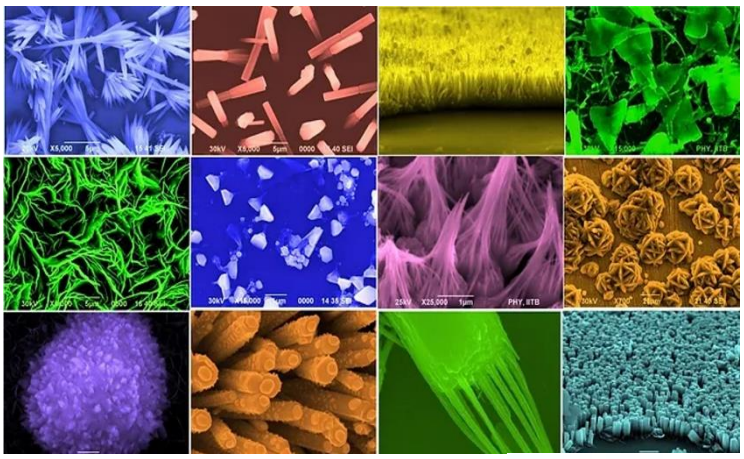
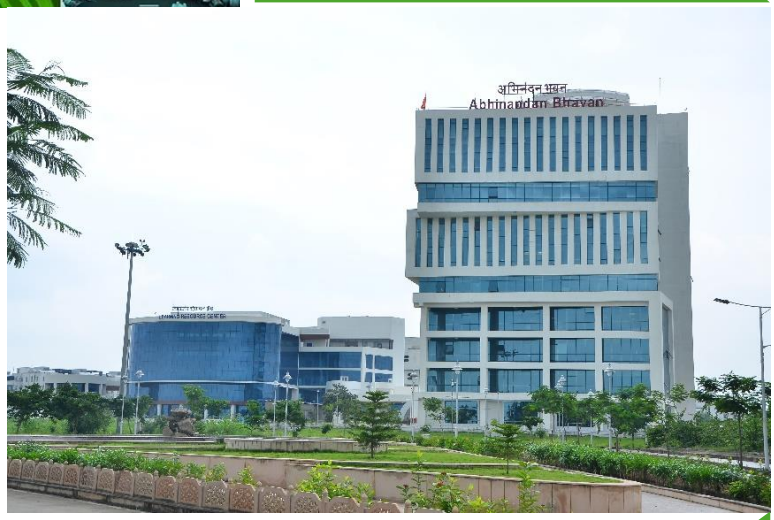
International Conference

On

ENERGY AND ENVIRONMENTAL MATERIALS

July 11-13, 2024





E_2M – 2024

ABSTRACT BOOK

Edited by: Dr. Ajay Kumar Kushwaha
Dr. Sunil Kumar
Department of Metallurgical Engineering and Materials Science
INDIAN INSTITUTE OF TECHNOLOGY INDORE

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International Conference

On

Energy and Environmental Materials

E_2M-2024

July 11-13, 2024

ABSTRACT BOOK

Organized by

Department of Metallurgy Engineering and Materials Science

INDIAN INSTITUTE OF TECHNOLOGY INDORE

In Association with

Department of Chemistry

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

Department of Physics

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MESSAGE FROM THE DIRECTOR

Professor Suhas S. Joshi *(FINAE, FNASI, FASME)*

Director

Indian Institute of Technology Indore

It gives me immense pleasure to invite all renowned scientists, academicians, and researchers from all over the globe to attend the International Conference on Energy and Environmental Materials (E_2M-2024) organized by Department of Metallurgical Engineering and Materials Science, IIT Indore.

E_2M-2024 aims to bring together experts, scholars, and researchers from various parts of the globe on a common platform to discuss the advances and challenges in energy materials and environment. It hopes to promote top-level research and globalize quality research, thus making presentations and discussions more competitive as well as focusing on the recent advancements in the field of materials science and engineering for future energy and environmental needs. Further, we hope that the conference will stimulate the development of new collaborations for undertaking innovative research, and open new avenues of research. I wish the participants will have an opportunity to listen to the distinguished experts and scientific discussions.

I wish the conference a great success.

Suhas S. Joshi

FOREWORD

Namaste, I extend a warm welcome to distinguished speakers, eminent participants, and members of the organizing committee in first International Conference on Energy and Environmental Materials (E_2M-2024). The objective of E_2M-2024 is to provide a platform to bring together academicians, scholars, and students of materials science and engineering to discuss and exchange innovative ideas. To understand the challenges related to energy and environmental materials. I hope this conference provides an exciting platform for new researchers to learn about the advancement in energy materials developments from the experts.

The conference designed to highlight the latest developments in *Synthesis & Characterization of Energy Materials, Energy Conversion & Storage, Green Hydrogen, Environmental Monitoring & Remediation, New Material for Energy Efficient Device*. Materials and energy are the two faces of the same coin which are closely associated with environmental impact. Therefore, advancement in materials and energy technologies are directly linked with creating a world with sustainable and environmentally friendly energy. To realize this concept, the sharing of knowledge become an important aspect, henceforth the idea of E_2M-2024 came into existence. The conference emphasizes promoting multidisciplinary research for finding sustainable energy solutions to real-world problems.

I would also like to express my deepest gratitude to all the speakers, participants, sponsors and organizers for your contribution to the conference.

With best wishes

Prof. Ajay Kumar Kushwaha

Convener, E_2M-2024

Associate Professor and HoD

Department of Metallurgical Engineering and Materials Science

Indian Institute of Technology Indore

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KEYNOTE SPEAKER

Prof. Satishchandra Ogale

Research Institute for Sustainable Energy, TCG-CREST, Kolkata, India and Indian Institute of Science Education and Research, Pune, INDIA

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Title: Designing Energy Materials and Interfaces for Superior Energy Harvesting and Storage

Abstract: Research on Clean and Renewable Energy Harvesting, Storage and Conservation has acquired CenterStage worldwide in view of the urgent need to mitigate the serious issues emanating from the unscrupulous use of polluting fuels and deteriorating environment. This research primarily embodies “Intelligent Materials Design, Innovation, and Engineering”. In addition to the key scientific aspects, affordability is also a very important criterion for this field if the laboratory advances are to meet the huge societal application scale. Therefore, much emphasis is being concurrently laid on the choice of earth abundant elements in such designs to the extent possible. Nanoscience has also made inroads into this energy arena in view of the tuneability it affords in realizing the desired functionality. Similarly materials dimensionality (0D, 2D, 3D and Mixed D) and associated uniquely different electronic states and properties has contributed immensely to the novelty of the designs. In this talk, I will outline this magical scenario with several examples in the domain of energy harvesting and storage derived from own research.

KEYNOTE SPEAKER

Dr. Tata Narasinga Rao

International Advanced Research Centre for Powder Metallurgy & New Materials (ARCI), Balapur P.O., Hyderabad-500005, INDIA

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Title: Translational Materials Research in Energy Storage Technologies crossing the valley of death

Abstract: The necessity of batteries is increasing due to the target set by the Government of India that 30% of the vehicles produced in India should be electric vehicles by 2030. Li-ion batteries are the key storage systems used in EVs due to their capability of storing high energy density and fast charging and discharging characteristics. While the demand is huge, India is totally dependent on imports of these Li-ion batteries. While government is encouraging establishment of Li-ion battery plants, the battery production in India is yet to pick-up. This is largely due to lack of indigenous technologies, which are essential to make the final batteries are cheaper or on par with the imported batteries. Material cost of a Li ion battery is ~ 60% of the overall cost of the Li-ion battery. While it difficult to compete in equipment manufacturing immediately, indigenous production of materials is essential and possible to reduce the import dependence of li-ion batteries. Alternatively, it is need of the hour to look into non-lithium based storage technologies (e.g., Na-ion batteries and supercapacitors) which are already being commercialized globally. In line with the above requirement and the ‘Atmanirbhar Bharat Abhiyan' or 'Self-Reliant India Mission', ARCI had developed indigenous technologies for the production of two key battery grade

electrode materials, Lithium Iron Phosphate (LFP) cathode and Lithium Titanate (LTO) anode powders for LIB. The unique know-how developed by ARCI involves solid state synthesis of LFP/LTO in a single step and these materials have been validated in coin cell and cylindrical cell configurations and they show promising electrochemical properties in terms of high discharge capacity, cyclic stability and excellent rate capability on par with the performances of commercial materials. Recently, LFP technology is transferred to one of the Indian companies, and the LTO technology is ready for transfer. ARCI has also embarked on the fields of supercapacitors (SC) and Na ion-batteries and developed graphene-like activated porous carbon by a low-cost chemical activation process from petroleum coke (petcoke) and Ni-Mn based layered metal oxide and Prussian blue analogue materials for these emerging storage technologies. ARCI has demonstrated, for the first time in India, a 1200F supercpacitor made from the above said petcoke, which is a requirement in EVs for regenerative breaking and enhancing the battery performance when used in hybrid mode. Fundamental challenges in technology development, addressing those challenges and technology commercization aspects will be discussed.

