) in conventional electrocatalysts has spurred the quest for cost-effective. In this study, we employed density functional theory to simulate the electrocatalytic performance of $Li_xMg_{(1-x)}Fe_2O_4$ for HER, marking the first such theoretical exploration of this material. Our analysis enclose diverse facets of the HER process, including the density of states, binding energies, band structure, charge transfer, and minimum-energy path. Notably, our findings consistently demonstrated a lower energy barrier for the HER activity, irrespective of the setup. These results provide compelling evidence that the suggested $Li_xMg_{(1-x)}Fe_2O_4$ structure holds the potential to enhance its intrinsic electrocatalytic activity, offering a promising way for sustainable and cost-efficient hydrogen production.

Keywords: *Ferrite; Electrocatalysis; Density Functional Theory; Electronic properties.*

K 030

Material Profilation using Structural and Thermodynamic Fingerprint

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ABSTRACT

The use of supercomputers and machine-learning aided quantum calculations has resulted to a wealth of data for materials. This has widens the gap between the generated information and the derived knowledge. We aim to implement a framework based on the geometric and electronic structural fingerprint of the materials. The framework will query the existing databases using the concept of similarity and map the connectivity of the materials space. As an implementation, we model the Gibbs free energy of the materials metal trihalide materials as the catalyst for water splitting reaction.

K 031

Ferrimagnetic Half-metals TaMnZ (Z = As, Sb, Bi) for Spintronic and Thermoelectric Application

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ABSTRACT

Half metals which are hybrids of metals and semiconductors has a variety of heat transport and spin transport properties. They can be investigated by first principle calculations. This research article covers the structural, mechanical, electronic, magnetic and thermoelectric properties of the half Heusler alloys TaMnZ (Z= As, Sb, Bi). The equilibrium lattice constants and corresponding ground state energies verifies that the studied alloys are stable in ferrimagnetic cubic phase. The band dispersion plots suggest that the compounds TaMnAs, TaMnSb and TaMnBi are half metals with indirect band gap having the band energies of 1.13 eV, 1.24 eV and 1.12 eV respectively in the spin down channel. As the materials have 100 % spin polarization and magnetic moment of -1 μ_B, they are suitable for making spintronic devices such as spin transistors and spin flip flops. Thermoelectric performance of the alloys in dependence of temperature have been studied by classical Boltzmann theory. The materials have low lattice thermal conductivity which was confirmed by Slack's equation. The obtained thermoelectric figure of merit for p-type TaMnAs, TaMnSb and TaMnBi are 0.7, 0.6 and 0.8 respectively at 1200K. Similarly, the figure of merit obtained for n-type TaMnAs, TaMnSb and TaMnBi are 0.6, 0.64 and 0.8 respectively at the same temperature. The favourable heat and spin transport properties of these alloys show that they are the potential elements in the thermoelectric modules of Seebeck generators and valves in the spin diodes and spin transistors.

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K 032

Identification of Dual Inhibitors Targeting VEGFR-2 and HDAC: A Computational Study

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ABSTRACT

The family of receptor protein tyrosine kinases (RTKs) known as vascular endothelial growth factor receptors (VEGFRs) controls tumor-induced angiogenesis. Each VEGFR family has unique characteristics. Among them, VEGFR-2 has been identified as a promising tumour therapy target. In addition, histone deacetylase (HDAC) enzymes play an indispensable role in biological processes such as gene regulation, transcription, cell proliferation, angiogenesis, migration, differentiation, and metastasis, suggesting that HDAC inhibitors may have therapeutic value. Therefore, it's necessary to discover novel approaches to enhance clinical results and reduce the harmful effects of VEGFR-2 and HDAC inhibitors. Due to their excellent pharmacodynamics, low toxicity, and anti-resistant actions, VEGFR dual-target inhibitors are gaining popularity as a viable treatment option, synergising with other medicines in tumour formation and progression. A group of VEGFR2/HDAC dual inhibitors with hydroxamic acid and N-phenylquinazolin-4-amine moieties was discovered in 2016. Pharmacophores of both inhibitors were recently synthesised to assess the inhibitory effects of phenylurea hydroxamic acids against VEGFR2 and HDAC. In 2022, inhibitors were developed and evaluated based on earlier reported pazopanib-based HDAC and VEGFR dual inhibitors. Herein, a novel series of dual inhibitors were identified, screened, and evaluated based on previously reported FDA-approved drugs. Molecular docking and molecular dynamics studies will be conducted to understand the molecular interactions between drug molecules and the targeted protein. The protein-ligand complexes will be subject to Gibbs free energy and entropy calculations during the binding mechanism of ligand in the cavity.

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K 033

Impact of Chemical Potential and Band Effective Mass in the Thermoelectric Heat Transport Properties of Narrow Band Gap Semiconductors – A Theoretical Approach

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ABSTRACT

The structural, electronic and thermoelectric properties of TiAgZ type half-Heusler compounds with 18 valence electrons was studied using Full Potential Linearized Augmented Plane Wave method (FP- LAPW) based on Density Functional Theory (DFT). The generalized gradient approximation of Perdew– Burke and Ernzerhof is used for calculation of the structural parameters and elastic properties of TiAgAl, TiAgGa, TiAgIn. The electronic properties reveal that the compound are narrow band gap semiconductors with direct and indirect band gap having the band energies of 1.39 eV, 0.19 eV, 0.08eV for TiAgAl, TiAgGa, TiAgIn respectively. On careful observation of the band structure one can predict that TiAgZ is a narrow indirect band gap semiconductor with electron transition along Γ-X symmetry point in the first Brillouin zone. Transport properties have been computed at different temperatures by using semi conventional Boltzmann theory within constant relaxation time approximation. The obtained thermoelectric figure of merit for TiAgAl, TiAgGa, TiAgIn are 0.4, 0.7 and 0.3 at 1000K. Hence these are suitable candidate for thermoelectric applications also.

Keywords: *half–Heusler compounds, Seebeck coefficient, density of states, figure of merit.*

K 034

Electing a Suitable Ionic liquid for Stabilizing Uio-66: A Computational Study

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ABSTRACT

Metal organic frameworks (MOFs) have emerged as a strong research material due to their exceptional porosity and tunable nature, MOF consist of metal cluster coordinated with organic linker, we can functionalize these linkers according to the application we are interested. With the beauty of having such fine qualities, it has various electrical, environmental and therapeutic applications, nevertheless there are several factors which can affect their performance such as moisture, chemical and thermal stability etc. To counter this issues several studies have been devoted on stabilizing the MOF, in this work we have considered UiO-66 (University in Oslo) as MOF because of its notable thermal and chemical stability and series of versatile ionic liquids (ILs) such as $[Emim]^+$ and $[Bmim]^+$ with $[X]^-$, where X = OAc, BF_4, PF_6, DCA, NO_2 and Cl have been impregnated in tetrahedral (~ 10 Å) and octahedral (~16 Å) pores of UiO-66. We have used first principle approach to study the synergism between UiO-66 and IL interface, spectral properties between the composites, charge transfer properties at the interface. We have observed that UiO-66 structure was not affected even after loading IL. Alkyl effect in IL and confinement effect is found to have played a crucial role in stability of the complex. Furthermore, when compared to cations, anions have profound liking towards MOF because of having high electronegative atoms. Result from this study will help us to understand the molecular level interaction between MOF and various ILs. In addition, suitable IL based composite will be used for the energy and environment related applications.

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K 035

Non-Covalent Interactions in Coronene-Ionic Liquids: A DFT Study

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ABSTRACT

The role of anions in ionic liquids (ILs) play an important part in the stability of the ILs@ Coronene (COR) surface. To get more insights on the complex stability, selection of a suitable density functional theory (DFT) method is important to study the interfacial influence of IL at the COR structures. Here, the interaction of ILs such as $[MMIm]^+$ $[X]^-$, $[EMIm]^+$ $[X]^-$ and $[BMIm]^+$ $[X]^-$ (where, X=OAc, $AlCl_4$, PF_6, BF_4, Cl, OTf, Tf_2N, DCA) with graphene model (i.e. COR) is studied. We found that the physisorption mechanism of ILs on the COR surface is mainly driven by the anions through different mode of interaction. Close scrutiny of the geometries shows that there are two modes of interaction at COR surface. The cation-anion exhibit strong interaction with the considered COR pane and the uptake depends on the size of the anion and cation of the ILs. The interaction between cation-anion forming C-H···F H-bonded interaction, which is undisturbed in fluorine (F-) based IL at the COR. whereas, non-fluorinated anions on the pane behaves differently than the former anions. This is due to the inter ion interaction as well as interfacial interaction between surface and ILs. The change in the cation-anion interaction span at the COR pane leads to the weakening of uptake strength. This is an important finding to identify the potential supercapacitor materials for energy storage applications. Furthermore, to get more insights on the structure, stability and spectra, we have employed binding strength analysis, vibrational frequencies, atoms in molecules (AIM), non-covalent interaction index (NCI) and symmetry adopted perturbation theory (SAPT0) analyses.

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K 036

Theoretical Predictions on the Ferrimagnetic Half metals ZrMnSi and HfMnSi for Thermoelectric and Spintronic Device Application

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ABSTRACT

Half metals are considered as the hybrids of metals and semiconductors. Here we have investigated the half metallic Heusler alloys ZrMnSi and HfMnSi with magnetic ground state are investigated through density functional theory. The different exchange–correlation functionals (GGA, LDA, PBESol and WC) are used to study these alloys. The equilibrium lattice constants and corresponding ground state energies are calculated using these four approximation methods. From GGA functional, the obtained band gap for ZrMnSi is 1.268 eV and HfMnSi is 1.311 eV. The reported alloys show semiconductor character in minority spin channel and also exhibit metallic character in majority spin channel. The studied alloys are mechanically stable and ductile in nature. The total magnetic moment of $-3\mu_B$ is obtained in the reported ferrimagnetic alloys. The obtained thermoelectric figure of merit for ZrMnSi and HfMnSi is 0.46 at 1200 K and 0.31 at 1200 K respectively, it shows that these alloys are the potential candidates for waste heat recovery application, and they are also useful for spin flip device application.

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K 037

A First Principles Prediction of Transition Metal-decorated Cyclo[18]carbon as a Toxic Gas Scavenger

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ABSTRACT

This study goes into the investigation of Transition metal-decorated Cyclo[18]carbon[1], or simply $C_{18}TM$ (TM = Ni, Pd, Pt) nanoclusters, and their interactions with toxic gases, including CO, NO, and NH_3. Our comprehensive Density Functional Theory analysis spans structural, electronic, topological, spectroscopic, and sensing properties, implemented by Gaussian 09 package[2], uncovers significant insights. One notable finding is the highly negative adsorption energies, indicating strong gas interactions. Particularly noteworthy is the substantial sensing response observed, with $C_{18}Ni$ showing potential for NO sensing and $C_{18}Pd$ for CO sensing based on conductivity. Employing the Quantum Theory of Atoms in Molecules (QTAIM), we gain insights into the strength of each interaction, while Raman spectra analyses shed light on the vibrational aspects of these interactions. Furthermore, our Non-Covalent Interaction (NCI) study elucidates the mechanisms underlying van der Waals interactions. Interestingly, the longer recovery times calculated, attributed to the highly negative adsorption energies[3], suggest that $C_{18}TM$ nanoclusters may find more utility in gas removal applications rather than rapid-response sensor applications.

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K 038

Deciphering the Apoptosis of Stem Cells in Bone Marrow against PARP Proteins in Acute Myeloid Leukaemia: A Computational Approach

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ABSTRACT

Acute myeloid leukaemia (AML) is a type of cancer that starts in the blood-forming cells characterized by the rapid growth of abnormal cells that build up in the bone marrow and blood and interfere with normal blood cell production. Inside the bone marrow, blood stem cells develop into new blood cells. During this process, the cells become lymphocytes, the blood-forming cells, which are types of myeloid cells. Myeloid cells can develop into red blood cells, white blood cells and platelets. These myeloid cells are the ones that are abnormal in AML. Poly (ADP-ribose) polymerase (PARP) protein plays an important role in causing AML. The PARP protein responds swiftly to the DNA damage. When a DNA is damaged, the DNA-binding domain of the protein binds with the B form of the DNA. When a compound binds strongly to the major groove or intercalating region of the DNA, the stem cell present inside the bone marrow diseased with AML undergoes apoptosis. To identify the potential DNA intercalator, a series of natural products are virtually screened using molecular docking and the compounds with the top binding scores are selected for ADMET profiling. The complexes were subjected to molecular dynamics (MD) simulations for 200 ns to examine their structural stability and dynamic behaviour. Various analyses such as root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), the radius of gyration (R_g) and hydrogen bonding interactions. Furthermore, to estimate the entropy of the system, Gibbs free energy calculations were also performed. This research will provide critical information about the DNA intercalators, which could potentially be incorporated into the treatment of AML.

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K 039

Hydration Pattern of Ionic Liquids in Biomolecules

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ABSTRACT

Ionic liquids (ILs) are a class of organic salts that are typically liquid at room temperature. Numerous ILs have synthesized and utilized for various applications in the field of energy, environment, biomedical and drug delivery applications. Particularly, Choline-based ILs have received widespread attention due to the advantages in low environmental impact, affordability, accessibility, solubility and ideal thermal stability. Choline (i.e. [Cho]) has shown the ability to stabilize the proteins and deliver drugs to specific targets in the body which can improve the effectiveness of drug therapies. In this study, we have selected three different ILs (i.e. [Cho] cation with anions such as acetate [OAc], taurate [Tau] and geranate [Ger]) with insulin dimer. To study the structure and stability, we have employed DFT and molecular dynamics simulations approaches. To get more insights on the molecular level interaction, we have explored the hydration patterns of these ILs with the aid of the DFT method and non-covalent interactions are characterized by the AIM and NCI analyses. The role of water molecules and the effect of the mixture of various [Cho] based ILs in the stability of the insulin dimer structure will be reported. Our study will provide the valuable information about the structure, stability, and function of IL in insulin dimer and how these molecular level interaction helps in transdermal and oral drug delivery systems.