KEYNOTE SPEAKER

Prof. Praveen C Ramamurthy

Indian Institute of Science, Bengaluru, INDIA

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Title: Organic Electronics: Molecules to Devices

Abstract: The critical aspect of the sensor lies in tailoring molecules to enhance selectivity towards specific analytes. A design approach is employed that considers charge distribution, size, geometric shape, and strategically placed functional groups to interact with the target analyte. Molecular architectures have been successfully designed to sense a range of analytes, including volatile organic compounds, nitrates, urea, tetracycline, metal ions (lead, mercury, iron, magnesium, and chromium), and bio-relevant substances such as E. coli, dopamine, sodium, and potassium. Understanding electronic interactions at the molecular level has enabled the precise development of organic sensors.

KEYNOTE SPEAKER

Prof. Manoj Kumar Ram

Poly-Materials App, LLC, USA

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Title: Design, Fabrication and Modern Applications of Sustainable High Power and High Energy-Based Supercapacitor

Abstract: A supercapacitor is an electrochemical device that stores and releases electricity like a battery, but the biggest advantage is it can be charged in a few seconds instead of hours like a battery. The supercapacitor can accumulate a full charge in seconds and subsequently deliver the burst of energy needed for starting a mass in motion, accelerating vehicles, and engaging power-take-off. Generally, supercapacitors are having low energy

density, but recent work has been focused on finding new hybrid material with increased surface area to enhance the energy density. Supercapacitors have numerous applications in portable consumer electronics, medical devices, appliances, and transportation technologies like electric hybrid vehicles, aerospace, and defense sectors. Successful supercapacitors can either replace automobile batteries or work in combination with them. Dr. Ram has been successful in developing high power and high energy-based supercapacitor using conducting polymer, carbon nanotube, graphene, dichalcogenide, and various nanomaterials. Dr. Ram has extensive experience in transforming the use of large surface area materials into supercapacitors and conducted research on conducting material using 2D/3D dichalcogenide, Mxene, graphene, and several polymeric composite materials. The properly designed synthesis of graphene or graphene oxide aerogel containing conducting polymer-dichalcogenide as electrode materials have shown high power and energy density, cycle number, and lifetime. The issues governing the performance of high energy density-based supercapacitors is dependent on types of electrode materials and fabrication techniques. The nanostructure effect used in the technology is unique and enabled to obtaining high specific capacitance-based supercapacitors. The novel technology promotes a synergistic interaction between nanocomposite electrodes and supercapacitors based on power density, energy density, and cyclability. Dr. Ram has used supercapacitor in thermal management of energy storage devices, power buffer and control system toolkit for DC systems which will be discussed at length.

KEYNOTE SPEAKER

Prof. Krishanu Biswas

Indian Institute of Technology Kanpur, INDIA

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Title: Multicomponent Quasicrystal as Template for 2D Multicomponent Alloys: Design, Microstructure and Applications

Abstract: Atomically thin metallic alloys have been considered important due to their prospective applications as interconnects/contacts in two-dimensional (2D) circuits, sensors, and catalysts, among others. The presence of weak interlayer interactions and in-plane covalent character in quasicrystals facilitate the synthesis of the two-dimensional (2D) multicomponent alloy by chemical exfoliation. I shall discuss large-scale formation of atomically thin 2D sheets by chemical exfoliation from the multicomponent Al70Co10Fe5Ni10Cu5 decagonal quasicrystalline alloy. The exfoliated ultra-thin two-dimensional multicomponent alloy (2D-QCs) exhibited an excellent OER/HER bifunctional catalytic activity in alkaline electrolyte, i.e., alkaline water splitting. The active surface area of the 2D sheets also provides a large number of active sites for the bifunctional catalysis of the oxygen and hydrogen evolution reactions. These 2D atomically thin sheets exhibit superior catalytic performance to their bulk counterparts. Molecular dynamics and DFT simulations of the 2D alloy support the experimental interpretation in terms of structural stability and catalytic properties. Synthesis of this type of new class 2D material provides a promising approach for the design and exploration of non-precious transition metal-based electrocatalysts for clean energy production. In addition, these 2D –QCs can be integrated with 2D MoS2 and WS2 to produce heterostructures for gas sensing applications. We shall discuss the devices and their efficacy for various gas sensing applications; H2, NO2 etc. The decoration of chemically exfoliated two-dimensional quasicrystals (2D-QCs) nanosheets on WS 2 flakes dramatically boosts the sensor response towards NO2 gas. In addition, the mechanism of gas sensing has been corroborated by deducing the interaction of NO2 molecules with QC nanosheet using density functional theory (DFT).

KEYNOTE SPEAKER

Prof. Sri Sivakumar

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Title: Development of Nanocatalysts for Cleaner Fuel

Abstract: Catalysis has significant impact on the quality of life and overall economic well being of the society. Four of the world's most successful industrial sectors i.e. petroleum, chemicals production (e.g. textiles, pharmaceutical, paper etc.), energy generation and food production rely heavily on catalysis. One of important challenge often faced in the area of catalysis is the development of highly active, selective, robust, low-cost and environmentally benign catalytic systems. A large surface-to-volume ratio is an essential prerequisite for an effective catalyst. Making catalysts in the form of nanoparticles provides a good way to achieve this aim. Recently, there is a large interest in the development of nanocatalysts. However, they face major challenges of sintering, leaching and deactivation during preparation or their utilization in catalytic reactions at high temperature. Further, modulating the metal-support interaction plays a major role in the determining the activity/mechanism of reaction. In this regard, I will focus on two approaches for the development of nanocatalysts. First part of my talk will focus on the development of sinter-resistant metal nanoparticles-loaded hollow zeolites for biomass conversion. The second part of my talk will address the development of ultrasmall bi/trimetallic nanocatalysts for hydrodesulfurization reaction.

KEYNOTE SPEAKER

Prof. Kothandaraman Ramanuja

Department of Chemistry, Indian Institute of Technology Madras, INDIA

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Title: Faradaic and Non-Faradaic Contribution to the Capacity of Novel Organic Cathode of Li-ion Battery

Abstract: A novel organic compound (trinapthylene-hexaone (TNH) based) with multi-redox sites was explored for energy storage in half-cell mode against Li. Notably, the Li//TNH cell exhibited a first cycle capacity of 1120 mAh g-1, maintaining nearly 510 mAh g-1 at 0.15 A g-1 over 100 cycles. The obtained capacity is way higher than the expected theoretical capacity of 343 mAh based on the redox nature of the molecule. The molecule undergoes an in-situ polymerization via peroxo linkage formation, leading to a 2D layered material. The additional capacity is hypothesized due to EDLC-type capacitance arising due to the polarization of pi-bonds along with the intercalation of Li^{+}.

KEYNOTE SPEAKER

Prof. Abir De Sarkar

Institute of Nano Science and Technology, Mohali, Punjab-140306, INDIA

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Title: DFT perspectives on valleytronics, piezoelectricity and flexible piezo-spintronics in selected functional 2D materials

Abstract: Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN2 monolayers exhibit valleytronic properties complementary to that in single-layer MoS2, while the merger of spintronic with valleytronic properties is observed in h-NbN and h-TaN monolayers. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS2/BP and MoSSe/BP vdWHs. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated together with the enhanced electrical conductivity arising from nearly free electron gas (NFEF) states. Origin of strain tunability in flat valence band and ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) will also be covered. The conflux of tunable Rashba effect and piezoelectricity observed in flexible MgTe, CdTe, and ZnTe monolayers signify its super high prospects for self-powered flexible-piezo-spintronics. The nature of metal-semiconductor contacts plays a crucial role in determining device performance. Non-resistive/Ohmic contact is found to occur in graphene/MgS vdWH, rendering it ideal for charge injection.

KEYNOTE SPEAKER

Prof. Pratima Agarwal

Department of Physics, Indian Institute of Technology Guwahati, INDIA

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Title: DFT Challenges in Dopant free c-Si heterojunction solar cells

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 world. 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). 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 the efficiency of MoOx/c-Si(n) solar cells will also be covered in this talk.

KEYNOTE SPEAKER

Prof. Ajay Kumar Mishra

University of Western Cape, Capetown, SOUTH AFRICA

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Title: Nano-engineered Materials for Wastewater Applications

Abstract: Nano-engineered materials have been used extensively for a variety of applications. Environmental pollution raised bigger concerns on the discharge of textile waste. Nanotechnology is fast growing on research and bringing sustainable solution in the minimization of the waste. The minimization of the risk of risk and health hazards with the development of industry, environmental pollution and energy shortages have raised awareness of a potential global crisis. Nano-engineered materials can be better solution in finding solution of environmental sustainability more specific to the textile waste remediation due to the large surface areas, diverse morphologies, abundant surface states, and easy device modeling. It is a challenge of great importance to identify and design nano-engineered materials that are efficient, stable, and abundant for the remediation of textile waste. The current talk will be focused on the recent advancement and applications of nano-engineered materials for wastewater applications.

KEYNOTE SPEAKER

Prof. Ajeet K Kaushik

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Title: Sustainable sensing for health and environmental management

Abstract: Presently nano-enabled smart sensing technology interfaced with other tools like the Internet of Things (IoT) and artificial intelligence (AI) are emerging significantly for efficient disease/problem management, even at point-of-care (POC) applications. Such systems are on the track of transformative research according to the goals of 5th and 6th-generation technology to track and manage health and the environment according to the goals of sustainability. In this direction, we are exploring electro-active electrodes for efficient bio (biosensor) and

chemical sensing with the capability of POC applications. Our developed sensing prototypes are well interfaced with a miniaturized potentiostat (M-P) which can be operated using a smartphone. Recently, to develop efficient infectious disease management, we have developed miniaturized nano-enabled biosensing systems to detect targeted biomarkers for diagnostics of infectious diseases like COVID-19 infection. Further, electrochemical sensing is explored for efficient sensing of water pollutants (heavy metals) and forever chemicals like microplastics selectively and at a very low level (ppm to ppb). We believe our developed biosensing and chemical sensing systems supported by AI and IoT approaches can be a potential tool for personalized health management and environment surveillance. The outcomes of these sensing technologies can be utilized for policy and timely decision-making efforts.

KEYNOTE SPEAKER

Dr. Jaspreet Dhau

Molekule Inc.,Tampa,Florida, USA

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Title: Fluorine-Free Firefighting Foam: A Sustainable and Eco-friendly Solution for Extinguishing Class-B Fires

Abstract: Aqueous film-forming foams (AFFF) have numerous applications in the industry and defense sectors. AFFFs are used predominantly as firefighting retardants that actively extinguish hydrocarbon fires. AFFFs are known for their ability to extinguish fires rapidly and effectively. Until now, the AFFFs made of fluorinated surfactants have demonstrated superior fire extinction performance capabilities because of the co-existence of hydrophobic and lipophobic head groups. The latter properties create a thin film that seals off the surface of burning hydrocarbon fuels. However, the inherent toxicity and poor biodegradability of the fluorochemicals, including perfluoroalkyl carbonates (PFAC), perfluoroalkyl sulfonates (PFOS), and fluorotelomer sulfonates (FTS), are a significant threat to the environment. Thus, a fluorine-free disruptive technology is urgently needed. Fluorine-free foams in the market do not produce thin-film blankets over the burning fuel and exhibit faster foam blanket degradation when compared to AFFFs. We have developed a fluorine-free ionic liquid-based firefighting foam for class B fuels such as jet fuel and gasoline (petrol). The spreading coefficient of the developed formulation is in the 2-3 mN/m range and has a better drainage time and seawater compatibility than the AFFF. The firefighting performance was evaluated on heptane, cyclohexane, and alcohol-free gasoline. The developed formulation forms a self-healing film over the burning fuel like the one observed in AFFF. The firefighting performance was evaluated on a large-scale fire (28 ft 2) test on jet fuel and gasoline fire. The developed formulation passed the MIL specifications on jet fuel and gasoline. The fire extinguishing time on a 28 ft 2 fire was 28 s sand 50 s on jet fuel and gasoline, respectively. The burn-back resistance time was 316 s on jet fuel and 418 s on gasoline.

KEYNOTE SPEAKER

Dr. Harish C. Barshilia

CSIR NAL, Bangalore, INDIA

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Title: Towards facile and eco-friendly renewable energy solutions: Recent advances in photo-thermal conversion coating technologies

Abstract: Solar radiation is converted into thermal energy and subsequently to electrical energy by solar thermal concentrating systems. Concentrated solar power (CSP) systems use solar absorbers to convert sunlight to thermal electric power. The solar collectors are coated with absorber coatings with high solar absorptance and low thermal emittance. Spectrally selective coatings, which are stable up to temperatures £400°C (in air and vacuum), have been developed in the past. However, in order to increase the efficiency of solar thermal power plants, solar selective coatings with high thermal stability are required. In recent years, great advances have been made in the field of nanostructured solar selective coatings with high solar absorptance and low thermal emittance at higher temperatures (T > 450oC). Amongst these, nanostructured transition metal nitride, oxide and carbide based tandem absorbers have emerged as novel high temperature solar selective coatings, which can be used for solar thermal power plants for electricity generation. Research is currently underway to increase the thermal stability of the coatings and subsequently to improve the efficiency of the solar thermal power plants. This talk will present an overview of the sputter deposited mid- to high-temperature solar selective coatings used for solar thermal applications. The presentation will also describe in detail our efforts in commercializing an absorber coating technology for domestic hot water applications.

KEYNOTE SPEAKER

Dr. Mohit Sharma

*Institute of Materials Research and Engineering, A*STAR, SINGAPORE*

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Title: High-throughput and Lightweight Composites for New-gen Aero-structure and Advanced Air Mobility (AAM).

Abstract: Advancement in composite technology is persistently implemented for industrial utilization e.g., lightweight structural part for aerospace applications. Recently, agencies are promoting usage of futuristic sustainable materials technologies to address the abrupt climate change and incremental energy demands. Fiber reinforced polymer composites, characteristically supports lightweight effectiveness. Continuous fibre reinforced thermoplastics (CFRTP) are strategically preferred due to their high specific strength, dimensional stability, elevated thermomechanical performance, recyclability to some extent and molding capabilities to conform intricate structure. Composites researcher and manufacturers are unceasingly exploring for efficient upscale processing technologies and innovative deployment methods for lightweight structural applications e.g., primary aviation structure and structure for electric powered vertical takeoff and landing eVTOL. The challenges coupled

with composite sustainability are landfill disposal, limited choice of commercially available bio compatible polymer/reinforcements and lack of recycled technologies to reused composites at end-of-life. Few allied R&D initiatives are consistently implemented to overcome the issues. For example, by utilizing thermoplastic-based composites manufacturing process, tailored fiber placement, utilization of innovative recycling techniques and compelling designs. The presentation will highlight the sustainable and lightweight composites for new-gen aero-structure and energy sector; AAM-eVTOL, Hydrogen transportation/storage, EVs techs.

INVITED TALKS

INVITED SPEAKER

Dr. Rohini Kitture

Wiley-VCH

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Title: Mastering Research Publishing: Insights from Editor's Desk

Abstract: Publishing research is crucial in academia as it facilitates knowledge sharing and progress in various fields. However, the intricacies of the publishing process often pose challenges for researchers. This presentation aims to provide valuable insights from an experienced editor to enhance the effectiveness of research publications.

The session will begin with an overview of Wiley's journals, offering attendees a range of potential venues for their research submissions. It will then delve into the detailed editorial review process, covering initial assessments and peer reviews, and clarifying reasons for desk rejections. By gaining a clearer understanding of these processes, attendees will be better equipped to avoid common pitfalls, thereby increasing the likelihood of their submissions being successful. Drawing on practical tips from editors, this presentation aims to empower researchers to improve their publication outcomes and maximize the impact of their work.