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K 040

A DFT Study on Thermoelectric Device Performance of α-GeTe/Sb Van der Waals Heterostructure

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ABSTRACT

Utilizing first-principles density functional theory in conjunction with the non-equilibrium Green's function method, we have undertaken an investigation into the thermoelectric properties of α-GeTe/Sb van der Waals heterostructure (vdWH) nanodevices. The electronic aspects of these thermoelectric devices were assessed through the examination of the Seebeck coefficient and electrical conductivity, which were derived from transmission spectra. Simultaneously, the thermal conductivity of the system was computed by analyzing the phonon transmission spectrum. By integrating both electron and phonon transmission spectra, we calculated the ZT values for the α-GeTe/Sb vdWH. Our findings indicate an enhancement in thermoelectric characteristics achieved through the construction of vertical van der Waals heterostructures. Remarkably, high ZT values are obtained due to the energy filtering effect at the interface. In this context, the vertical van der Waals heterostructure featuring a smaller contact area and slightly reduced phonon thermal conductance ultimately exhibits superior thermoelectric performance. This improvement is attributed to a reduction in phonon transmittance and a narrower spectrum range of effective phonon transmission. Our theoretical work introduces an innovative approach and offers valuable theoretical insights for the advancement of high-performance, high- density integrated circuits in the microelectronics industry.

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K 041

Thermoeletric Properties of Layered Compound $GaGe_2Te$: A First Principles Study

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ABSTRACT

The increasing demand in energy in the present modern world due to the decrease of fossil fuels forced the researchers across the globe to look for renewable energy sources. Thermoelectricty is one such source where one can see a direct conversion between thermal and electrical energies. Lot of layered materials such chalcogenides, pnictides etc. have shown promising thermoelectric efficiency. In the present study, we focus on the thermoelectric properties layered compound $GaGe_2Te$. The compound $GaGe_2Te$ is synthesized experimentally recently [1]. The structure of $GaGe_2Te$ exist in trigonal crystal structure with space group 164. The optimized structure is probed for electronic, phonon and thermoelectric properties. The band gaps of the compound are 0.03eV and 0.99eV respectively with PBE and HSE functionals respectively. We have calculated thermoelectric properties such as Seebeck coefficient, electrical conductivity, electronic and lattice thermal conductivities, and power factor (shown in Fig.1) using BotlzTraP2 code [2].

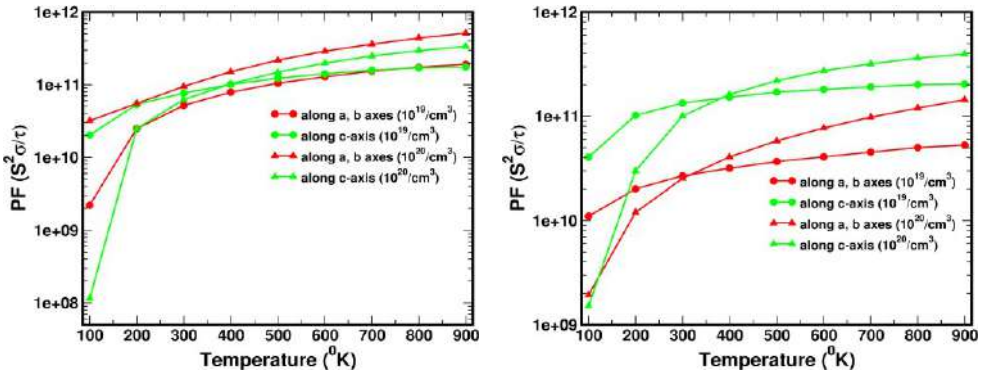

Figure. 1: The power factor of $GaGe_2Te$ compound along a and c-axes for (a) electrons and (b) holes.

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K 042

Topological Nodal Line Features in Semimetal LiYGe

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ABSTRACT

The field of topology in condensed matter physics has generated a lot of interest during the past decade because of their rich novel physics. The topological quantum materials have dragged the attention of worldwide researchers not only due to their exotic transport properties but also their possible applications in quantum computing etc. Three types of semimetals in the field of topology are discovered namely, Dirac semimetals, Weyl semimetals and nodal line semimetals. The topological properties of LiYGe compound are explored through first principles calculations. Nodal lines can cross the Brillouin zone (BZ) in the shape of a closed ring or a line. The nodal line compound LiYGe exists in hexagonal structure.

The nontrivial nature of the bands without SOC is seen along Γ-M and Γ-K directions which is shown in Fig. 1(a) in red and blue color bands. The bands where this red and blue color are touching will give nodal line behavior in the Brillouin zone. With the application of SOC, the nodal line becomes gapped line as can be seen from Fig. 1(b). The topological features such as Z2 index, surface states etc. will be further discussed.

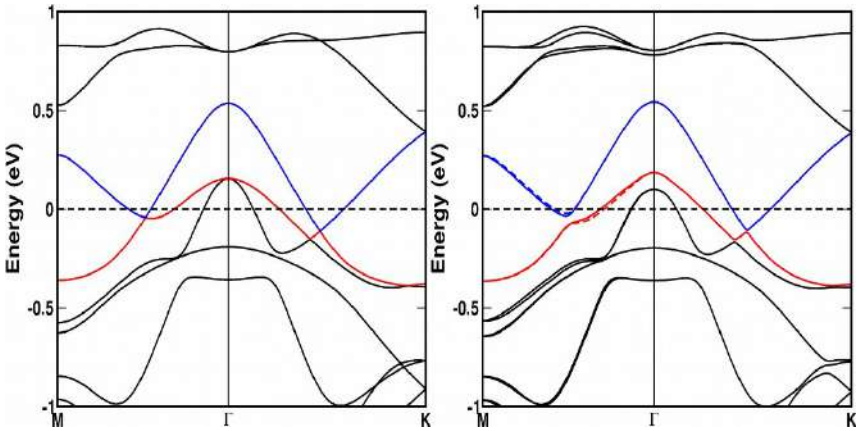

Figure. 1: The band structure of LiYGe compound (a) without SOC and (b) with SOC.

K 043

The Impact of Strain on the Thermoelectric Properties of HfNBr Monolayer: A First Principles Study

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ABSTRACT

Two-dimensional (2D) materials have garnered significant interest and research due to their unique properties and potential for thermoelectric (TE) energy harvesting. Most of the investigated compounds for TE applications are binary and exhibit isotropic behavior. Here, in this study, we investigate the TE properties of ternary transition metal halide HfNBr monolayer under varying strain using first-principles calculation in conjunction with semiclassical Boltzmann transport theory. We examined the impact of uniaxial compressive and tensile strain on the electronic, mechanical and transport properties of the HfNBr monolayer. We focused on the orthorhombic form of HfNBr, exhibiting the anisotropic transport properties. HfNBr is found to be an indirect band gap semiconductor by employing the Heyd-Scuderia-Ernzerhof (HSE06) exchange-correlation functional. Due to its layered structure, HfNBr exhibits highly anisotropic values of Seeback coefficient, electrical and thermal conductivity. A high power factor and low thermal conductivity of the investigated monolayer is obtained via strain engineering. This contributes a reasonably high thermoelectric figure of merit (*ZT*), making HfNBr very promising in thermoelectric energy harvesting. Thus, the present study may provide valuable insights in exploring the impact of compressive and tensile strain on the transport properties of ternary transition metal nitrides and their prospective energy harvesting applications.

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K 044

Topological properties of nodal line semimetal LaMgGa: A first principles study

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ABSTRACT

The topological quantum materials have dragged much attention worldwide due to their novel rich physics. Topological semimetals are systems in which the conduction bands and the valence ones cross each other in the Brillouin zone (BZ). When a material's conduction and valence bands cross as a discrete point, it is called a Dirac/Weyl semimetal; when they cross as a closed curve, it is called a topological nodal-line semimetal. The electronic and topological properties of LaMgGa are explored through first principles calculations. The compound LaMgGa exists in hexagonal crystal structure.

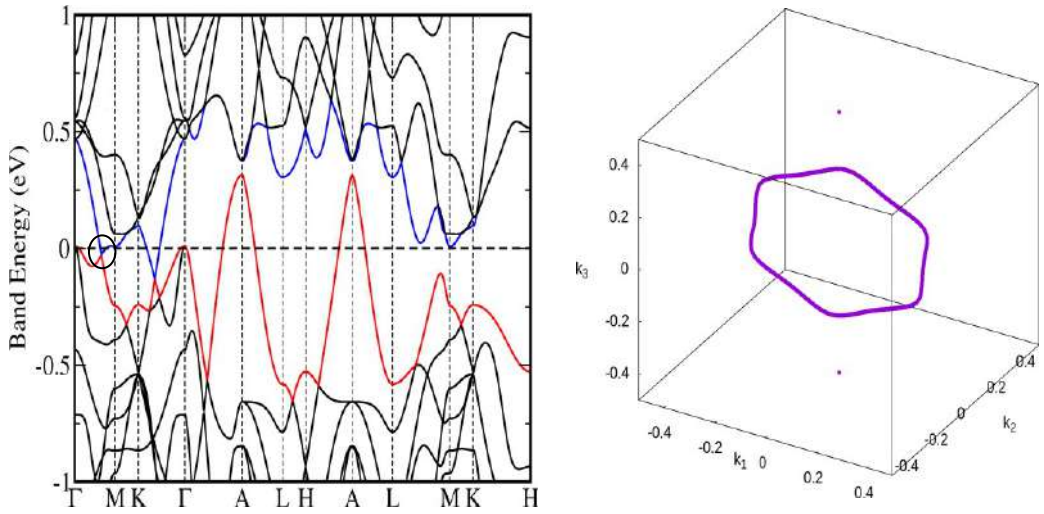

Figure. 1: The band structure of LaMgGa compound (a) without SOC and (b) its nodal line without SOC.

The nontrivial nature of the bands without SOC is seen along Γ-M and Γ-K directions which is shown in Fig. 1(a) in red and blue color bands. The bands where this red and blue color are touching will give nodal line behavior in the Brillouin zone which is shown in Fig. 1(b). The other topological properties such as surface states, Z_2 index further confirmed the nodal line behavior in the studied compound.

K 045

In Silico Docking Analysis of Bioactive Compounds from *Syringodium isoetifolium* Against Breast Cancer Protein - HER2 Kinase and HSP90

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ABSTRACT

All over the world Cancer is the second leading cause of death. Early detection and treatment of cancer extends millions of people life. Current strategy explains that they were 20 million peoples were diagnosed with cancer. The efficacy of cancer treatment is much lowered due to its negative aspects, for example nausea, hair loss edema, fatigue, constipation, diarrhea, mouth throat problems, nerve problems and pain. Nowadays, natural remedies have been overwhelming success for various diseases in our society. The secondary metabolites present in the herbs has all the pharmacological activities which double our life span. *Syringodium isoetifolium* is one of the major tropical seagrasses which belongs to the family Cymodoceaecea, and otherwise called as Noodle grass. Many phytocompounds present in the seagrass *S.isoetifolium* which has been identified by LC-MS analysis. The current study is focused on the interaction between the compounds identified in HAE of *S.isoetifolium* with the breast cancer protein such as HER2 Kinase receptor and HSP90 by *Insilico* study. Molecular Docking studies of HAE of *S.isoetifolium* with major compounds like 7-Hydroxycoumarine, 4-Hydroxycoumarine, Arecoline, Nootkatone, Phloretin and Zerumbone was done. The docking studies affirmed the restraint of target protein HER2 Kinase receptor to identify the anticancer activity of 4-Hydroxycoumarine, 7-Hydroxycoumarine, Arecoline, Nootkatone, Phloretin and Zerumbone. The order of binding energy was Nootkatone> Zerumbone > Phloretin > 4-Hydroxycoumarine >7-Hydroxycoumarine >Arecoline.

Keywords: *Cancer, S.isoetifolium, Molecular docking, HSP 90, HER2 Kinase receptor, Nootkatone, Zerumbone.*

K 046

Exploring Nodal Line Behavior in LaMgTl Semimetal through First Principles Calculations

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ABSTRACT

Topological materials, including topological insulators (TIs), topological semimetals (TSMs) and topological superconductors (TSCs) have been attracting tremendous research interests due to their protected boundary states and prospects for the future applications in quantum devices. A theoretical study using Density Functional Theory (DFT) is used to explore the electronic, topological properties in the nodal line semimetal LaMgTl. The compound exhibits hexagonal crystal structure as shown in Fig. 1(a) with space group 189.

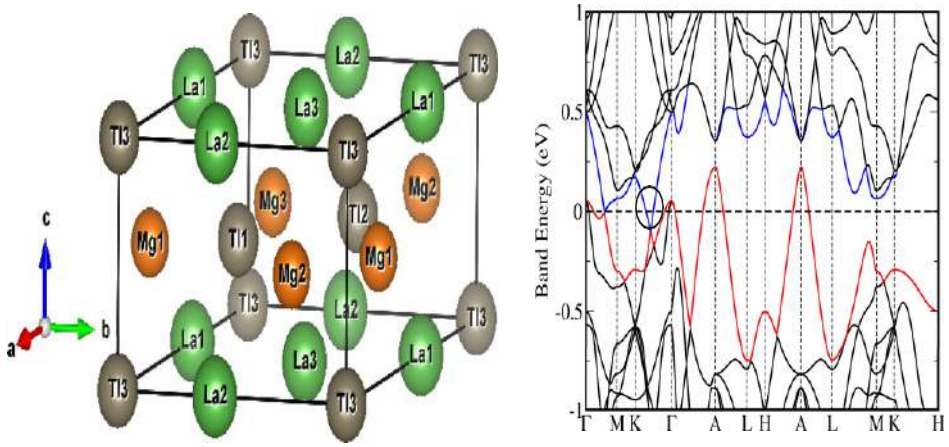

Figure. 1: The band structure of LaMgTl compound (a) without SOC and (b) its nodal line without SOC.

The nontrivial nature of the bands without SOC is seen along Γ-M and K-Γ directions which is shown in Fig. 1(b) in red and blue color bands. The bands where this red and blue color are touching will give nodal line behavior in the Brillouin zone. The other topological properties such as Berry phase, surface states, Z2 index further confirmed the nodal line behavior in the studied compound.

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K 047

Phase Field Modelling of Microstructure Evolution during Multilayer Deposition of IN718 during Directed Energy Deposition

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ABSTRACT

In Additive manufacturing (AM), Directed energy deposition (DED) is widely used for manufacturing components which require very close tolerance [1, 2]. This process involves deposition of material onto a substrate using a strong energy source like laser/electron beam. During the process, the material, which is introduced as either as a powder or wire, undergoes cycles of intense heating and cooling. Phase field modelling allows to monitor these changes occurring in the microstructure during these rapid solidification conditions, which is otherwise difficult to observe in real time. In the present study, the focus is on investigating the solidification microstructure formation during DED processing of a Nickel based superalloy (IN718), considering the case of multilayer deposition. Due to high energy source, deposition takes place by solidification which involves partial remelting of previously deposited layer. The main aim is to observe the evolution of primary γ phase after successive melting and solidification. In order to reduce the computational effort, Inconel 718 is assumed here as a 5-component system consisting of two solid phases (γ and Laves), barring the parent liquid phase. Rosenthal approach is used here to calculate the temperature profiles at different regions within a layer. Material properties like density, viscosity and thermal conductivity are also considered for calculation. For the first layer, the Laves phases are found to be deposited near the interdendritic regions of γ dendrites owing to their low solubility in γ phase. Whereas these precipitates get redistributed for the subsequent deposition as they get segregated due to remelting. The experimental micrographs of DED samples, obtained through Field Emission scanning electron microscopy (FESEM), validates the simulated outcomes with reasonable accuracy.