INVITED SPEAKER

Dr. Suman Singh

CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Chandigarh, INDIA

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Title: Materials engineering for energy harvesting application

Abstract: The depletion of fossil fuels, environmental pollution, and climate change highlight the urgency for efficient energy harvesting technologies. Water splitting is key, converting renewable energy into hydrogen gas through electrolysis powered by solar or wind energy. Water splitting can be performed using various ways like electrochemical electrolysis, electrolysis at room temperature without using external energy, biological water splitting. This generates storable, clean energy without greenhouse gas emissions. Material engineering advances the field by creating catalysts and electrodes that improve water-splitting efficiency, driving sustainable energy solutions. In water splitting, novel materials are crucial for developing efficient catalysts that can drive the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) efficiently and sustainably. The design and optimisation of catalysts, including transition metal oxides, metal chalcogenides, and carbon-based materials, are imperative for enhancing the kinetics and stability of water-splitting processes, thereby facilitating the generation of clean hydrogen fuel. Our team is working towards designing various catalysts like GCN, MXenes, MBenes, metal oxides etc and electrodes of various materials and designs.

INVITED SPEAKER

Prof. Tokeer Ahmad

Jamia Millia Islamia, New Delhi, INDIA

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Title: Scalable Green Hydrogen Production using Photo- and Electro-Chemical Water Splitting

Abstract: Semiconductor based photochemical and photoelectrochemical water splitting is an ultimate source of hydrogen generation as renewable green energy for tackling the ongoing fuel crisis. g-C3N4 is an ideal candidate for overall water splitting as a result of the excellent alignment of its band edges with water redox potentials. However, a single catalyst with a limited number of active sites does not exhibit significant photo/electrocatalytic activity for hydrogen production. Therefore, we have developed the semiconductor heterostructures of g-C3N4 with CuFe2O4 , Cu2O, CdSe, CdS and MoS2 NPs and QDs as the highly efficient nanocatalysts for enhanced hydrogen evolution reactions. The monophasic heterostructures have been designed in different weight ratios with fairly uniform distribution of nearly spherical particles and high specific surface area which creates an interfacial charge transfer between two semiconductors. As prepared heterostructures showed significant hydrogen evolution which is evident by observing high apparent quantum yield, low onset potential, lower overpotential and high electrochemical active surface area that will be presented in detail.

INVITED SPEAKER

Prof. Dipankar Mandal

Institute of Nano Science and Technology, Mohali, INDIA

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Title: A New Era of Machine Learning integrated Cognitive Nanogenerators

Abstract: Achieving seamless human-machine interaction relies on the pivotal role of machines in recognizing and responding to human emotions. However, the integration of emotions into robotics presents challenges, given the intricate and subjective nature of human emotional experiences. To propel the development of cognitive robotics capable of perceiving and responding to human emotions, there is a pressing need for advanced emotional sensors driven by machine learning algorithms. By seamlessly integrating advanced machine learning algorithms with the piezoelectric nanogenerators, our approach endeavours to build a robust AI model capable of accurately identifying and classifying a diverse spectrum of emotions. Experimental results attest to the feasibility and efficacy of our integrated machine learning approach in accurately identifying and distinguishing between different emotions based on physiological activities for instance voice analysis component extracts nuanced features from speech patterns, encompassing pitch, tone, and intonation, while arterial pulse analysis captures temporal variations linked to emotional responses. This integrated methodology enhances emotion recognition capabilities, providing a holistic comprehension of the user's emotional state and exhibits promising applications across various domains, including human-computer interaction, healthcare, and affective computing.

INVITED SPEAKER

Dr. A S Prakash

CSIR-Central Electrochemical Research Institute, Chennai, INDIA

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Title: Advancements in Sodium-ion Battery Technology: Novel Cathode Materials to Full-Cell Systems

Abstract: Sodium-ion batteries (SIBs) have emerged as promising alternatives to lithium-ion batteries, offering potential advantages in resource abundance and cost-effectiveness. The pursuit of high-performance cathode and anode materials compatible with sodium-ion insertion/extraction processes has spurred innovation, showcasing notable potential in materials such as layered transition metal oxides, polyanionic compounds and hard carbons. This talk focus on the design and development of new cathode materials compositions and hard carbon production for sodium-ion battery demonstration. Further, ongoing developments in electrolytes, with a focus on enhancing sodium-ion transport and stability, coupled with novel cell configurations and sodium-ion full-cell systems, aim to overcome challenges associated with capacity and cycle life. Despite this progress, several challenges persist, including the quest for achieving high energy density, a comprehensive understanding of and effective mitigation strategies for electrode degradation mechanisms, and the optimization of large-scale manufacturing processes. This work emphasizes the ongoing efforts and potential breakthroughs in sodium-ion battery technology.

INVITED SPEAKER

Prof. Anantharaj Sengeni

IIT Kanpur, INDIA

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Title: Electrocatalysts are worthless without accurate and precise testing!

Abstract: The rapid surge in reports on energy conversion electrocatalytic reactions, spanning OER, ORR, HER, CO2RR, NOxRR, NRR, AOR, 2e- WOR, etc., with poor precision and accuracy in testing is alarming. Daily, hundreds claim breakthroughs with new electrocatalysts. However, a grave concern arises from the unwitting errors in electrochemical screening, often conducted by non-experts. This compromises the reliability of reported figures of merit regarding activity, stability, and selectivity. The sheer volume of such reports is staggering and warrants immediate attention. This presentation will highlight prevalent screening errors and propose simple yet crucial practices, supported by fundamental electrochemistry principles, to mitigate them.

INVITED SPEAKER

Prof. Raj Kumar Gupta

BITS Pilani, INDIA

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Title: Ultrathin films of graphene system and applications

Abstract: Graphene is considered to be a wonder material which promises numerous novel applications. When spread onto a two-dimensional surface, graphene yields a remarkable increase in surface-to-volume ratio, amplifying surface activities manifold. The abundance of π-electrons on the basal plane of graphene enhances bio-molecular interactions through π-π stacking, bolstering its potential for bio-sensing applications. Additionally, graphene exhibits superior biocompatibility compared to other nanomaterials, further underscoring its suitability for such applications. In this talk, I will discuss the fundamentals of ultrathin films of monolayer, bilayer and twisted bilayer graphene at different interfaces. The bio-sensing and potential of 3D graphene for energy storage will also be discussed.

INVITED SPEAKER

Prof. Babasaheb R. Sankapal

Visvesvaraya National Institute of Technology, Nagpur, INDIA

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Title: 'Material Mutualism' -State of art for energy conversion & storage

Abstract: Energy crises is main issue that whole world is facing. In this regards energy conversion through photovoltaics and energy storage through supercapacitor can play a major role. If solar cells are colorful and attractive and supercapacitors are completely solid-state and flexible then they will have added advantage. Hence, start of art will be demonstrated through simple and low-cost chemical routes towards 'Material mutualism' concept for energy conversion by means of dye sensitized solar cell and energy storage through supercapacitor applications. Hence, the development of colorful solar cells through the concept of dye sensitized solar cell will be explored using chemically deposited ZnO with wide spread dyes. Energy storage process rely on two distinct mechanisms, electric double layer capacitance (EDLC) and pseudo capacitance but EDLC possess high stability but suffers through low capacitance; on contrary, pseudo has high capacitance but suffers through low stability. Mostly, EDLC uses carbon-based materials whereas pseudo uses metal oxides, chalcogenides and polymers. In hybrid, it can be possible to integrate both materials which takes advantages of both mechanisms through 'material mutualism' concept leading to high capacitance along with high stability which will be demonstrated towards flexible solid-state supercapacitor applications.

INVITED SPEAKER

Prof. Rohit Mehra

Dr. B R Ambedkar National Institute of Technology, Jalandhar, INDIA

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Title: Estimation of Environmental Radioactivity levels in Air, Water and Soil for the Assessment of Health Risks to the Human Population

Abstract: Solid State Nuclear Track Detectors have existed on earth, moon and other solidified species (e.g. meteorites) due to cooling down of insulation material in space in the form of minerals (mica, quartz, etc.). Passive radon monitoring using SSNTDs was initiated by three American scientists namely, R. L. Fleisher , R. M. Walker and P. B. Price (1965a, 1965b) and ultimately, patented by Becker (1969, 1970). Typical organic materials used for radon dosimetry are made of bisphenol-A polycarbonate (Lexan, Makrofol), cellulose nitrate (LR-115, CN-85) and polyallyl di-glycol carbonate (PADC or CR-39). Bare mode Single cup diffusion chamber and Twin cup dosimeters for estimation of indoor 222Rn/220Rn concentrations in air have become obsolete today owing to their several drawbacks such as unwanted interferences from progeny, atmospheric turbulence effects and negative 220Rn concentrations. To overcome these technical limitations, a new pin-hole based 222Rn/220Rn discriminating dosimeter with single entry face was designed by Sahoo et al. (2013). It is one of the most versatile devices in mixed field environment of 222Rn and 220Rn in air. Further the Radium, Thorium and Potassium in natural soil also contribute to the radiation doses to the human population. The use of Gamma Ray Spectroscopy is a very accurate method for the estimation of Radium, Thorium and Potassium concentration in soils and thereby estimating the Annual Doses to the human population.

Keeping toxic nature of uranium in mind, a survey of groundwater consumed by inhabitants is also conducted. A comprehensive analysis of uranium burden in a human adult is done by determining natural uranium concentration. The annual effective doses are computed both age-wise and organ-wise. Internal organ/tissue doses give an insight of radioactive targets which may act as bio-indicators of uranium toxicity in human body. The transfer coefficients of different body organs are calculated using hair compartment model of uranium and compared with those obtained using ICRP's biokinetic model. The results of the study not only fulfil an environmental cause but also, a social cause to identify regions of concern, regions of negligible uranium concentrations and those for which data is currently unavailable, but nevertheless, may become prospective uranium sites and should be investigated. Numerous dosimetric, radiobiological and epidemiological studies have been carried out by many researchers to establish guideline values for various radionuclides, identify regions of concern develop biokinetic models, and project national baseline values. This study summarizes some important studies conducted in India by our group at NIT Jalandhar.

4INVITED SPEAKER

Dr. Jeoti Kanta Mohapatra

Molekule Inc. USA

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Title: Emerging Applications of Magnetic Nanowires

Abstract: When a piece of ferromagnetic material reduces its size to nanometer scale, its magnetic ordering will be altered and its magnetic properties will be consequently changed, because ferromagnetism is a size-sensitive physical phenomenon related to electronic exchange, magnetocrystalline anisotropy, and magnetostatic interactions, which are all effected by geometric parameters of the material at nanometer scale. In this talk, we will discuss the scientific and technological problems of ferromagnetic nanowires, from their synthesis strategies to the geometric confinement in 1D that give rise to new magnetic effects, including the size, surface, and shape effects on magnetic properties, particularly on magnetic anisotropy and coercivity. Various ferromagnetic materials are studied, including metals, alloys and ceramics. These low-dimensional nanoscale magnets can find broad applications in green energy, information storage, and biomedicine. On the other hand, low-dimensional objects can be used as building blocks to assemble new types of advanced magnetic structures.

INVITED SPEAKER

Prof. Prem Pal

IIT Hyderabad, INDIA

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Title: Simple and cost effective silicon surface texturing methods for solar cell

Abstract: Silicon-based solar cells dominate the modern solar cell market. Surface texturization is one of the popular methods to reduce optical reflections from silicon surface to enhance the efficiency of the solar cell. {100} oriented silicon wafers are primarily used in crystalline silicon solar cell. Wet anisotropic etching is most extensively used in surface texturing of silicon because of its high throughput and lower cost. Potassium hydroxide (KOH) and tetramethylammonium hydroxide (TMAH) are two most widely etchants for the surface texturing of silicon. In these two etchants, TMAH is preferred when complementary metal-oxide semiconductor (CMOS) process compatibility and very high etch selectivity between silicon and silicon dioxide are the major concerns. Surface texturing using low concentration TMAH and KOH (< 0.5%) results in high surface roughness. This is a remarkable observation that can be applied in solar cell industries to minimize the reflection from silicon front surface. In the present research, we present a cost effective methods for the surface texturing of Si{100} in extremely low concetration KOH and TMAH. The main objective of this study is to achieve an optimized etched surface topography at lowest possible etching concentration and etching time to minimize the reflectance for application in solar cells. Very low average solar weighted reflectance (Rsw) is obtained on the samples etched in 0.5 TMAH and 0.5% KOH. In comparison to the previous studies, reflectance values obtained in this work are quite promising for large area surface texturing of silicon solar cell panels for enhancement in their efficiency.

Moreover, the use of very low concentration alkaline solution minimizes the chemical waste. This also helps in adopting the technique for fabricating anti-reflective silicon surfaces at large scale.

INVITED SPEAKER

Prof. Biswajit Mondal

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Title: Waste to Wealth: Electrochemical Upgradation of Biomass and Waste Plastic to Valuables with the Co-production of Hydrogen

Abstract: The electrochemical oxidation of lignocellulose and plastic waste to value-added chemicals represents a promising approach to addressing critical environmental challenges. However, selective oxidation to specific products at higher current densities remains challenging. Oxidative cleavage of C(OH)-C moiety of various lignocellulose and mixed biodegradable and bio-nondegradable plastics can be a tackling strategy. In this study, we demonstrated electrochemical oxidation with a monometallic Ni(O)O-H for cellulose-based biomass, a series of lignin-based model complexes, lignin-derived secondary alcohols (KA oil), mixed plastic wastes based on the O-H bond dissociation energy of the catalyst. The catalyst performs exceptionally well for the selective oxidation of cellulose and lignin-based model complexes like HMF and PED at 100 mA cm-2 with 87 – 100 % yield. KA oil oxidation to adipic acid with 54% yield was observed at constant current electrolysis of 20 mA cm-2. Also, plastic waste precursors having C(OH)-C bond oxidation were investigated using the same catalyst to selectively obtain the oxidized product. This was further applied to mixed plastic waste upgradation to generate formate and acetate with Faradaic efficiency of 66% and 74%, respectively, and 100% yield in terephthalic acid along with the co-production of hydrogen.

INVITED SPEAKER

Prof. Sandan Kumar Sharma

IIT Patna, INDIA

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Title: Tribological Performance of Transparent YAG Ceramics: A Study for Energy-Efficient Optical Applications

Abstract: Transparent ceramics with improved tribological properties are essential for protective optical elements like windows and domes. Yttrium Aluminum Garnet (YAG, Y 3 Al 5 O 12) ceramics, prepared via reaction sintering of high-purity Al 2 O 3 and Y 2 O 3 powders, exhibit these properties. Hardness and fracture toughness were measured using indentation. This study examines the friction and wear behavior of YAG ceramics in unlubricated sliding against chrome steel (100Cr6) balls at loads of 5, 10, and 15 N. The coefficient of friction (COF) ranged from 0.423 to 0.693, and the specific wear rate ranged from 9.44 x 10 -5 to 1.82 x 10 -4 mm 3 /Nm. At lower loads, tribochemical layer formation via a wedge mechanism reduced the COF. Increasing the load to

10 N stabilised the iron oxide layer, maintaining a consistent COF. At 15 N, the COF increased due to YAG microchips formed by contact stress and material removal. Further, Raman analysis confirmed oxide layer formation on the wear surfaces.

INVITED SPEAKER

Dr. Aayushi Arora

Royal Society of Chemistry

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Title: RSC: Integrating Chemical Sciences Community and Beyond

Abstract: Royal Society of Chemistry (RSC) is one of the leading society publishers serving the community since mid 1800s delivering impactful, accessible content in our journals, books and data products, and an excellent customer experience. The portfolio comprises of more than 60 journals which encompasses core chemistry, energy and environmental sciences, engineering and interface, pharmacy, analytical chemistry and several others integrated together. We work towards growing and supporting our membership to reflect the diversity of the chemical sciences. We work with communities to offer an excellent chemistry education to all, driving greater diversity and improving skills in the chemical sciences. We aim to increase the diversity of people choosing and fulfilling their potential in the chemical sciences for a truly inclusive community. The presentation will focus on the initiatives that the Royal Society of Chemistry undertakes as a society publisher to enable change in chemical science education and practice to ensure a diverse and skilled workforce. We also endeavour to provide the opportunities and tools for the chemical science community to network, create and exchange knowledge, adapt and thrive. It would also cover information on energy and environmental sciences portfolio which includes the journals that are in this portfolio, various India Highlights, Themed collections of these journals, new RSC launches and related topics. Lastly, discussion about our publishing resources that can help authors and reviewers to publish with us effectively and efficiently.