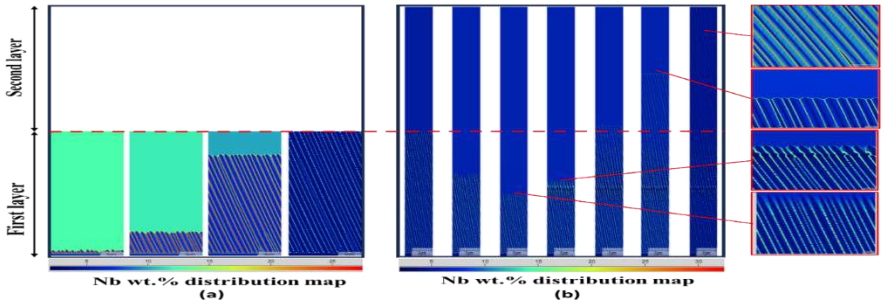

Fig. 1: Longitudinal view of solidification microstructure in DED processed IN718 sample showing (a) First layer and (b) Second layer which involves remelting of first layer.

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K 048

Computational Modelling of Superlattice WSe_2-WTe_2 to Explore Charge-Transport Anisotropy

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ABSTRACT

Recently, superlattice has become a very promising material for electronics and transport applications in semiconductor technology. Superlattice structure provides distinctive supremacy to nurture the underlying physics in their sublayers arising from the interfaces. However, large-scale industrial applications require information related to stability and performance near room temperature. In this context, we have studied the electronic structural and carrier transport properties of the hexagonal phase of WSe_2 and WSe_2-WTe_2 superlattice using density functional theory calculations combined with Boltzmann transport theory. Firstly, we showed that our optimized crystal structures of WSe_2 and WSe_2-WTe_2 are dynamically stable and optimized lattice parameters match with existing data available in the literature. Here, we solve the Boltzmann transport equation parametrized by deformation potential (DP) theory to compute carrier mobility and observe that DP model compromises the accuracy and overestimates the longitudinal acoustics phonon limited mobility by two orders. To address this concern, we incorporate scattering by longitudinal optical phonon exclusively to accurately compute mobility using Fröhlich interaction. Our proposed model is very simple and effective in reproducing mobility, which matches with experimental results. This approach is computationally very cheap and provides an alternative route to obtain mobility accurately, without using highly expensive EPW code.

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K 049

Machine learning Approaches for Anti-inflammatory Small Molecule Prediction

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ABSTRACT

Inflammation responses occur under the normal conditions when tissues are damaged; these responses cause chronic autoimmune and inflammation disorders. Several anti-inflammatory small molecules have been found in the process of the inflammatory response, and these small molecules have been used to treat some inflammatory and autoimmune diseases. Numerous tools for predicting anti-inflammatory peptides (AIPs) have emerged in recent years. However, conducting experimental validations in the lab is both resource-intensive and time-consuming. This study introduces a predictive model for identifying anti-inflammatory small molecules. The proposed model can facilitate the screening of compounds in the context of drug discovery for inflammatory diseases. The primary dataset used for model training and testing consists of 2000 anti-inflammatory inhibitors and 2000 non-inhibitors. Several machine learning classifiers have been employed to build these models. Initially, we developed models using 2-D chemical descriptors and achieved a maximum AUC of 0.81 on the test dataset. Notably, our Gradient Boosting model outperforms other prediction models. The results underscore the reliability of the proposed model as a predictor for identifying small molecules with anti-inflammatory properties.

Keywords: *Anti-inflammatory, autoimmune disease, small molecules, machine learning, k-fold cross validation.*

K 050

Effect of Defects to Tailor the Structural and Electronic Properties of Zigzag GaN Nanoribbons

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ABSTRACT

Defects are an integral part of any nanomaterial under pragmatic conditions. The presence of defects can significantly alter the electronic properties of nanomaterials for various applications. Therefore, in the present manuscript, we have investigated the effect of vacancy and Stone-Wales defects (SWD) on the structural and electronic properties of zigzag GaN nanoribbons (ZGaNNR). It is revealed that the incorporation of considered defects is an exothermic process and the proposed structures are energetically feasible to be obtained. Furthermore, the electronic properties of ZGaNNR are highly influenced via the incorporation of vacancy or SWD. A semiconductor to metallic transition for the vacancy defects whereas reduction in the band gap has been witnessed for SWD. It is worth mentioning here that for Ga (N) vacancy, the major contribution to the conduction channel arises from the N (Ga) p-orbital. Our findings indicate that apart from tailoring the electronic properties, these defects can also be used to induce n-type or p-type doping character in the material.

Keywords: *GaN, nanoribbon, electronic structure, vacancy defect, Stone-Wales defect.*

K 051

Computational Prediction of Anticancer Small Molecules using Machine Learning

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ABSTRACT

Cancer remains a significant global health challenge. Conventional cancer therapies typically rely on approaches like radiotherapy or the use of anticancer medications to combat malignant cells. However, these methods are often costly and can lead to adverse side effects, imposing substantial burdens on patients. The discovery of anticancer peptides (ACPs) represents a notable breakthrough in the treatment of tumors. Yet, the conventional process of discovering ACPs through experimentation is frequently characterized by its time-consuming and costly nature. To address this challenge, we embraced a machine learning-based approach to construct an anticancer model using small molecules. Anticancer small molecules (ACSMs) represent a class of compounds meticulously designed to specifically target and inhibit cancer cells. In this study, we have used 2000 anticancer inhibitors and 2000 anticancer non-inhibitors. All the models were trained on 80% of training data using various machine learning algorithms and evaluated on 20% of test data. To ensure the robustness of our models, we subjected them to both internal validation via 10-fold cross-validation and external validation. The performance of our developed models was measured using key metrics such as accuracy, AUC (Area Under the Curve), sensitivity, specificity, and MCC (Matthews Correlation Coefficient). The results of this study offer valuable insights into the potential of our approach for predicting anticancer small molecules. thus, advancing the field of cancer research and drug discovery.

Keywords: *Anticancer peptides, Anticancer small molecules, Machine learning, 10-fold cross-validation.*

K 052

Design of biodegradable Mg-alloys for orthopedic applications: an ANN and MOGA approach

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ABSTRACT

Among the new age orthopedic materials, magnesium and its alloy earned importance due to their huge possibilities for the last few decades. Due to their almost similar density as human bone, high strength to weight ratio and nontoxic degradation nature in aqueous environment, they have huge potential as the biodegradable implant material. Here in this work designing of Mg-alloy with required degradation rate inside human body with adequate strength is made by materials informatics approach. Artificial neural network (ANN) and multi objective genetic algorithm (MOGA) have been used to optimize the performance of the alloy as a short-term implant material for hard tissues. Four different predictive data-driven models for yield strength, % elongation, ultimate tensile strength and corrosion rate is developed by ANN using published data. The effect of the different alloying elements has been studied using sensitivity analysis. In order to design the Mg-alloy with adequate strength along with controlled low corrosion rate, MOGA is used to search the optimum composition of the alloy.

Keywords: *Magnesium alloy, mechanical properties, corrosion rate, materials design, artificial neural network, multi objective genetic algorithm.*

K 053

Molecular docking, Conceptual Density Functional theory, Molecular dynamics simulation and Free Energy Calculation study of Bioactive compounds as novel JAK2 inhibitor

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ABSTRACT

Colorectal cancer is the third most common types of cancer worldwide, after lung and breast cancer. Evidence has shown that JAK2/STAT3 have an important effect in the activation of the colon cancer. It promotes tumor progression by promoting cell survival and resistance to chemotherapy. Recent studies have shown that inhibiting JAK2 pathway leads to a reduction in tumor cell proliferation and growth, and can also promote apoptosis in colon cancer cells. In the present study Molecular docking, Cross docking was performed and top ten compounds were selected depending upon their binding affinity and selectivity. The top compounds were subjected to Conceptual – Density functional theory. Besides, the Molecular dynamic simulation was also carried out for the selected leads. The top leads predicted to be a selective inhibitor for JAK2 protein targeting colorectal cancer.

Keywords: *Colon cancer, JAK2, Virtual screening, Molecular docking, DFT, MD Simulation*

K 054

An in Silico Strategy to Identify JAK1 Specific Inhibitors for Breast Cancer

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ABSTRACT

Breast cancer is the most prevalent form of cancer and the leading cause of cancer-related fatalities. Existing breast cancer treatments have inherent drawbacks, highlighting the need for the development of new drugs. In breast cancer cells, activation of the inflammatory cytokine IL-6 class by ERBB2 receptor tyrosine kinase signalling requires JAK1. JAK1 contributes significantly to the progression of metastatic cancer and the continuous activation of the STAT3 oncogene. This underlines the fact that JAK1 can be utilised to target breast cancer. Using computational approaches, we performed virtual screening against the Zinc database to identify potent and selective lead compounds against the JAK1 protein. Molecular docking with Autodock tools 1.5.7 was used to classify compounds according to their binding affinity. Using pkCSM tool, further drug likelihood was evaluated. Followed by cross-docking to verify selectivity and cDFT analysis to ascertain the inhibitory efficacy of leads using the B3LYP method with the 6-31G (d,p) basis set in Gaussian 16. PASS analysis was also done to predict the biological activity based on chemical structure of compounds. To validate the molecular interactions between selected inhibitor compounds and the JAK1 structure, molecular dynamic simulations with Gromos96 2005 force field have been performed using Gromacs 2016. Moreover, binding free energy calculations for JAK1-lead complexes were performed using the MM/PBSA method. The results of this study indicate that C78, C66 and C93 are probable drugs. Therefore, JAK1 inhibition has been proposed as a potential breast cancer target. Additional validation employing *in vitro* studies could aid in identifying the bioactivity of selected leads, thereby enabling their use in the treatment of this disease condition.

Keywords: Breast cancer, cDFT, JAK1, Molecular docking, Molecular dynamics simulation

K 055

A DFT Insight into the Influence of Chemical Disorder on the Structural and Magnetic Properties of X_2crsb (X = Co, Fe) Heusler Alloy

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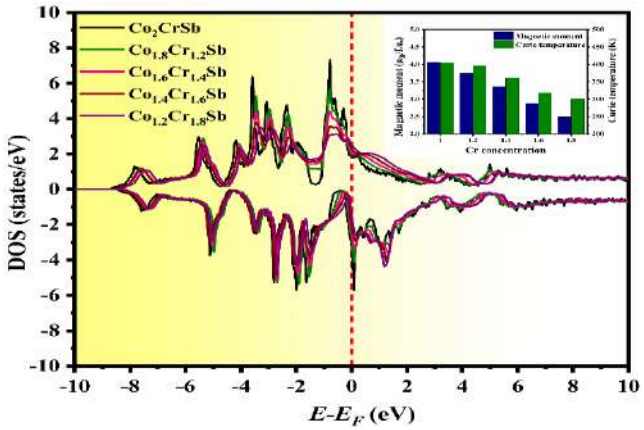
ABSTRACT

The Heusler alloys with $L2_1$ phase are gaining great attention towards spintronics and magnetocalorics, ascribed to their ferromagnetic and half-metallic behavior. In this context, the electronic and magnetic properties of X_2CrSb (X = Co, Fe) alloy is investigated using Spin polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) package. Moreover, the effect of chemical disorder ($X_{2-x}Cr_{1+x}Sb$ (x=0, 0.2, 0.4, 0.6, 0.8)) on their inherent properties is also investigated systematically. The magnetic moment of the alloy decreased linearly with Cr concentration. Despite the disorder induced in the system, the half-metallic property is preserved; with a slight reduction in band gap in both the systems. The positive exchange coupling parameter indicated the strong ferromagnetic interactions in all the alloys. However, the interaction strength gets reduced with increasing disorder. This resulted in decrease of Curie temperature (T_C) in disordered X_2CrSb alloy. Notably, $Co_{1.2}Cr_{1.8}Sb$ is found to exhibit T_C around room temperature (i.e.): 300 K. This outcome of the present study calls for experimental validation on $Co_{1.2}Cr_{1.8}Sb$ system and to unveil its potential towards solid state refrigeration.



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K 056

AIE-Active Ferrocene π-Extended Phenyl Conjugated Indanedione Chromophores: Synthesis, Photophysical, Electrochemical, NLO and Computational Studies

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ABSTRACT

The donor-π-acceptor (D-π-A) based ferrocene double phenyl conjugated indanedione chromophores [$Fc(Ph)_2$dione (**1**) and $Fc(Ph)_2(OCH_3)_2$dione (**2**)] were synthesized and characterized. The charge transferability of the chromophores **1-2** was examined in absorption and emission spectra using various solvents from non-polar toluene to more polar dimethyl sulfoxide. This shows a red shift with a more significant effect in emission spectra (40 nm) due to a high excited state dipole moment (1). The low fluorescence was observed in the chromophores **1-2** due to the photo induced electron transfer (PET) process, it was enhanced by the aggregation induced emission process (AIE) [THF: H_2O at 30 % (**1**), 40% (**2**)] due to the formation of aggregates. The aggregate formation was confirmed by the TEM images of the chromophores **1-2** in [THF: H_2O at 30 % (**1**), 40% (**2**)], which also shows higher quantum yield due to the principle of Restricted Intramolecular Rotations (RIR). The fluorescence lifetime studies were examined to find the amount of time the molecules spend in the excited state, and the quantum yield was calculated. The electrochemical studies were carried out to find the redox potential of the chromophores **1-2**, which is utilized to calculate the band gap values (2). The SHG efficiency was obtained by the Kurtz and Perry powder technique. In addition, the theoretical studies were done using density functional theory (DFT) and time-dependent DFT and TD-DFT at B3LYP, CAM-B3LYP, and LC-BLYP/6-31+G** level of theory to find out the dipole moment, polarizability and hyperpolarizabilities (3).