INVITED SPEAKER

Prof. Ram B. Choudhary

IIT (ISM) Dhanbad, INDIA

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Title: Nature-Inspired Carbon Electrode Materials as Green Precursors for Green Supercapacitors

Abstract: Supercapacitors, also known as ultracapacitors, are the high-capacity capacitors with the capacitance value unusually higher than solid-state capacitors but reasonably restricted to lower voltage limits. These are the energy storage devices for harvesting electrochemical energy and empowering electrical energy at quite a high power density. Flexible structures, light weight, 3D-stretchability, good mechanical strength, high thermo-chemical stability, ultrafast charge-discharge with long cycle life are some of the most enchanting and desirable features that causes to accept them attractively and globally for a broad range of high-power applications. In this context, nature-inspired active electrode materials with bio-inspired configuration, organic frameworks, and

mechanically flexible and stretchable carbon materials click best for the successful fabrication of supercapacitors. Notably, carbon electrodes are the key components for the design and development of the supercapacitors owing to their excellent porous morphology, large surface area, good electrical conductivity, high mechanical strength, and ease of processability. Nonetheless, with the continuous advancement in green chemistry aimed to overcome environmental issues in the fabrication of supercapacitors comprising of green precursors like agricultural wastes, non-edible forest products, microbial residues, and bio-mass accumulates are in good practice owing to their high carbon content and discrete functionalization. Furthermore, biomass-based carbon precursors exhibit multiple electroactive functional groups such as –CH, -CO, -CO3, -COOH, -OH, -NH2, -SH, -SiH etc. which when subjected to pyrolysis, break into elemental species of oxygen (O), nitrogen (N), sulphur (S) etc. and get incorporated or doped into the carbon lattice. Upon activation, these display hierarchical porous structures that facilitate ion transport and shorten the diffusion pathways for inflated charge storage. The relevance of green energy is more applicable in green material solutions to energy problem. Since green energy is a multidisciplinary, rapid-research forum for the science and engineering of green materials and green devices used in all forms of energy production, harvesting, conversion, storage, utilization and relevant policy. These feedstocks potentially yields with numerous admissible advantages in the design-development of green energy storage devices thereby diminishing undesirable and excessive volume of the bio-wastes in the environment. In the present discussion, it is emphasized to justify the viable approaches towards broad spectrum of the green and sustainable carbon materials as potential source for energy storage in supercapacitors. It will also manifest varying mode and mechanism of actions and ensuing the advantages of the material features for green energy storage system delineated for evergreen and efficacious energy storage devices with the least environmental repercussions and reverberations comprising of 2-D and 3-D hierarchical porous activated carbons from agricultural and bio-waste products and their fibrous contents with ameliorated electrochemical performance. The major objectives behind such harnessing, designing and recycling the readily accessible nontoxic residues as green precursors in the nature focuses onto meet the multiplying energy demands as one of the major components for value added energy storage devices. Finally, it will also be discussed with the current limitations and future prospects for designing nature-inspired carbon electrode materials for supercapacitor applications.

INVITED SPEAKER

Prof. Ardhendu Sekhar Giri

IISER Bhopal, INDIA

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Title: Low-cost activated carbon doped TiO2 nanocomposite and its photocatalytic degradation of Antibiotics under UV-light irradiation

Abstract: The degradation of an antibiotic drug was investigated by low-cost nanocomposite material. The visible light responsive non-metal activated carbon doped TiO2 nanocomposite photocatalyst with wide band gap energy was synthesized via the coprecipitation method with an equal mass ratio of activated carbon and TiO2. Under optimal conditions, the photocatalytic experiment was carried out in a batch reactor in the presence of irradiation of 15W UV light. A significant effect of carbon caused a notable reduction in the optical band gap of doped with TiO2. The composite showed the maximum removal of 87.6% tetracycline drug in 45 min. The optimal catalyst dose and drug concentration were found to be 1.25 g and 100 mg/L, respectively, but the optimal reaction time, 45 min, and pH=6.5 are very significant in the presence of UV light. The kinetic experimental data showed the best fitting for both pseudo-first-order (ka=21.83 min−1) and pseudo-second-order (0.23 g/g min) models with a

high accuracy based on R2 values. Freundlich model showed a maximum adsorption capacity (qm) of 94.87 (mg.g-1) for tetracycline drug removal on the heterogeneous surface with higher accuracy than the Langmuir model. Adsorption followed by degradation was shown at optimized pH, while intraparticle diffusion phenomena act as the rate-limiting step. Moreover, a proposed drug degradation mechanism based on the formation of hydroxyl free radicals is suggested, and LC/MS analysis identified fourteen intermediate products during drug degradation. At the same time, the antibacterial activity test showed that the generated degradation products were less toxic compared to the tetracycline molecule.

INVITED SPEAKER

Prof. Bikas C. Das

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Title: Memristors and Memtransistors: Exploring Versatile Behaviors and Neuromorphic Potential

Abstract: Memristors (MRs) and memtransistors (memTs) are emerging as transformative elements in the landscape of data storage and neuromorphic computing systems, thanks to their distinctive attributes and adaptable behaviors. These nanoelectronic devices demonstrate non-volatile resistance switching, mirroring the synaptic plasticity observed in biological brains. Leon Chua's conceptualization of memristors in 1971 laid the groundwork for their exploration, and they have since garnered attention for their capacity to emulate biological synapses with nonlinear conductance alterations in response to voltage pulses, facilitating the modulation of synaptic weights. Memtransistors, a more recent innovation, amalgamate the functionalities of both memristors and transistors, offering enhanced capabilities. Moreover, MRs and memTs have the potential to transcend the constraints of conventional computing architectures, such as the von Neumann bottleneck and power inefficiency. In this presentation, I will delve into the recent strides made in MR and memT technology, encompassing advancements in materials engineering, device fabrication, and circuit design methodologies. Through this exploration, we aim to elucidate the transformative potential of these devices in reshaping the energy-efficient future of advanced computing paradigms.

INVITED SPEAKER

Prof. S. N. Pandey

Motilal Nehru National Institute of Technology Allahabad, Prayagraj, INDIA

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Title: Oxide/ hydroxide/ oxyhydroxide materials for energy storage: Supercapacitor

Abstract: Sustainable energy storage and conversion devices without sacrificing current environment condition have always been a crucial need for society. Among the numerous energy storage technologies, supercapacitors have gained very much interest by the scientific community, especially because of their remarkable qualities, including substantial power density, the ability to charge-discharge quickly, and an extended cyclic stability. The electrode material is the key component of supercapacitor device. Carbon and its derivative, polymers, metal oxides/hydroxide etc. are different types of supercapacitor electrode materials. Metal oxides have much higher capacitance and energy densities compared with that of carbon materials. During the past years, the electrochemical performance of various metal oxides/ hydroxides/ oxyhydroxides has been explored. Fractal analysis is an analytical tool that can extract more information about the surface differently from the traditional analysis. This analysis provides a deeper understanding how the morphology of the surface varies with different physical and chemical properties. The electrochemical and fractal analysis of oxide/ hydroxide/ oxyhydoxide materials will be discussed.

INVITED SPEAKER

Prof. Koyel Banerjee Ghosh

Indian Institute of Technology Hyderabad, INDIA

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Title: Advancing spin-controlled electrocatalysis via. chirality-induced spin polarization

Abstract: Electrocatalysis is one of the potential avenues to store electricity produced from renewable energy sources in the form of fuel. Electrocatalytic oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) are the foundations of renewable energy technology. However, both processes have significant activation barriers that severely limit the overall performance of energy conversion devices that utilize ORR/OER. Though traditional catalyst design prioritizes crystal and electronic structure, understanding the detailed mechanism requires consideration of spin selection rules as the ground electronic state of diatomic oxygen is a triplet. It has been explored that by utilizing chiral molecules, the multielectron reduction process of diatomic oxygen (ORR) and oxidation of water (OER) can be improved. The justification behind the use of a chiral catalyst as the spin-filtering electrode is the chiral-induced spin selectivity (CISS) effect. It has been demonstrated when electrons are transported through a chiral molecule, due to spin-polarization, one spin of the electron prefers to go through one enantiomer and the other prefers to go through the opposite enantiomer. This is known as the CISS effect. Hence, the spin-dependent electron transfer processes may take place at the liquid/solid interfaces during electrocatalytic oxidation of water or reduction of oxygen while using the chiral molecular functionalized electrode. In this presentation, I will highlight some examples of electrocatalysis that will demonstrate the enhancement of the catalytic property resulting from the spin-controlled charge transfer.