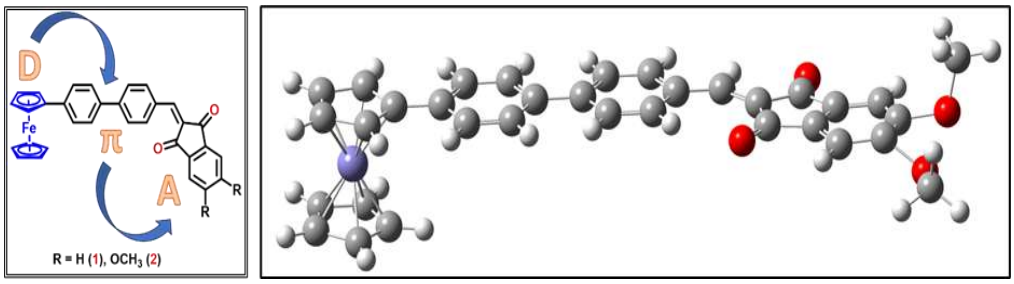

Fig. 1. Chemical structure and optimized structure of the chromophores.

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K 057

NLO-Active Ferrocene Appended Donor-π-Acceptor (D-π-A) Chromophores: Synthesis, Structural, Luminescence Second Harmonic Generation, and Theoretical Studies

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ABSTRACT

A New nonlinear optical (NLO) active chromophores, featuring phenyl and methoxy phenyl substitutions at the D-π-A motif [(Fc-C(C_6H_4-R)=CH-CH=C(CN)-C_6H_4-Br) {R=H (**1**), OCH_3 (**2**)}] were synthesized and subjected to detailed structural analysis. Further, the crystal structure of the chromophore **2** was confirmed using single-crystal X-ray diffraction analysis, which shows triclinic crystal system with centrosymmetric (P-1) space group. Both the chromophores exhibited suppressed emission in the solution state due to the twisted intramolecular charge transfer (TICT) phenomenon induced by the cyano vinylene group. Upon aggregation induced emission (AIE) in THF/H_2O mixture (80% ratio), chromophores **1** and **2** showed significantly enhanced fluorescence, attributed to its restricted intramolecular rotation (RIR) processes. Quantum yield values increased by factors of 1.8 (**1**) and 2.3 (**2**) in the aggregated state compared to the solution state, with corresponding lifetime decay values of 5.4 ns (**1**) and 5.1 ns (**2**). Cyclic voltammetry revealed a single-electron transfer mechanism from Fe^{2+}↔Fe^{3+}. Moreover, second harmonic generation (SHG) efficiency was explored using the Kurtz and Perry powder technique with KDP as reference. Though crystallization was in centrosymmetric space group, presence of non-covalent interactions such as C–H·····π interactions, inter and intra-molecular hydrogen bonding in the crystal packing suppresses the antiparallel alignment making it NLO active. Additionally, Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) calculations, employing different functionals (B3LYP, long-range corrected CAM-B3LYP, and LC-BLYP), were done to determine hyperpolarizability, dipole moment and molecular electrostatic potential of the chromophores.

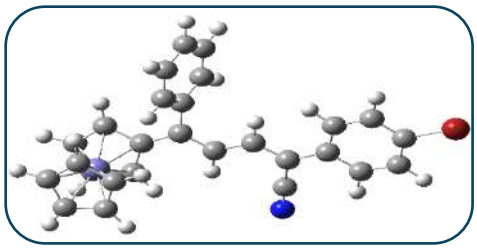

Fig. 1. Optimized structure of chromophore 1

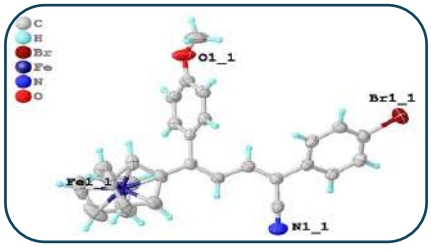

Fig.2. Crystal structure of chromophore 2

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K 058

A First Principle DFT Approach for Using Functionalized Graphyne as a Drug-Carrying Vehicle

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ABSTRACT

In this study, the effectiveness of Graphyne as a drug carrying vehicle is investigated based on first principle density functional theory calculations. Graphyne, a carbon allotrope is a two-dimensional material with sp and sp2 bonded carbon atoms arranged in crystal lattice. It has now gained significant attention and interest as a promising material among researchers due to their unique characteristics and potential applications in many fields, especially in drug delivery and possess exceptional properties including high-thermal stability, low toxicity, large surface area, biocompatibility and tunable electrical properties. The present graphyne system is functionalized with biologically available functional groups such as hydroxyl(-OH), thiol(R-SH), carboxyl(-COOH), amino (-NH_2) and carbonyl(C=O) and nucleobases such as cytosine,guanine,adenine and thymine in order to improve their solubility properties, which is an essential condition for a for drug delivery nanocarrier. The total energy and chemical potential of 2 ×2×1 γ- Graphyne comes to be -7527 eV and -4.67 eV.The minimum total energy difference by repeated random perturbation of the structure confirms stability. The band structure of the most stable γ-graphyne suggests a semiconducting behaviour with an energy gap of 0.45 eV. The electronic states of γ-graphyne pristine monolayer shows nearly symmetric behaviour with respect to valence and conduction band energies near to the Fermi level within an energy range ±1 eV.

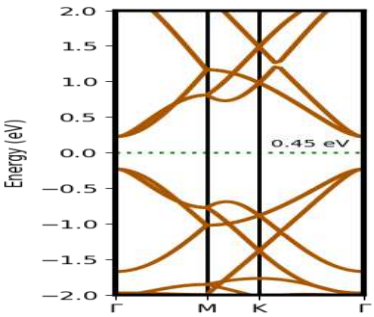

Fig.1- Band structure of γ - 2×2 Graphyne

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K 059

Titanium-Based Semiconductors: Unveiling a New Compound Semiconductor Family

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ABSTRACT

Half-metallic ferromagnets have become increasingly important in spintronic applications [1]. Based on Heusler compounds, R.A. de Groot et al. have proposed several compounds as half-metallic with a large probability of spin-polarization [2,3]. The binary compounds offer convenience in synthesis and their integration into the electronic industry, as in the case of CrAs [4]. The success of CrAs has inspired us to explore the possibility of finding binary half-metallic compounds for spintronic applications. Using first-principle calculations, we are proposing a new family of compound semiconductors based on titanium. When Ti is alloyed with Ge and Sn in the zinc blend symmetry, the alloys become semiconducting. With the nominal chemical formula of 1:1, TiGe and TiSn are modelled using two different exchange-correlation functionals, namely LDA and GGA. From the total energy vs. volume curves, we have optimised the lattice parameter. From the electronic band structure and the density of states, we have determined the nature of the band gap for TiGe and TiSn. The exhibited band gaps of TiGe and TiSn are direct band gaps in nature and relatively small in magnitude. We have made an attempt to add magnetism to this new family of semiconductors by doping magnetic impurities like Mn and Cr. When the Mn concentration is 12.5% in TiGe, they have exhibited a total magnetic moment of 3.02 μB per unit cell, and for TiSn, it is 3.01 μB per unit cell. Interestingly, after adding the magnetic impurities, TiGe and TiSn have become half-metallic, with a band gap existing in the spin-down channel. Therefore, with or without a small band gap, TiGe and TiSn can find application in infrared photodetectors and sensors. Further, with magnetic impurities, both systems have shown spin-polarisation in one of their spin channels, signifying their applicability in spintronic applications.

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K 060

Spin Flipping in Fe_2X(Sb, Ge) Binary Half-Heusler Alloys

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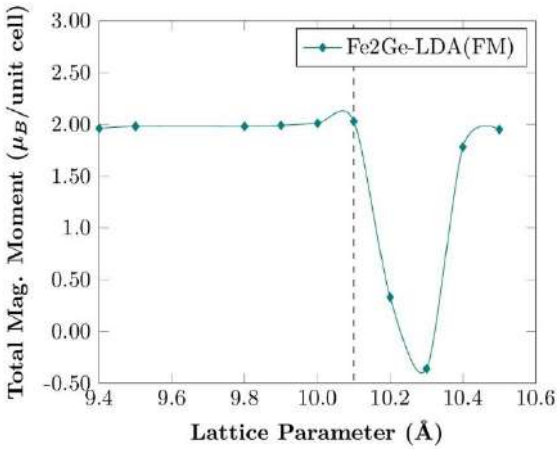
ABSTRACT

Half-Heusler materials are the excellent class of materials which has potential application in the field of spintronics [1]. We have studied the electronic and magnetic properties of binary half-Heusler Fe_2X (Sb, Ge) alloys. The electronic structure of both the alloys have shown half-metallic nature and particularly Fe_2Sb followed the Slater-Pauling rule [2]. The total energy calculations confirm that the ferromagnetic state is the ground state. Additionally, we have studied the meta magnetic behaviour of these alloys and we have observed an abrupt change in the magnetic moments of Fe atoms and this spin flipping phenomenon could be more beneficial for magnetostriction applications.



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K 061

Tetragonal Defect Chalcopyrites CdX_2Te_4 (X = Ga, In): Electron and Phonon Transport Properties

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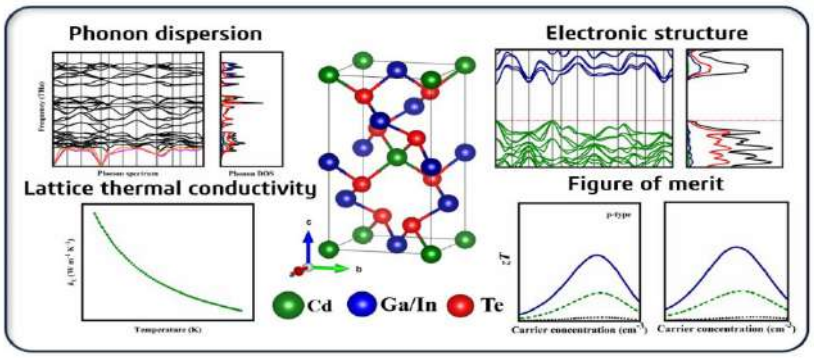
ABSTRACT

Ever-increasing energy consumption with carbon emissions is intended to search and develop alternative energy technologies for a sustainable civilization. Due to the various advantages, such as the low maintenance associated with zero-emission, thermoelectric devices have resembled alternative energy conversion techniques for the past few decades. One of the well-known challenges that should be addressed for effective energy conversion is the lower conversion efficiency of thermoelectric materials. To develop appropriate thermoelectric material, it is essential to understand the structure-property relationship. In this way, the present work systematically demonstrates the defect chalcopyrite's ($Cd(Ga/In)_2Te_4$) electron and phonon transport properties using the density functional theory computations. The stability of the structures is examined mechanically, dynamically, and thermally. The tetragonal defect chalcopyrites have a mixed bonding nature and a larger Gruneisen parameter, which indicates a significantly larger lattice anharmonicity.



Further, the phonon modes coupling, moderate group velocity, Debye temperature, and specific heat supports low lattice thermal conductivity of the systems. This low k_L and optimum power factor yield noticeable thermoelectric performance (zT>1). This study not only reveals the thermoelectric properties of the defect chalcopyrites, also demonstrates the fundamental understanding between structure and properties. This study can pave the way for the experimentalist to get a clear picture of materials exploration.

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K 062

Basis Set Selection for Raman Response of Agrochemicals using DFT/B3LYP Calculations

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ABSTRACT

India is an emerging economy and agriculture plays a significant role in it. Farmers use agrochemicals in an unregulated and excessive amount to increase the yield of crops, which causes considerable contamination in the food being grown and also in the water bodies in nearby areas. Exposure to excessive levels of these agrochemicals can lead to a variety of health problems, including cancer, respiratory problems, neurological disorders, and reproductive problems. A study by the Environmental Working Group (EWG) in 2019 found that exposure to atrazine, a common herbicide, in drinking water is linked to an increased risk of non-Hodgkin lymphoma, a type of cancer [1]. Raman spectroscopy can help identify and quantify the chemical composition of materials with high sensitivity, selectivity, speed, and accuracy. Hence, it is an excellent technique for onsite measurements of harmful agrochemicals in both solid and liquid samples. Density functional theory (DFT) can model the Raman response of the agrochemicals, however, the selection of the basis set is essential to ensure an accurate analysis. Further, the Raman study of these chemicals used by Indian farmers is lacking. The current article aims to establish the accuracy of various data sets (Pople's basis sets, Los Alamos National Laboratory basis sets, and other large basis sets) to model agrochemicals including, herbicides, insecticides, and weedicides. Fig. 1 establishes the accuracy of DFT analysis for the Raman response of herbicide Atrazine which was calculated using Pople's basis set and B3LYP exchange correlation functional.

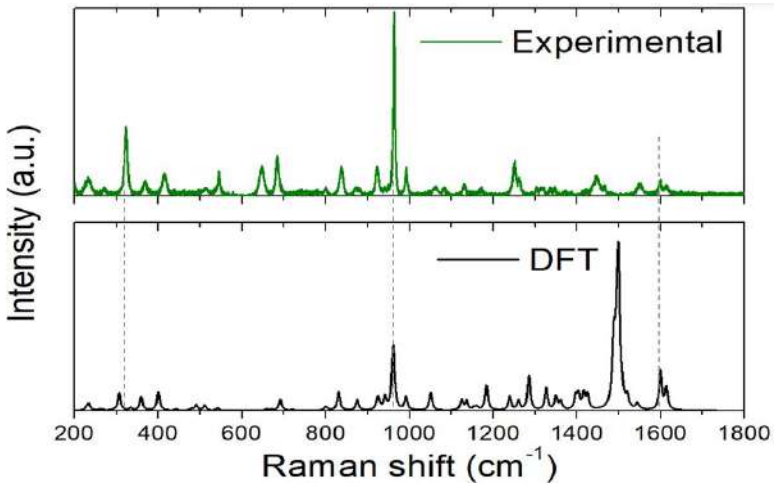

Fig. 1 Comparison of a) experimental and b) theoretical Raman response of Atrazine

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K 063

Characterization and Applications of a New Semiconductive BiZnO-$SnFe_3O_4$ Nanocomposite Material by Co-Precipitation Method

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ABSTRACT

An innovative semiconductor BiZnO-$SnFe_3O_4$ nanocomposite material has been prepared by the co-precipitation method. The characterization of HR-SEM and HR-TEM studies revealed that BiZnO -$SnFe_3O_4$ possesses a nano-spherical shaped structure. Energy dispersive X-ray analysis confirmed the presence of Zn, Bi, Sn, Fe Cu, Cr, and O. The photoluminescence analysis showed the possible recombination of electron-hole pairs by the transfer of electrons and holes between BiZnO and $SnFe_3O_4$. The ultraviolet-visible diffuse reflectance spectral UV and solar irradiation demonstrate the superior photocatalytic activity by Trypan Blue (TB) dye. As a photoelectrode, BiZnO - $SnFe_3O_4$ demonstrated a high efficiency short circuit to produce CV and dye-sensitized solar cells via electrocatalytic applications., irradiation as solar cell applications

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K 064

Toxic Heavy Metals Detection Using Boron Nitride ($B_{12}N_{12}$) Nanocage Towards Environmental Remediation Applications - A DFT Study

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ABSTRACT

High atomic weight metallic chemical elements otherwise Heavy metals that could pose risks to the environment and living organisms. Some of the metals (Iron) that pose health risks to human are necessary at trace level but are toxic at higher levels, while others are toxic with no known benefits (Nickel, Lead and Manganese). The present work deals with the investigation on the adsorption of Toxic Heavy Metals (THMs) at the surface of Boron Nitride ($B_{12}N_{12}$) nanocage using Density Functional Theory (DFT) implemented in Gaussian 16 software package. where the THMs ($MnCl_2$, $FeCl_2$, $NiCl_2$ and $PbCl_2$) are act as adsorbate and $B_{12}N_{12}$ cage act as adsorbent. The optimized geometry of THMs, $B_{12}N_{12}$ nanocage and their complexes ($B_{12}N_{12}$+THMs) were obtained at B3LYP/LANL2DZ level of theory associated with the Polarizable Continuum Model (PCM) by considering water as a aqueous medium. The interaction is maximum for the adsorption of $MnCl_2$ [-55.03 kcal/mol] at the surface of $B_{12}N_{12}$ nanocage. Based on the adsorption energy (kcal/mol), the Heavy metals are arranged in the order of $MnCl_2$ > $FeCl_2$ > $NiCl_2$ > $PbCl_2$. The negative sign indicates that there is a strong interaction between THMs and the $B_{12}N_{12}$ nanocage. Moreover, the calculated optical properties of THMs adsorbed $B_{12}N_{12}$ nanocage using time - dependent density functional theory reveal that the absorption spectra of $B_{12}N_{12}$ nanocage undergo appreciable changes after adsorption of THMs. Therefore, $B_{12}N_{12}$ may serve as a potential candidate in the realm of environmental remediation applications in the near future.

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K 065

DFT Study of $TmGa_3$ Intermetallic Compound

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ABSTRACT

Intermetallic alloys and compounds of transition metal elements fall into an interesting category of materials with a large number of technological applications. These materials gain attention because of their exotic mechanical, electronic and magnetic properties (Watson and Bennett 1978). The cubic intermetallic compound $TmGa_3$, which crystallize in $AuCu_3$ structure as shown in the Figure 1, is interesting because of its relatively strong quadrupolar pair interactions. The stability of the structural and electronic properties of ErX_3 (X = Ga, In and Sn) intermetallic compounds have investigated by Shukla et.al [1]. Deutz et.al [2] have studied the low temperature specific heat, a.c. susceptibility and magnetization data for $TmGa_3$. In the present work we have investigated the structural, electronic, elastic and mechanical properties of isostructural and isoelectronic magnetic $TmGa_3$ intermetallic compound, by using first principles density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method. The calculations are carried out within LSDA for the exchange correlation potential. Our calculated ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') are in good agreement with the available experimental and other theoretical results. The computed electronic band structure and DOS reveal that the compound is metallic in nature. We also predicted the elastic constants and mechanical properties for this compound using LSDA approximation. The compound is found to be brittle in nature in accordance with Pugh's criteria.

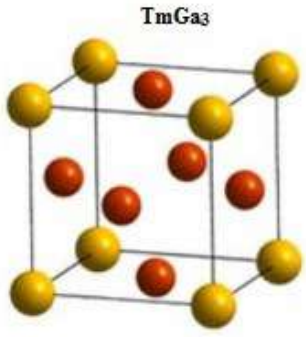

Figure 1. $TmGa_3$ Intermetallic Compound crystallize in $AuCu_3$ Structure

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K 066

Analysis of Wettability of Rough Surfaces Using Lattice Boltzmann Method

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ABSTRACT

The surface wettability can be engineered to enhance the separation of contaminants from water. Hydrophobic surfaces can effectively separate oil from water in oil-water separation processes. In this study, we present the numerical investigation of the surface wettability with irregular triangular micropillars using a two-dimensional (2D) pseudo-potential multiphase lattice Boltzmann method with a D2Q9 model for various solid-fluid interaction parameters of the range from -1.30 to -2.20. Firstly, the simulation of the equilibrium state of a water droplet on a smooth surface is considered with various interaction parameters to examine the accuracy of the present numerical model. We then imposed the microscale irregular triangular pillars at the bottom of the surface with different heights of the pillars to study the behavior of water droplets on the micropillars. We have taken a water droplet of radius 100 lattice units in the domain of 800x800 lattice units for the study and analyzed the wettability by measuring the contact angle. The study shows that increasing the solid-fluid interaction parameter of the pillars dramatically reduces the contact area between water droplets and solid walls due to the momentum redirection phenomenon.

Keywords: *Wettability; Contact angle; Water droplet; Lattice Boltzmann method*

K 067

Investigations on the salt of 4-Bromoaniline with maleic acid

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ABSTRACT

In the present work 4-Bromoaniline salt, 4-Bromoanilinium maleate (4- BAME) is crystallized by slow evaporation solution growth method which is examined by both theoretical and experimental methods. This is caused by proton transfer from maleic acids to amine group (4-bromoaniline). The molecular structures were optimized using the Density Functional Theory (DFT) with a 6-311++G(d,p) basis set and the B3LYP function. A geometrical characteristic of the molecule was also examined along with their intermolecular hydrogen bonds. These investigations demonstrate that the N–H…O and O–H…O hydrogen bonds stabilize the molecules. These interactions also analyzed by Hirshfeld surface and finger print analysis. The UV spectra of the crystal reveal that the crystal has wide transparency in visible region and optical band gap is 4.3 eV obtained from the Tauc's plot. The thermal behavior of crystal is evaluated by TG/DSC techniques and the melting point is 163°C. Quantum chemical methods were used to calculate the vibrational modes. There is a strong agreement between the calculated vibrational spectra and the optimized molecular geometry and the experimental results. Intramolecular charge transfer (ICT) and hyperconjucative contact were interpreted using the natural bond orbital (NBO) approach. The detailed understanding of the nature of H-bond interactions is provided by this approach. Using the HOMO-LUMO plot, the compounds' chemical potential, electronegativity, and chemical hardness were ascertained. Small band gap values in the frontier molecular orbitals indicate potential biological or pharmacological activity of the compounds.

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K 068

Frequency Splitting in Dissimilar Coupled Disks

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ABSTRACT

Optical micro resonators with closed concave boundaries have the ability to trap light strongly inside. Once the trapped light inside the structure is interfered at a specific frequency, it can be retained inside the resonator with minimum loss [1]. But there is an extension of light waves happening to the surrounding medium in the form of an evanescent field [2]. Any disturbances on the evanescent field cause changes in the spectral features of the resonant mode either in the form of mode broadening [3], mode shifting or mode spitting [4]. These changes in the resonant mode are monitored, analysed, and used as a sensing signal. In this study, we used a coupled microcavity system that consists of disks with different refractive indices. Finite difference time domain simulations were employed to measure spectral features of this system. We chose disks with refractive indices 1.49 and 1.59. The radius of the first disk was taken as 1.6μm and the radius of second disk was adjusted to 1.621μm to match the individual resonant frequencies at 580 nm (Fig.1a). When a coupled disks is formed frequency splitting has been observed as shown in Fig. 1b.

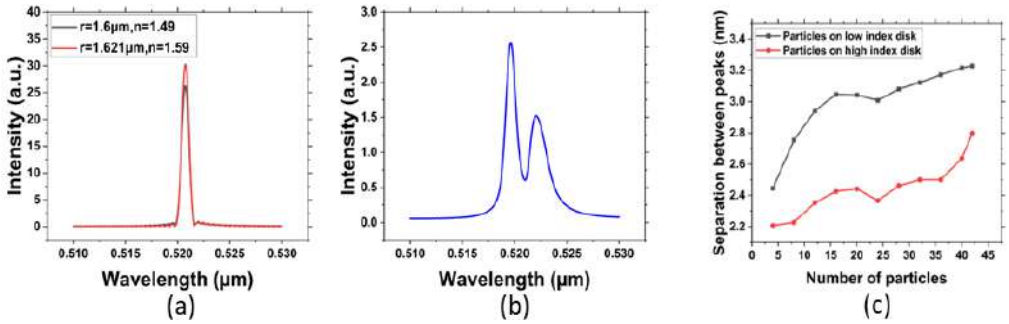

Fig.1 (a) Resonant spectrum of each disk. (b) Frequency splitting of coupled disks. (c) Plot of separation between peaks against number of particles placed on low index and high index disks separately.

Next, we performed calculations to determine the spectral separation of whispering gallery modes (WGM) in this unique coupled system. We systematically attached nanoparticles with a diameter of 40nm and refractive index of 1.45 at the bright spots of the WGM pattern on each individual disk. As shown in Fig.1c, it is clear that there is a difference in spectral separation when nanoparticles are placed on disks with high and low refractive indices respectively. Furthermore, we observed that the spectral separation increases as more nanoparticles are added. This characteristic demonstrates the potential of this structure as a refractive index sensor.

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K 069

Theoretical Investigation on Ag-decorated Blue Phosphorene for Biosensing Application

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ABSTRACT

Two-dimensional (2D) materials are a novel class of nanomaterials that are employed in a variety of applications and research domains, including biomedicine, biosensing, and chemical sensing, as well as energy storage and electronics etc...2D materials have numerous advantageous physical, chemical, electronic, and optical properties, such as large specific surface areas, excellent electrical and thermal conductivity, ease of functionalization, and tuneable electronic structures, making them promising candidates for the development of high-sensitivity sensors.2D materials include transition metal dichalcogenides (TMDs), boron nitrides (BN), carbon nitrides (CN), and monoelemental Xenes (phosphorene, antimonene, arsenene, bismuthene, silicene, germanene, and others).Researchers are studying 2D Blue Phosphorene because it is anisotropic, and has tuneable qualities. The blue phosphorene (BP) is one of the allotropes of layered phosphorene. It is employed to detect the existence of liver cancer biomolecules like octenol, decane, and hexanal. These biomolecules adsorption are examined with the density functional theory (DFT) method.In this work, the structural geometry and electronic properties of monolayer BP, and Ag decorated blue phosphorene is theoretical analysed by using DFT. we have explored BP's structural geometry and electronic properties with various concentrations of Ag dopants from 1.56% to 4.68%.The adsorption behaviour of octenol, decane, and hexanalon BP-NS is explored based on adsorption energy, band gap variation, charge transfer, density of states spectrum, and electron density. These analyses will show that these materials are good candidates for biosensing applications.

K 070

Adsorption Studies of Toxic Harmful Gases HCN, SF_4 and AsH_3 on $MoTe_2$ Monolayer: A First Principles Investigation

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ABSTRACT

The emission of hazardous gases from various sources, especially industries, and automobiles, has a detrimental impact on the environment, which results in severe health complaints. To gauge the air quality in both indoors and outdoors, it is vital to employ extremely sensitive and specific gas-sensing devices. A wide range of nanomaterial were used for gas sensing applications. However, it is noted that Transition metal dichalcogenides (TMDCs) were widely used in gas sensors for the detection of various toxic gases. Because, TMDCs have large specific surface area and excellent surface energy levels, longer bonds, and a smaller band gap. Molybdenum Ditelluride ($MoTe_2$), an exfoliate TMDC has recently garnered significant attention in the fast growing fields of two dimensional electronics and has received extensive attention in gas sensing. In this study, we employed the first principle calculation for sensing the harmful gases like HCN (Hydrogen cyanide), SF4 (Sulfur tetrafluoride), and AsH_3 (Arsenic trihydride) on $MoTe_2$ monolayer. Further to improve the sensing ability, we employed doping on $MoTe_2$ monolayer and adsorption characteristics for all the doped systems, were analysed systematically. Our results demonstrate that $MoTe_2$ material has a potential to be an efficient gas sensor.

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K 071

Gas-Sensing Properties of NO on Ce-doped Zinc Oxide: A DFT Study

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ABSTRACT

One of the most prevalent pollutants that pollute the environment is nitrogen oxide. NO and NO_2 gases, which are hazardous to both human health and the environment, are included in NO_x. Therefore, the rare earth element Ce doped metal oxide semiconductor (MOS) ZnO was employed to reveal their NO gas sensing properties. Based on density functional theory (DFT) calculations optimized surface of ZnO (0001), Ce-doped ZnO (0001), and adsorbate structure of NO were calculated, and also adsorbate NO on the modified ZnO (0001) surface was calculated. Furthermore, the gas sensing properties were examined through adsorption energy, Bader charge analysis, charge density difference (CDD), charge transfer, band structure, and total density of state. For the Ce-doped ZnO (0001) surface the NO adsorption energy is more negative than the bare ZnO. Also, from Bader charge analysis, we calculate the charge transfer value from the substrate to adsorbate increases after doping of rare earth element Ce. Favorable electronic properties and suitable adsorption energy of Ce-doped ZnO can be a potential gas sensor for NO molecule. As well as DFT calculations were compared with the existing results of experiments.

Keywords: *Metal oxide semiconductor, DFT, REE, and Gas sensing*

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K 072

Computational Intelligence in Designing New Nanostructures

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ABSTRACT

New potentially 2D nanostructures based on carbon, molybdenum and silicon are generated by the intelligent computing method based on a memetic strategy combining the evolutionary algorithm and the conjugate-gradient optimization technique for the molecular model [1][2].

The main goal of design is to find stable arrangements of atoms under certain imposed conditions. The objective function is formulated as the total potential energy of an atomic system. The optimized nanostructure is considered as a discrete atomic model. In the case of carbon interactions between atoms are modeled using the AIREBO potential. Validation of the obtained results of new 2D graphene-like materials are presented, along with their mechanical properties [3].

Apart from graphene one of the most prominent 2D material is the Single-Layered Molybdenum Disulfide ($SLMoS_2$), which reveals polymorphism at the nano-level. The paper presents optimization technique which allows to obtain SLMoS2 heterostructures with desired mechanical properties. The behaviour and energy of the atoms is determined by the REAX-FF potential. Examples of such periodic $SLMoS_2$ 2H/1T heterostructures are presented [4]. New nanostructures based on silicon are also presented using the presented intelligent methodology and interatomic potentials [5].

Funding: The research is funded within the National Science Centre, Poland, project No. 2021/43/B/ST8/03207.