INVITED SPEAKER

Prof. Anurag Srivastava

Atal Bihari Vajpayee Indian Institute of Information Technology and Management Gwalior, INDIA

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Title: Air and Water pollutant Detection: 2D Materials as the Potential Candidate

Abstract: Detection of minor gas leaks in a hazardous work environment has been a challenging research problem for many decades as it involves health, safety and environmental risks. The past decade has shown enormous research contribution in terms of publication to achieve high quality sensor. A report of the World Health Organisation has revealed Gwalior is the most polluted city in India in terms of air pollution along with other 12 cities of India. The report also suggests that the Indian population living outside Kashmir and the Himalayan belt are exposed to air pollution beyond the WHO safe limits. Meanwhile, Delhi, touted as the most polluted city in the world, doesn't feature in the list of cities with highest air pollution levels. Also, no other metro city features in the notorious list. Both experimentalists as well as theoreticians have attempted their level best to design and miniaturize sensor materials. Some of them got well recognition but still the goal to achieve quality sensor is far apart. Conventional sensors based on semiconducting metal oxide thin films, organic polymeric materials, silicon and carbon black-polymer composites have been preceded by nanostructure sensors for past decade. In this race, carbon nanostructures have evolved as prominent candidates due to its extraordinary chemical and physical properties. 2D-nanostructures served fascinating research prospects for scientific community in past few decades. Starting with carbon nanotube (CNT) and graphene, different new 1D and 2D nanostructures have been introduced with novel chemical and physical characteristic, and successfully tested as quality sensor materials and are essential for miniaturizing electronic devices. The present talk will include our group's recent computational work on 2D nanostructures for their sensor application in detecting various Air and water pollutants, using density functional theory approach.

INVITED SPEAKER

Prof. Anil K. Yadav

Chaudhary Charan Singh University, Meerut UP, INDIA

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Title: Phosphors for Energy efficient LEDs and Lighting Applications

Abstract: The depletion of fossil fuel resources highlights the requirement of switching to sustainable energy sources due to sever drawbacks of fossil fuel such as environmental pollution, resource scarcity and climate change. Energy crises arise from a number of variables including geopolitical tensions, supply disruptions, and increasing energy demand beyond available supply. In order to handle energy crises materials play a crucial role by enabling the development of alternative energy sources, energy storage technologies, and energy-efficient systems. For instance, Phosphorescence materials also known as phosphors play a crucial role in the realm of energy materials due to their significant contribution to energy-efficient lighting technologies such as Light

Emitting Diodes (LEDs). LEDs are completely changing the lighting industry by offering more energy efficiency and longer operational lifetimes compared to traditional lighting sources. Phosphors are essential components in LEDs as they enable the conversion of blue or ultraviolet light emitted by the LED chip into a broad spectrum of visible light, thereby producing white light suitable for various lighting applications. Phosphors are essential to the efficiency of LEDs since they improve both their overall efficiency and color rendering capacity ensuring that the emitted light closely matches natural sunlight, which is crucial for applications such as indoor lighting, automotive lighting, and displays. Researchers are continuously exploring new phosphor compositions and synthesis methods to achieve higher efficiency, better colour quality, and enhanced stability under various operating conditions. Additionally, efforts are underway to develop phosphor materials with improved thermal properties to mitigate efficiency droop, a phenomenon where LED efficiency decreases at higher operating currents. In summary, phosphor materials are integral to the development of energy-efficient lighting technologies such as LEDs. Their role in converting primary light sources into high-quality, visible light underscores their importance as energy materials in the pursuit of sustainable and efficient lighting solutions.

INVITED SPEAKER

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Title: Efficient Modulation of Hydrogenation/dehydrogenation Kinetics Using Nanoengineered Materials in MgH2 Solid-State Hydrogen Storage

Abstract: Hydrogen as the energy carrier is getting attention because of its intrinsic characteristics, such as the maximum gravimetric energy density and the abundance of precursor sources, i.e., water, for producing green hydrogen using renewable energy. However, its potential relies on safe use for different applications. Solid-state hydrogen storage materials are considered the safest medium of hydrogen. Magnesium hydride, i.e., MgH2, is a promising material with around 7.8 wt% hydrogen storage capacity, which is nearly twice the target of 4 wt% hydrogen storage, proposed by DoE, USA. However, this material suffers from high-temperature hydrogenation/dehydrogenation kinetics, thus making it difficult for practical applications. We innovated the methodology of designing nanocomposites of MgH2 with nanoengineered carbonaceous and hybrid carbonaceous-metallic nanoparticles. The developed nanocomposites showed a significant reduction in desorption temperature (50 C or more) in desorption temperature with respect to pristine MgH2, for which desorption is > 300 C. This improvement in hydrogenation/dehydrogenation is attributed to the synergistic interaction between grain and nanoengineered modifies. Thus, the present approach of modulating hydrogenation/dehydrogenation may provide a roadmap for the synergistic modification of Mg/MgH2 system towards enhanced kinetics without hampering storage capacity.

INVITED SPEAKER

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Title: In-situ Liquid-Phase Transmission Electron Microscopic Observation of Si-H2O reaction for On-Demand H2 Production

Abstract: With the immense technological revolution, the excessive use of fossil fuels as the primary energy source has caused a significant increase in CO2 and other greenhouse gases in our atmosphere. To address the associated climate change and fossil fuel depletion hydrogen technology has emerged as one of core research topics among researchers. However, its practical application is still in its infancy due to the lack of a safe and efficient method for storing and delivering hydrogen. The most efficient approach to tackle these challenges is through on-demand H2 production. Nano-Si particles are an excellent candidate for H2 production due to their large yield. In terms of mass, one gram of Si produces an impressive 1.75 L of H2. We have achieved a H2 flow of 1.6 L/g of Si using NaOH and other additives such as NaCl. Our method allows for instantaneous H2 production, and the rate can be effectively controlled by adjusting the reaction's pH value and temperatures. To gain a comprehensive understanding of the reaction under various pH conditions and in the presence of different additives, we utilized in-situ liquid-phase transmission electron microscopy (LPTEM). This technique allowed us to demonstrate the entire reaction in real-time, enabling observation of H2 formation and structural changes in Si. Furthermore, by combining the LPTEM observations, energy loss electron spectroscopy (EELS) analysis and other materials characterizations, we propose a detailed reaction mechanism. We measured the purity of the produced gas using gas chromatography mass spectrometry (GC-MS) and found it to be 99.58%. These findings suggest a viable option for instant H2 production in portable fuel cells using Si cartridges or pellets.

INVITED SPEAKER

Prof. Sachin Gupta

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Title: Novel spintronic materials for next generation technological applications

Abstract: Spintronics is an emerging field in electronics, which incorporates a spin degree of freedom of an electron in addition to traditional charge degree of freedom, offering numerous advantages such as nonvolatility, high data processing speeds, low power consumption, and high storage density. The advancement of spintronics is closely intertwined with the development of functional material systems, crucial for designing proof-of-concept devices. Materials characterized by high spin polarization, Curie temperature, and topological properties can play pivotal roles in the advancement of spintronic devices. In this talk, I will delve into various spintronic materials, examining their structural, magnetic, and transport properties, and elucidating their potential significance in spintronic applications.

INVITED SPEAKER

Dr. Shamima Hussain

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Title: Advanced material for next generation devices

Abstract: The advancement of next-generation devices is heavily reliant on the development of new materials that offer superior properties and functionalities. The future technology is being governed by material exhibiting exclusive properties. These advanced materials are pivotal in the development of next-generation devices across various fields , viz., electronics, energy, healthcare, and aerospace. By leveraging their unique properties, researchers and engineers can create devices that are more efficient, durable, and capable of performing complex functions, thus driving technological progress and innovation. In this talk , our focus would be directed towards some applications based on material synthesised in the laboratory. The idea is to set the young minds in the direction to explore other similar material to create a healthy society.

INVITED SPEAKER

Dr. Himanshu Tyagi

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Title: Wide-field Imaging with Super-resolution Enabled by Raman Signals (WISER)

Abstract: Raman scattered signals from advanced materials and biological systems serve as highly reliable fingerprints, utilizing a label-free and non-destructive process. However, traditional confocal Raman microscopy is significantly constrained by its small imaging area (limited to the laser beam's diameter focused on the sample) and diffraction-limited resolution. Attempts to increase the imaging area through point-by-point scanning result in poor resolution Raman maps and are further hampered by the slow mapping speeds. While advancements like tip-enhanced Raman spectroscopy (TERS) address the spatial resolution issue, they are still hindered by slow scanning speeds and challenges such as probe fragility, the need for flat samples, and high technical complexity and costs. Therefore, a method that offers improved resolution and larger area maps without high complexity and costs is highly desirable. We present WISER (Wide-field Imaging with Super-resolution Enabled by Raman Signals) to address these challenges. WISER achieves broader area Raman maps by using a wide-field Raman technique instead of the traditional confocal approach. By combining wide-field Raman with an imaging interferometer, we enable high-speed Raman mapping. This optoelectronic image acquisition process avoids the slow speeds and imperfections caused by mechanical movement in conventional Raman mapping. Super-resolution Raman maps are achieved through a structured illumination approach, where a digital mirror device modulates the incident wide-field laser illumination. Using the WISER technique, Raman maps of various samples (e.g., nanodiamonds, 2D MoS2, CNTs) show up to a 2-fold improvement in spatial resolution compared

to conventional methods. Our approach, which integrates structured illumination microscopy with hyperspectral Raman, promises wider area Raman maps with better resolution than traditional Raman microscopy.