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K 073

Computational Investigation of CO_2 Activation on Pristine and Cu Decorated Ψ-Graphene, Ψ-Graphone and Ψ-Graphane

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ABSTRACT

Investigating new two-dimensional nanomaterials for efficient CO_2 capture is useful in not only to maintain the balance of oxygen and carbon dioxide in atmosphere but also in searching an alternate source of fossil fuels. Here, we have employed first-principles calculations to study the CO_2 adsorption capacity of pristine and Cu decorated bare ψ-graphene, half-hydrogenated ψ-graphene (i.e. ψ-graphone) , and fully hydrogenated ψ-graphene (i.e. ψ-graphane). Our results categorize the CO_2 adsorption on these three nanosheets in weak physisorption. Neither full nor half hydrogenation of ψ-graphene is capable of increasing the activity of ψ-graphene towards CO_2 capture but by the decoration of copper (transition metal atom) over ψ-graphene, the adsorption capacity of CO_2 increases up to three times. But no considerable increment is observed in binding energy of CO_2 after the decoration of copper on its hydrogenated forms. Our theoretical investigation may inspire the experimentalists to synthesize ψ-graphene based adsorbents and gas sensors for CO_2 capture and detection.

K 074

Strain Engineering in 2D Analog of Bulk Manganese (III) Oxide-Mn_2O_3 and its Heterostructure with Graphene

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ABSTRACT

2D-Mn_2O_3 is a newly exfoliated two-dimensional magnetic indirect bandgap semiconductor. A comprehensive structural analysis of bulk manganese (III) oxide-Mn_2O_3 under strain has been conducted through first-principles calculations utilizing density functional theory (DFT). The calculations reveal it is ferromagnetic in the ground state, displaying a substantial total spin magnetic moment of 16 μ_B per unit cell. Furthermore, it emerges as an intrinsic magnetic semiconductor, featuring a significant band gap of 0.98/3.6 eV in the majority/minority spin channels. In this study, we explore the effects of tensile and compressive strains on the magnetic state and band gap of materials. Our findings reveal a strong influence of both strains on the band gap, whereas the ground state of the 2D-Mn_2O_3 compound remains largely unaffected. However, the substantial band gap poses a significant constraint on its potential applications. To overcome this limitation, we have addressed existing uncertainties by creating a suitable van der Waals (vdW) heterostructure with graphene. We anticipate that the resulting 2D-Mn_2O_3 composite, currently under investigation, will have a broad range of applications in spintronics and memory-based technology.

K 075

Shape Reversibility and Functional Characterization of Shape Memory Alloys

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ABSTRACT

A series of alloy system take place in a class of functional materials due to stimulus response to external effect. Shape memory alloys take place in this class by exhibiting a peculiar property called shape memory effect. This phenomenon is characterized by the recoverability of two certain shapes of material at different conditions. Shape memory effect is initiated on cooling and deformation processes and performed thermally on heating and cooling, with which shape of material cycle between original and deformed shape in reversible way. Therefore- this behavior can be called Thermoelasticity. These alloys are used as shape memory devices in many fields such as medicine, metallurgy, building industry. This property is result of successive thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling with cooperative movements of atoms by means of lattice invariant shears in <110 > -type directions on the {110} - type planes of austenite matrix, along with lattice twinning, ordered parent phase structures turn into the twinned martensite structures, and the twinned structures turn into the detwinned structures by means of stress induced martensitic transformation, with stressing material in the martensitic condition. Shape memory alloys become noticeable as smart materials in mechanical applications in many fields of industry.

These alloys exhibit another property called superelasticity, which is performed by stressing and releasing material at a constant temperature in parent phase region, and shape recovery is performed simultaneously upon releasing the applied stress. Superelasticity is performed in non-linear way; stressing and releasing paths are different in the stress-strain diagram, and hysteresis loop refers to energy dissipation. Superelasticity is also result of stress induced martensitic transformation and ordered parent phase structures turn into detwinned martensite structure with stressing in the parent phase region.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures at high temperature parent phase field. Lattice invariant shear and twinning is not uniform in copper based ternary alloys and gives rise to the formation of complex layered structures, depending on the stacking sequences on the close-packed planes of the ordered parent phase lattice. The layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on copper based CuAlMn and CuZnAl alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging duration at room temperature. This result refers to the rearrangement of atoms in diffusive manner.

Keywords: *Shape memory effect, martensitic transformation, thermoelasticity, superelasticity, twinning, detwinning.*

K 076

First Principle Calculation of Evolution of Magnetic Properties of 2-Dimensional ZrI_2

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ABSTRACT

Multiferroic materials are of great interest due to their potential application, as well as for fundamental studies. Various two-dimensional (2D) materials have exhibited numerous interesting properties not observed in bulk materials **[1]**. 2D β-ZrI_2 has recently attracted a lot of attention due to its potential for multiferroic properties. Ferroelectric materials with spontaneous electric dipole moments switchable by an external electric field offer a broad range of technological applications, such as, field effect transistors, spintronics and electro-optical devices **[2]**. In this work, we report on the first-principles evidence of robust vertical ferroelectricity in layered ZrI_2. The out-of-plane polarization in ZrI_2 is found to be rigid upon interlayer sliding, and the low energy barrier for its ferroelectric switching combined with a small band gap can hold out the prospect for slidetronics applications. Our theoretical study reveals that the ferroelectric activity in ZrI_2 stems from a subtle interplay of charge redistribution and ionic displacements. The electronic structure shows that 2D β-ZrI_2 material have semiconducting behaviour with small band gap Eg<3. Optical properties study shows that this material has strong absorption in visible and UV region. Additionally, we have reduced the band gap of this material by using strain engineering. Due to reduction of band gap this material able observes all wavelengths in visible light region. Finally, we computed AIMD simulation to understand the ferroelectric switching and Curie temperature of this material. All our results show that 2D β-ZrI_2 material can be possible potential candidate for room-temperature spintronic, photovoltaic and optoelectric device application.

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K 077

Basis Set Selection for Raman Response of Agrochemicals using DFT/B3LYP Calculations

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ABSTRACT

India is an emerging economy and agriculture plays a significant role in it. Farmers use agrochemicals in an unregulated and excessive amount to increase the yield of crops, which causes considerable contamination in the food being grown and also in the water bodies in nearby areas. Exposure to excessivelevels of these agrochemicals can lead to a variety of health problems, including cancer, respiratory problems, neurological disorders, and reproductive problems. A study by the Environmental Working Group (EWG) in 2019 found that exposure to atrazine, a common herbicide, in drinking water is linked toan increased risk of non-Hodgkin lymphoma, a type of cancer [1]. Raman spectroscopy can help identify and quantify the chemical composition of materials with high sensitivity, selectivity, speed, and accuracy. Hence, it is an excellent technique for on site measurements of harmful agrochemicals in both solid and liquid samples. Density functional theory (DFT) can model the Raman response of the agrochemicals, however, the selection of the basis set is essential to ensure an accurate analysis. Further, the Raman study of these chemicals used by Indian farmers is lacking. The current article aims to establish the accuracy of various data sets (Pople's basis sets, Los Alamos National Laboratory basis sets, and other large basis sets) to model agrochemicals including, herbicides, insecticides,and weedicides. Fig. 1 establishes the accuracy of DFT analysis for the Raman response of herbicide Atrazine which was calculated using Pople's basis set and B3LYP exchange correlation functional.

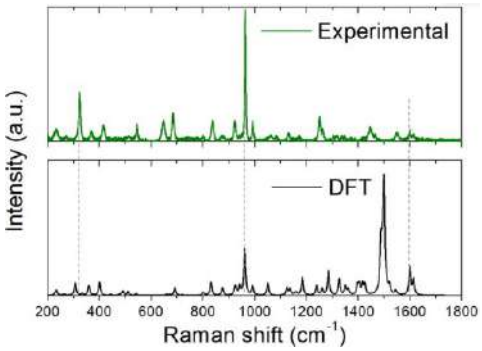

Fig. 1 Comparison of a) experimental and b) theoretical Raman response of Atrazine

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K 078

Modelling Of Additive Manufacturing and Welding Processes

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ABSTRACT

Due to the multiscale nature of these metal manufacturing processes — the impact of manufacturing process parameters on the microstructure, further, which has either a beneficial or deleterious impact on the manufactured parts' performance — the software suite must be capable of modelling all the scales [1]. This calls for the requirement of a variety of computational modelling techniques such as discrete element methods, AI/ML, kinetic monte carlo simulations, phase-field methods, and multiphase finite volume methods [2,3]. The two objectives of the present study were (i) Modelling of the powder-bed laying process using Discrete Element Method (ii) Modelling of the microstructure evolution during welding and additive manufacturing processes using Kinetic Monte Carlo simulations. The aim of this development process through the extension of open-source software packages. This work included developing, validating, and extending the features to include more physically relevant modelling capabilities and also document the procedure for re-use and incorporation into the application. The user provides process parameter inputs, such as the raster pattern, size of powder particles, type of laser, etc. through the user- interface. The power-laying process is then modelled using DEM, the results are then extracted as an STL file and fed into an open-source mesher, SnappyHexMesh. This prepares a mesh consisting of hexahedral and polyhedral elements, suitable for a solver developed in the finite-volume framework provided by OpenFOAM. The powder bed formation process has been found to have three consecutive stages: packing, layering and compression. Two main applications were developed, modelling of the powder-bed laying process and modelling of microstructure growth in additive manufacturing and welding processes. These modelling techniques will play a vital role in any additive manufacturing software suite and in the research related additive manufacturing. Similar such features may also be found in Flow-3D's 'Additive' software package.

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K 079

Thermoelectric Properties of Line-Node Dirac Semimetal and Topological Insulating Phase in Hexagonal Pnictide CaAgAs

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ABSTRACT

The structural, electronic, and transport properties of CaAgAs, a recently predicted topological nodal line semimetal, have been investigated using first-principles density functional theory (DFT) with spin-orbit coupling (SOC) and Boltzmann transport theory. The material exhibits a topological phase transition from a nodal line semimetal to a topological insulator phase as a result of the SOC effect. The Voigt-Reuss-Hill approximation is used to compute various mechanical properties. The calculated Seebeck Coefficient~153.19 μV/K, Power factor ~0.64×1011 W/m.K2.sec and lattice thermal conductivity ~6.20 W/m.K suggest that CaAgAs have superior thermoelectric performance compared to other well-known predicted thermoelectric materials. The calculated thermoelectric properties observed in CaAgAs are attributed to the topological phase transition induced by SOC. This discovery highlights the material's promising application as a high-performance thermoelectric material, opening avenues for further exploration and development in the field of energy conversion and utilization.

Keywords: Topological Insulator, Thermoelectric Properties, DFT, FPLAPW.

K 080

Identification of Secondary Structure Element in Proteins using Solid-State NMRChemical Shielding Anisotropy Calculated using DFT Methods

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ABSTRACT

NMR Chemical Shielding Anisotropy (CSA) offers valuable insight into the local electronic environment at atomic level and in particular, the ^{13}C and ^{15}N CSA tensor of protein backbone act as highly reliable indicators of protein secondary structure. This study investigates the sensitivity of CSAtensors of backbone $^{13}C^{\alpha}$ and amide ^{15}N as a function of backbone dihedral angle ϕ and ψ in alanine from different proteins using ab initio method. DFT-GIAO calculations on proteins reveal that the $^{13}C^{\alpha}$shielding along the C^{α}-N bond vector, C^{α}-C^{β} bond vector and C^{α}-H^{α} bond vector exhibits higher sensitivity to protein secondary structure than the three principal components. Similarly, the projectionof ^{15}N shielding on N-C^{α} bond vector, N-H bond vector and ^{15}N shielding perpendicular to peptide planealso quite sensitive to the secondary structure of the polypeptide segment. Furthermore, our DFT calculations on proteins show that 2D correlation plots of CSA tensor parameters of backbone nuclei $^{13}C^{\alpha}$, $^{13}C'$ and ^{15}N are useful to differentiate the two major secondary structure elements.

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K 081

Strain Effect on the Electronic Structure and Thermoelectric Properties of *Half*-Heusler Alloy

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ABSTRACT

Before realizing any device's actual application, it is necessary to understand its performance by simulation or first-principle investigation. Most sensor devices are nanomaterials, especially thin film-based, which are under strain due to lattice mismatch between the sensor material and the substrate on which thin film is grown. This mismatch offers strain to the film material and affects the material's properties and overall performance [1-3]. In this work, we comprehensively explored strain engineering's impact on the band structural characteristics of the CoHfSi *half*-Heusler alloy. Employing the self-consistent ultra-soft pseudopotential method and generalized gradient approximation within density functional theory, we investigated the effect of both uniform and tetragonal (compressive and tensile) strains on the electronic structures, phonon dispersion and thermoelectric properties. A *p-type* semiconducting ground state with an indirect band gap of ~ 1.13 eV between the Γ- and X-high symmetry points is estimated. Under the compressive strain, the band gap decreased to 0.98 eV, whereas it increased to 1.22 eV for the tensile strain. Conversely, uniform strain exhibited an opposite effect on the electronic structure; there is an increase in the band gap from up to 1.25 eV under compressive strain and a decrease up to 0.85 eV for the applied tensile strain. The figure-of-merit decreases in both types of applied strains between 1-5 %. Phonon dispersion analysis confirmed the thermodynamic stability of CoHfSi under strain, showing positive frequencies in both uniform and tetragonal strain scenarios. Additionally, this study provides novel insights into the strain-induced effects on the thermoelectric properties of CoHfSi at elevated temperatures.

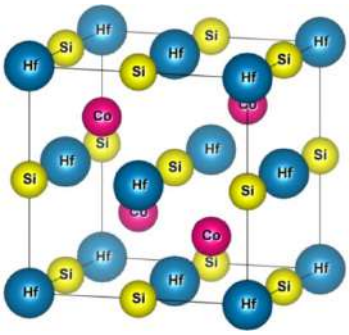

Figure 1: Crystal structure of CoHfSi

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K 082

DFT Studies On Anthraquinone Derivative: Spectroscopic Analysis of UV-Visible, NMR, IR-Raman, Mulliken Atomic Charges, HOMO-LUMO and ESP Map

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ABSTRACT

Density functional theory has been used to optimize the geometry of anthraquinone derivative, 2-amino-9, 10-anthraquinone (2AAQ) at 6-311G++(d, p)/B3LYP basis set. Semi-empirical and HF method also has been used to optimize the geometry. UV-Visible spectra of the molecule have obtained using optimized geometry from DFT method in different solvents. UV-Visible spectra have been studied from TD-DFT method at 6-311G++ (d, p)/B3LYP basis set. The ground state dipole moment obtained from DFT, semi-empirical and HF method is smaller than the excited state dipole moment obtained from TD-DFT method. The NMR, IR-Raman spectra were obtained from DFT method at 6-311G++ (d, p)/B3LYP basis set in acetonitrile. Different vibrational modes were obtained from IR-Raman spectra. IR and Raman vibrational modes observed for different types of bond in molecule like, C-H, C=C, C=O, NH_2. H^1 and C^{13} NMR shielding values were evaluated from NMR spectra using GIAO method. Molecular properties such as molecular polarizability, acidity-basicity, and other characteristics can be determined from Mulliken atomic charges. Small value of HOMO-LUMO energy gap in gas phase and solution indicated that easier for the electron to jump from HOMO-LUMO level. Electrophilic and nucleophilic sites of the molecules were identified from molecular electrostatic potential map.

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K 083

Spinterfacial Effect on Transport Properties due to Molecular Adsorption: A First-PrinciplesStudy

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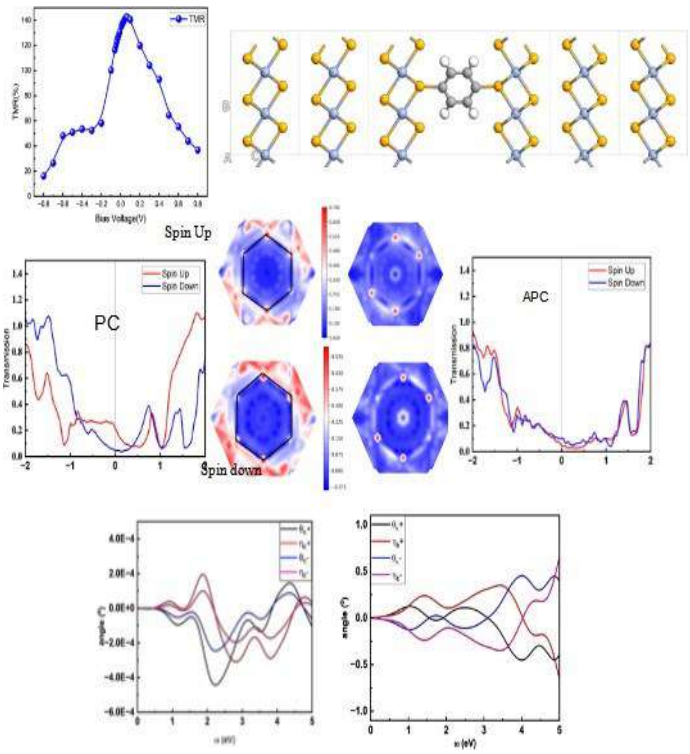
ABSTRACT

With the discovery of Graphene, 2D materials were able to draw major attention for their interesting properties and plenty of applications. Getting 2D ferromagnetic materials is often quite difficult, though ferromagnetism can be seen only in few-layers or sometimes in the monolayer limit. Magnetic anisotropy energy and exchange interaction energy are the two key factors for maintaining long-range magnetic ordering. Interestingly the 2D magnetic materials show very high anisotropy energy with a unique easy axis. In this work, we study the layer-wise and strain-dependent electronic and magnetic properties, and secondly, the manipulation of magnetic properties due to the adsorption of the molecule by the substrate. Further, we study the changes in the physical properties due to the increase of van-der Waal layers. We make use of the combined approach of DFT and non-equilibrium Green's function (NEGF) formalism to determine the Tunnel Magneto Resistance (TMR) by constructing several magneto-tunnel-junction (MTJ) devices with transition metal dichalcogenides as electrodes and single molecules (*e.g. benzene*) in the central region. Magneto-Optical Kerr effect (MOKE) signals are calculated using full potential all-electron code *Exciting,* taking muffin-tin radii of Bohr. The *Exciting* code uses *the time-dependent density-functional theory* (TDDFT) to calculate the Kerr angle (θ_K) and ellipticity (η_K) in the presence of positive and negative magnetic fields.



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K 084

Investigaton of Structural & Electronic Properties of Janus CrXY(X, Y = Se, Te And X ≠ Y) Using First-Principles Approach

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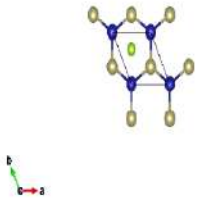
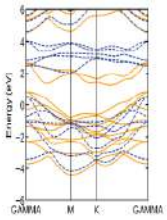
ABSTRACT

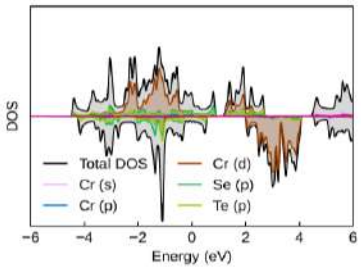
To investigate the structural and electronic properties of 2D Janus Transition Metal, CrTeSe, first-principles calculations were performed using the Vienna ab-initio Simulation Package (VASP). The results showed that CrTeSe has a stable monolayer structure with a lattice constant of 6.26 Å. The electronic band structure of CrTeSe is characterized by an indirect band gap of 1.62 eV. The density of states (DOS) analysis revealed that the valence band of CrTeSe is mainly composed of Te-5p and Se-4p orbitals, while the conduction band is mainly composed of Cr-3d orbitals. The Bader charge analysis showed that the charge transfer from Te to Cr atoms is responsible for the formation of the Janus structure. The calculated work function of CrTeSe is 4.73 eV, which is higher than that of CrTe2 and CrSe2, indicating that CrTeSe is a more n-type semiconductor. The results of this study suggest that 2D Janus Transition Metal, CrTeSe, is a promising candidate for applications in optoelectronics and nanoelectronics.



CrTeSe relax



CrTeSe band structure



DOS Calculation of CrTeSe

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K 085

An Ab-initio Study of Nickel Nano Clusters for Hazardous Gas Sensor Application

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ABSTRACT

In the present study, we have investigated the adsorption properties of HCN and CNCl molecule on pure Ni_6 cluster using DFT calculation. The geometrical optimization of Ni_6 clusters and the complex of Ni_6 M (M=HCN, CNCl) were performed by Gaussian 09 software using the B3PW91 level of theory consisting of Becke hybrid exchange functional and LANL2DZ Basis set which includes relativistic effects[1] .In this study, the electronic structure and sensing properties of Nickel cluster Ni_n(n=2-6) using Density Functional Theory (DFT) are presented. Since Nickel Nano clusters involve chemical reactions with polluting gas molecules Hydrogen Cyanide (HCN) and Cyanogen chloride (CNCL) are adsorbed[2]. We observed the binding energy for Ni_6 is -2.67 eV among all the clusters considered energetically favorable for the adsorption of gas molecules.Among all the different clusters Ni_6 has good suitability by HCN gas molecule strongly interacted with Ni_6 nanocluster as compared to the CNCl with the adsorption energy of -2.66 eV. The recovery time for this configuration is 1.7×10^{28} s at 310K temperature. The calculated formation energy for Ni_6 is E= -2.67 eV/atom. The negative and high value of formation energy confirms its stability .[3]Among all of nanoclusters HCN gas molecule strongly interacted with Ni_6 nanocluster as compare to the CNCl with the adsorption energy of -2.66 eV. The recovery time for this configuration is 1.7×10^{28} s at 310K temperature.The HCN gas molecule strongly interacted onto the Ni_6 nanocluster with -2.65 eV energy which is chemisorption[4] in nature. Furthermore, the longer recovery time suggests that Ni_6 nanocluster could be considered as a promising candidate for removal material for HCN gas molecule from the environment, whereas shorter recovery time for CNCl gas molecule suggested that it can be used for detection.

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K 086

Computational Studies of the Optical Properties of 4-Cyano-4-Hexylbiphenyl using combined Dft and Molecular Dynamics Simulation

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ABSTRACT

In this study, we investigated the optical properties of the liquid crystal 4-cyano-4-hexylbiphenyl (6CB) from the n CB homologous series using the Vuks equation [1]. Our methodology was based on the works of Shin-Pon Ju [2]. We obtained the polarizability and anisotropy polarizability of the liquid crystal through DFT calculations, using B3LYP with the basis set 6-31G (2d, p), which was implemented in Gaussian 09. To determine the density and order parameter of the liquid crystal, we employed Molecular Dynamics simulation using the United Atom Model suggested by Tiberio et al. [3] and implemented in the software NAMD. The experimental results are in agreement with the theoretical results.

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K 087

An in vitro cytotoxicity study on PANI/ TiO_2 nanocomposites against HCT- 116 cancer cells using MTT Assay

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ABSTRACT

Polyaniline/ TiO_2 nanocomposites were synthesized with different TiO_2 weights (20 %, 40 %, 60 %, and 80 %) using an in situ chemical polymerization method. The prepared composite samples were characterized by FT-IR, XRD, TEM, FE-SEM with EDAX, UV-Vis and PL properties. The FT-IR spectrum confirms the presence of metal oxide in the structure of the composites. The intensity of polyaniline increases with increasing metal oxide content. The promotion of electrons from the ground state to the excited state of the composites was confirmed by UV-Vis studies. The FE-SEM study shows a spherical morphology. X-ray diffraction patterns show that the nanocomposites exhibit preferential orientation growth along the (110) plane with a hexagonal wurtzite structure. The antibacterial activity is enhanced with increasing concentration of TiO_2 nanoparticles. The anticancer effect on HCT-116 cell lines is more effective when using PANI/ TiO_2 nanocomposites. EDAX study confirms the presence of elements Ti, C and O in the structure. The conductivity of the composites decreases with increasing the content of TiO_2.

Keywords: *PANI/TiO_2 nanocomposites; FE-SEM;XRD; TEM; Antibacterial activity; Anticancer effect ;MTT assay;*

K 088

Structural, Electronic, Magnetic and other Physical Properties of 211-MAX phase Cr_2TlN with GGA+U approximation

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ABSTRACT

In this study, we investigated the magnetic and electronic properties of Cr_2TlN using PBE-GGA and GGA+U exchange-correlation functionals. The predicted material was found to be dynamically stable as it doesn't have either negative or imaginary frequencies in the phonon dispersion spectra. The electron band structures and density of states analysis suggest that Cr_2TlN exhibits metallic characteristics due to the hybridization of Cr-d with N-p and Cr-d with Tl-p states at Fermi level. The results indicate that a ferromagnetic and antiferromagnetic spin order of Cr atoms is the preferred state for the bulk and supercell of the Cr_2TlN compound, respectively. In the ferromagnetic phase, the calculations show an increase in the total magnetic moment of Cr_2TlN from 1.14 to 3.51 μB per atom with different values of U. Additionally, our research has demonstrated that the anticipated material displays characteristics of ferromagnetism when U is equal to 0 eV. However, the substance behaves as an antiferromagnet as U increases from 0 to 1 and 2 eV. Furthermore, we investigated the mechanical properties of Cr_2TlN, including the elastic constants C_{ij}, which adheres to the Born-Huang criteria for mechanical stability. The Young modulus, rigidity modulus, and bulk modulus are successfully assessed using the Voigt-Reuss-Hill approximation. The ductility and brittleness of the compound is evaluated through Pugh's and Poisson's ratios, revealing that Cr_2TlN displays ductile behavior. The low values of Young's modulus and minimum thermal conductivity suggest that Cr_2TlN could be the best candidate for thermal barrier coating applications. We hope that this theoretical investigation offers valuable insights for future experimental research on Cr_2TlN.

Keywords: Magnetic MAX phases, Hubbard parameter, antiferromagnetism.

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K 089

Effect of stacking order in VSe_2 system – A First Principle approach

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ABSTRACT

2D materials are bringing revolutions to numerous advanced applications due to their fascinating physical, chemical and electronic properties. These materials open up new arena in research especially due to their tunable properties. MX_2, the transition metal chalcogenides, display a characteristic layered structure. It consists of one transition-metal atom sandwiched between two chalcogen atoms forming covalent bonds, held together by van der Waals forces [1]. Previous reports have shown that by changing the interlayer stacking orders in bilayer CrI_3, the interlayer exchange interaction between ferromagnetic and antiferromagnetic can be tuned [2,3]. Recently, a similar study has been performed in CrI_3 where the magnonic behaviour is seen to be strongly dependent on the stacking configuration [4]. Motivated by all these findings, in this work we report the connection between the stacking order and magnetic properties of VSe_2 system via first-principles calculations.

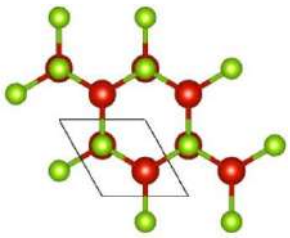

Figure - Top view of hexagonal VSe_2 bilayer, where red ball belongs to V atoms and green ball belongs to Se atom.

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K 090

Experimental and Theoretical Characterization of 1,3-Diphenyl-3-(phenylsulfonyl)propan-1-one

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ABSTRACT

Compound 1,3-Diphenyl-3-(phenylsulfonyl)propan-1-one (DPP) was studied by recording its FT-IR (4000-400 cm^{-1}), FT Raman (4000-50 cm^{-1}) and UV-Visible spectra (200-400 nm). Barrier heights around flexible bonds were estimated by evaluating torsional potentials using optimized structure. Density functional theory, utilizing B3LYP exchange-correlation functional along with 6-311++G(d,p) basis set, was used to determine the ground state structure parameters, general valence force field, harmonic vibrational frequencies, potential energy distribution, intensities of infrared and Raman bands, oscillator strengths and absorption maxima for electronic transitions in a solution of DMSO-d_6 with TD-DFT, frontier molecular orbital characteristics, NLO behaviour, NBO parameters, Fukui functions, molecular topology and MESP analysis. The observed and estimated quantities for structural parameters, IR, Raman and UV- Vis transitions showed good agreement. All the frequencies of the molecule were assigned unambiguouslyfor the first time using PED and eigenvectors. The NBO study confirmed that the chemical was suitable forNLO applications. The drug characteristics of the molecules were evaluated by using drug-likeness, alongwith its ADME properties and Bio-activity. The target protein and the ligand Interactions were investigated using molecular docking and Respective binding sites and residues were evaluated.

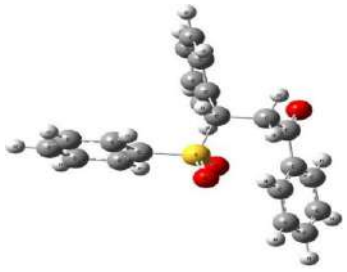

Figure 1. Optimized molecular structure of DPP (EDPP = -3905.302 × 13 kJ mol-1)

Keywords: *Vibrational Spectra, DFT, Molecular Docking, Home Lumo energies, NBO analysis.*

K 091

MAML-based Meta-Learning for Nanomaterial Classification in Transmission Electron Microscopy Images

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ABSTRACT

Understanding the properties and behavior of nanomaterials hinges on accurate and efficient classification in transmission electron microscopy (TEM) images. However, conventional deep learning methods often demand large, specific datasets for each nanomaterial type, hindering their applicability and adaptability. This work introduces a groundbreaking approach leveraging Model-Agnostic Meta-Learning (MAML) for nanomaterial classification in TEM images. MAML empowers models to learn "how to learn," enabling them to rapidly adapt to novel nanomaterial types with limited data. We propose a MAML-based model that utilizes a diverse set of base nanomaterial classes to acquire transferable knowledge, which is then fine-tuned on specific target classes with minimal samples. Our experiments demonstrate that this MAML-based model outperforms conventional deep learning methods, particularly when encountering unseen nanomaterial types. It exhibits significant improvements in both accuracy and generalizability, showcasing the potential of MAML for nanomaterial classification with limited data. This opens doors for efficient and precise characterization of nanomaterials in TEM images, paving the way for advancements in various nanotechnology-driven fields.

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M 001

Comparative Study of 2D $Ti_3C_2T_x$ MXene prepared via Solvothermal and HF-etching for Rapid Methylene Blue Degradation under Visible Light

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ABSTRACT

Two methods were used to successfully construct a two-dimensional pure MXene $Ti_3C_2T_x$ in this work: a solvothermal etching process that lasted 48 hours and used low-toxicity etching chemicals ($NaBF_4$, HCl), and a stirring-based HF etching process that lasted 24 hours. According to our analysis, we discovered that the solvothermal etching procedure yields higher porosity as the surface area increases. In addition, Mxene with the lowest particle size and the most defects, which served as active sites has been reported. The absence of active sites was Mxene's primary issue, which is resolved in this work. Using 10 mg of solvothermally generated Mxene within 30 minutes under visible light by electrostatic contact, these properties affected the degradation process, resulting in a 99.5% degradation of methylene blue (MB) in a 20 µM aqueous solution of MB. There has never been a prior report regarding the perfect material. This study's results might shed light on how to put MXene to use in real-world water purification applications. In addition, MXene showed great recyclability, which allowed for its continued usage, making it an efficient material for industrial applications.

Keywords: *$Ti_3C_2T_x$, MB dye degradation, removal mechanism, visible light photocatalyst*

M 002

Thermoelectric Transports in Chemical-Free Fabricated Non-Periodic MoS_2 Holey Structure

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ABSTRACT

The frontiers have explored the properties in crystals, bulk or with controlled mono-, bi-, few layers in MoS_2. The recent interesting reports on evaluation of structural effect has competitive performance to improve thermoelectric properties. Here, we report chemical-free holey structured MoS_2 fabricated by single step chemical vapor deposition (CVD) technique. The formation of holey structure is confirmed by Field emission Scanning Electron Microscopy (FESEM) and the estimated area of hole is lie in the range of ~(0.1 – 3.2) nm^2. The maximum electrical conductivity (σ) of 346.42 S/m is achieved at 300 K where metal to semiconductor transition is noticed. On other hand, the maximum Seebeck coefficient (S) of 1103 μV/K is attained at 595 K and the highest power factor of 267 $\mu W/mK^2$ at 300 K. Meanwhile the suppressed phonon transport is noted where the phonons can be trapped behind the hole due to small phonon MFP than the distance between adjacent holes. This creates a local negative temperature gradient under necking effect opposing the linear temperature gradient across the film. The very high Seebeck coefficient, electrical conductivity, and power factor of 6-layered MoS_2 with a holey system have proven the decisive role of domain arrangements in the thermoelectric properties.

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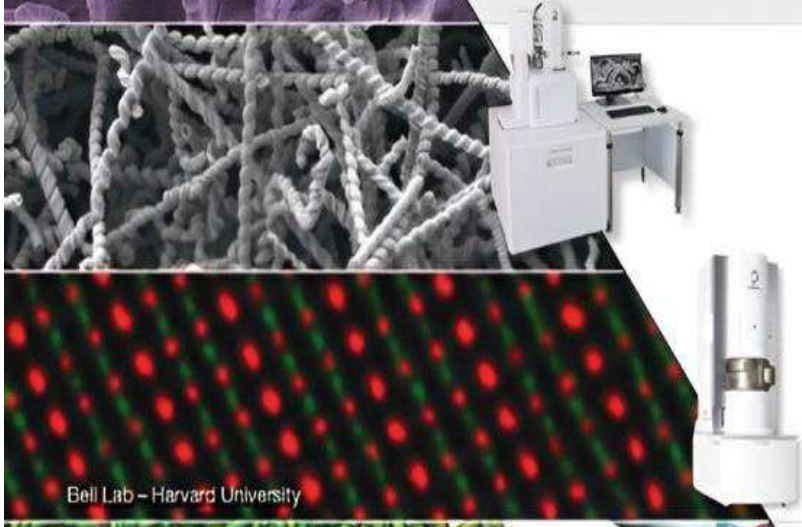

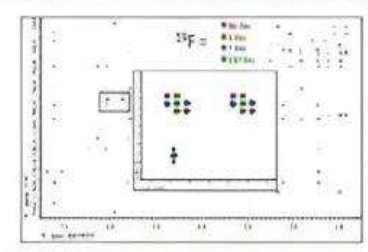

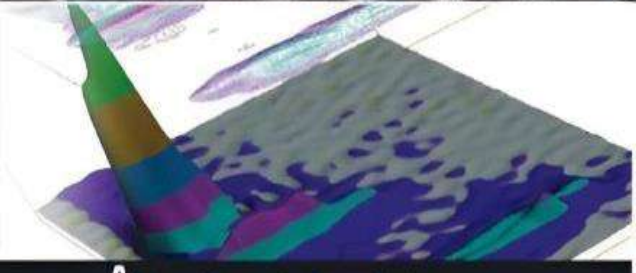

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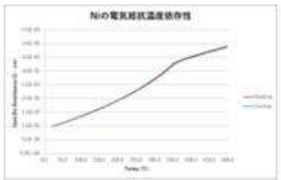

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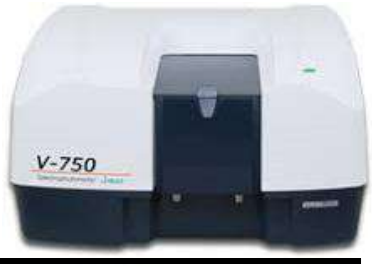

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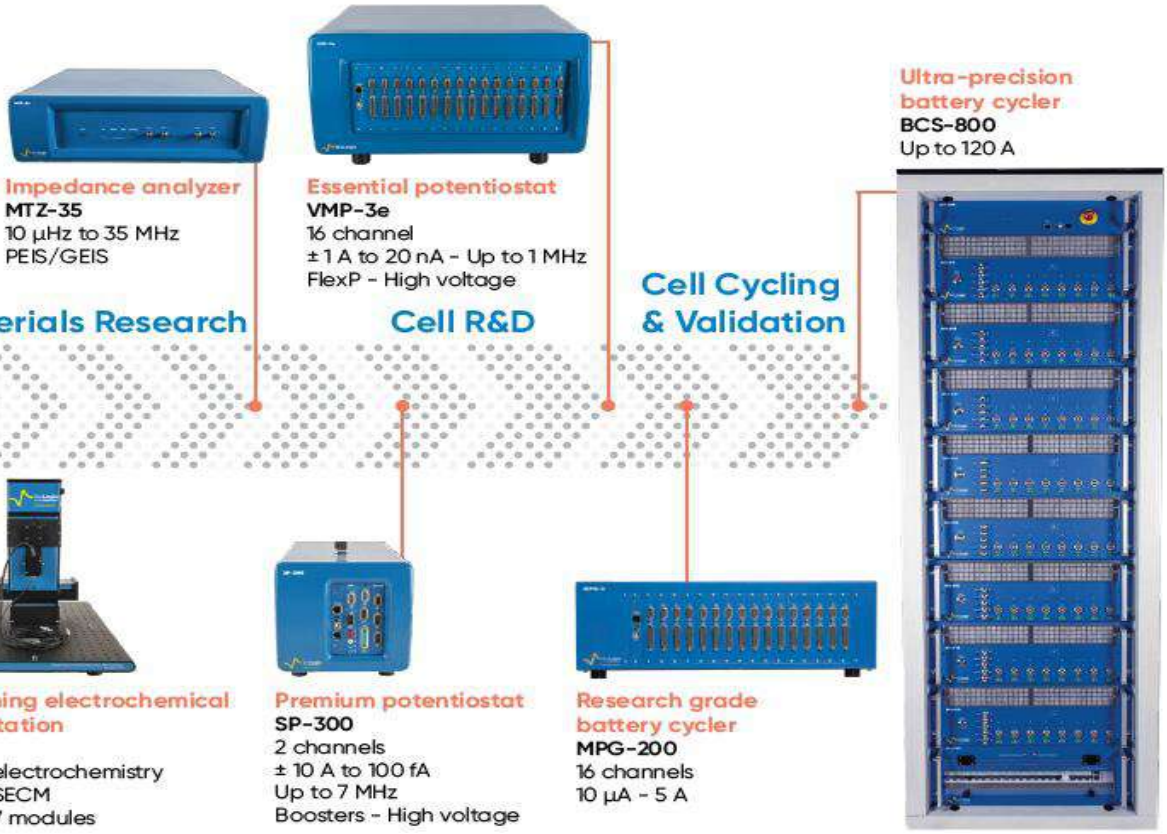

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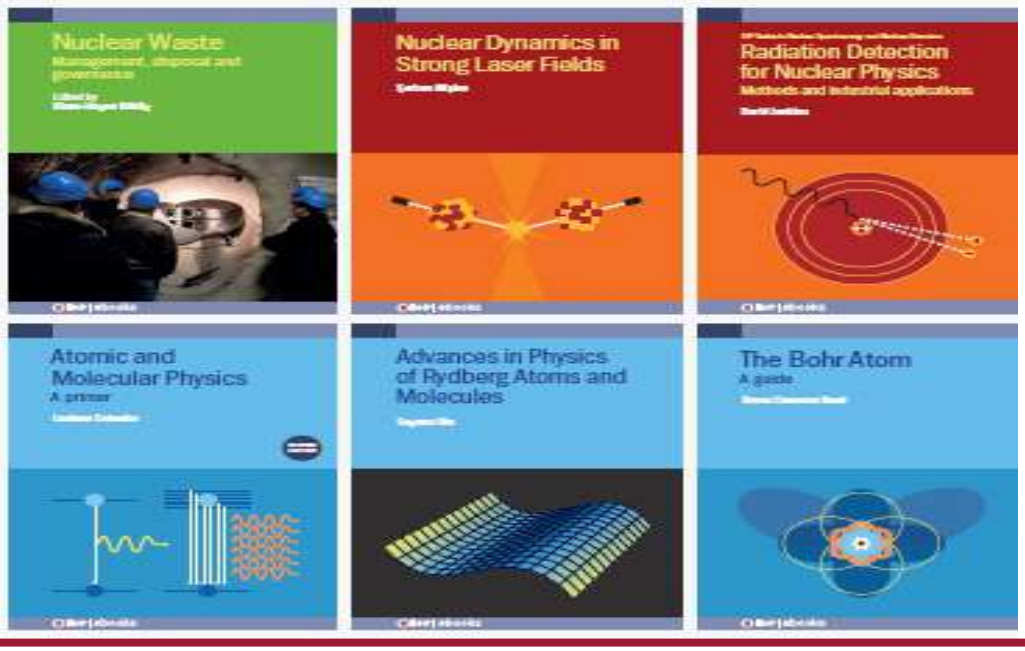

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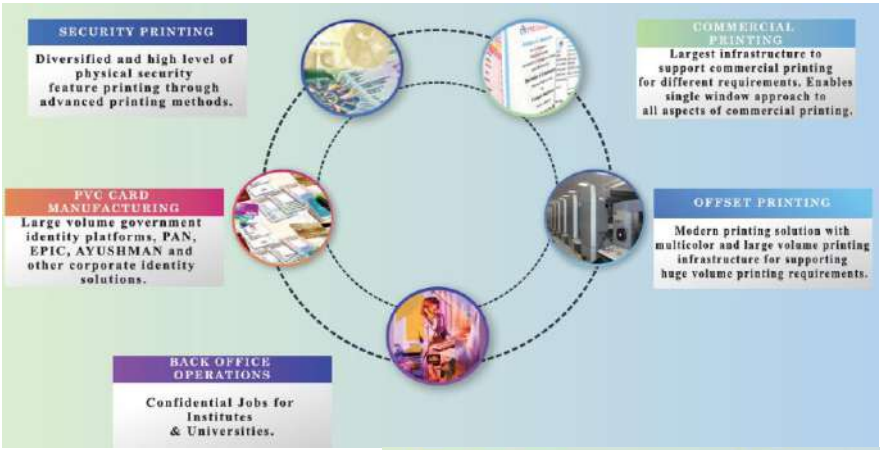

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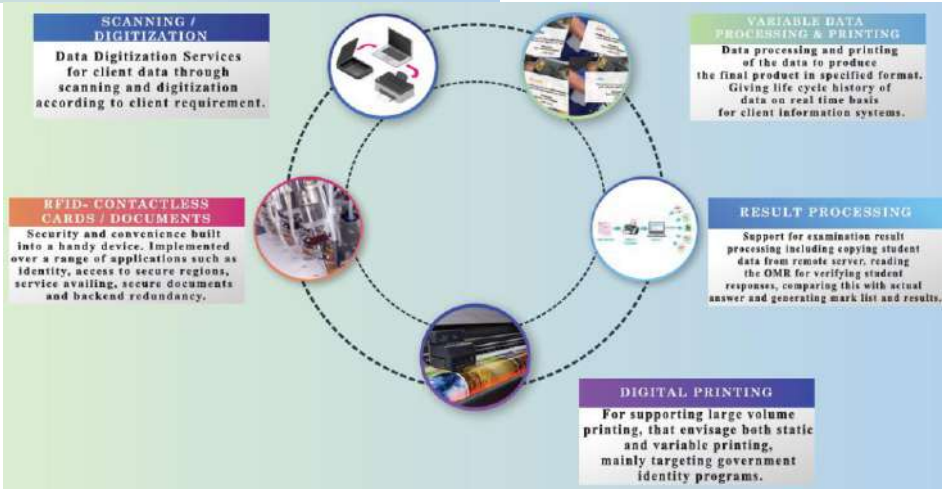

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