INVITED SPEAKER

Prof. Nirmal Ganguli

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Title: Antiferromagnetic spintronics promising superfast computation at miniscule energy

Abstract: The future of human civilization will be dictated by how we solve the energy problem we are faced with. Besides harvesting energy, an important aspect of the solution lies in making our routine tasks more energy-efficient. The initial exponential increase in computer speed has reached a plateau, while the energy consumption by personal computers and supercomputers is exponentially increasing, owing to the use of more of them. The emerging technologies based on antiferromagnetic spintronics may offer a solution in this regard. Based on the principle of altering the antiferromagnetic spin texture and domains using spin-orbit torque, devices utilizing antiferromagnetic spintronics may operate at THz range with minuscule power consumption. We will show a few examples of designing oxide heterostructures where antiferromagnetic spintronics may be realized based on our first-principles density functional theory calculations.

INVITED SPEAKER

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Title: Future Materials for Thermoelectric and Hydrogen Storage

Abstract: The human sustainability and development are strongly dependent on energy use. This involves the development of technology that harnesses renewable energy sources such as sun light, wind, tides, hydrogen, and waste heat recovery. While solar, wind, and tidal energy technologies have previously been developed and deployed, nano thermoelectric materials are still in their early stages of development. Hydrogen is a readily available and efficient source of renewable energy. Nonetheless, its flammability poses a significant concern, necessitating the development of materials for appropriate hydrogen production, storage, and detection in order to compete with fossil fuels and introduce a hydrogen-based economy. During the discussion, I will go over the various materials of thermoelectric and hydrogen storage, beginning with their fundamental principles of both technologies. It will go over the materials involved, such as binary chalcogenides and composite materials. Metal hydrides and oxide, hydrogen storage, and sorbent materials are all now being investigated for hydrogen-powered technology. The advantages and disadvantages of different materials, as well as prospective solutions to various issues in thermoelectric and hydrogen storage, will be discussed.

INVITED SPEAKER

Prof. Utpal Sarkar

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Title: Carbon based material for nanoelectronic and optoelectronic applications

Abstract: Carbon based allotropes like graphene, graphyne, twin graphene etc. gained special attention to the researcher now-a-days because of their application in several fields. This talk aims to provide the atomistic insights of the electronic and optical properties of these systems through density functional theory framework. Due to the presence of B or N or BN at different sites, the conductivity of doped system can be tailored from metal to large band gap semiconductor depending on substitution type, doping site and concentration. Its structural constitution offer a wide range of bandgaps apart from doping or application of strain. We observed these materials are suitable as dielectric medium in nanoscale capacitors. These findings paves the way to utilize these designed structures in various electronic applications. Moreover, the presence of dopant atom shifted the onset of absorption spectra from infrared to UV region via visible region and found to be suitable in optoelectronics.

INVITED SPEAKER

Prof. Swagata Roy

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Title: A Cutting-Edge Approach to Self-Harvesting and Renewable Energy Storage Devices Using b-Nucleated High-Dielectric PVDF Composites

Abstract: Self-sufficient devices that harvest and store energy in a single unit are crucial for powering microelectronics. Herein, a pioneering approach is employed to achieve that goal. Self-charging photo power cells built upon electroactive and high dielectric doped polyvinylidene fluoride (PVDF) and its co-polymer (PVDF-HFP) composite films are the prime components explored in this research direction. Unlike traditional methods (that use separate components for harvesting and storage of energy), this approach exploits the unique properties of PVDF/PVDF-HFP composites to harvest and store renewable solar energy in a single unit by promoting the formation and enhancement of this distinct β-phase and augmenting its dielectric properties. This integrated approach offers significant recompenses in terms of device simplicity, efficiency gain, and miniaturization. Our group has made significant strides in this specific field by exploring novel strategies for promoting b-phase nucleation in PVDF/PVDF-HFP through the addition of dopants viz., montmorillonite (MMT) and Ni(OH)2 nanoparticles modified MMT, which led to remarkable enhancements in b-phase formation (~ 85.22%) and improved dielectric properties. In furthermore studies, Folic acid (FA) modified PVDF composites was used as the base material to fabricate an organic photovoltaic self-charging energy storage cell (OPSESC) and an impressive energy density of 7.84 mWh g-1 and specific capacitance of 61 F g-1 was obtained. Another study focused on the in-situ synthesized ZnO nanoparticles within PVDF thin films, resulting in the development of a self-charged photo-power bank (SPPB) showcasing excellent storage capabilities with power density of 3.04 W

m-2. Likewise, insitu-MgO2 nanoparticles-PVDF composite films were employed to fabricate a state-of-the-art self-charging photo-power bank. High energy density of 240 mWh m-2 and a remarkable charge density of 1350 C m-2 has been achieved combined with rapid self-charging capacity and exceptional long-term cycling stability for 30 days. These results suggest a novel research direction where the miniature devices are capable to harvest and store renewable energy in a single unit without any electric biasing to power up microelectronic appliances like LEDs and watches. Looking ahead, we aim to further optimize these b-phase nucleated materials for even higher energy conversion efficiencies, improved durability, and scalability for mass production which will surely usher the path for powering wearable microelectronics and serve to the ever increasing energy demands of the future world.

INVITED SPEAKER

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Title: Development of fully biodegradable magnesium(Mg)-molybdenumtrioxide (MoO3) transient battery

Abstract: A high-performance fully biodegradable Mg–MoO3 battery that consists of all dissolvable materials including Mg, MoO3, Mo, sodium alginate hydrogel, PLGA, and polyanhydride encapsulation layer. The battery is capable of providing a high stable output voltage up to 1.6 V as well as desirable capacity (6.5 mAh cm−2) and prolonged lifetime up to 13 d. The battery is capable of driving typical ultralowpower implantable electronics with robust functions. Demonstrated operations include a red LED, a calculator, and an ECG signal detector amplifier. The battery exhibits desirable biocompatibility and is fully biodegradable both in vivo and in vitro. The battery can potentially be used as an on-board power source to achieve self-powered therapeutic systems for tissue regeneration, presurgery, or postsurgery monitoring over extended periods. This would otherwise be impossible due to the limitations of currently available power tools. The novel materials' strategies and fabrication schemes of the battery system offer a promising approach for advanced power supplies and provide a critical step along the route to achieve fully-functional transient systems that could play an essential role in green electronics, minimizing the environmental impacts and implantable bioresorbable therapeutic and diagnostic systems eliminating secondary surgery for device removal.

INVITED SPEAKER

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Title: Electrospun lead-free ceramic Nano fibres for energy harvesting applications

Abstract: Man and Materials have symbiotic relationship throughout the edges. The progress of human civilization is closely linked to the developments in Materials. Now a day, many scientists and researcher are investigating materials at a very small scale. Such technological advances are known as nanoscience and nanotechnology. Electrospinning (E-spin) is a unique technique to fabricate polymeric as well as ceramic nanofibers. Research on electrospun nanofibers is a very active field in material science owing to their novel applications in diverse domains. The focus of this talk is to provide an insight of the investigation of Lead-free Sodium Bismuth Titanate materials in different forms. Also, it gives an insight into E-spin technique by understanding the working principle, influencing parameters and applications of nanofibers in energy harvesting applications.

CONTRIBUTED PAPERS: ABSTRACTS

THEME-A: Synthesis & Characterization of Energy Materials

Enhancing Bifacial Perovskite Solar Cell Efficiency from 18% to 26% and Beyond through Albedo Incorporation

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Abstract: Hybrid perovskite solar cells stand out as a compelling option for the next era of thin-film photovoltaic technology, thanks to their outstanding optoelectronic features and cost-efficient manufacturing procedures. In response to market demands for commercialization, current research endeavors prioritize the development of high-throughput fabrication techniques that align compatible with perovskite chemistry. This study introduces high-performance bifacial perovskite solar cells utilizing a transparent rear electrode composed of room-temperature RF sputtered transparent conductive layers with superior mobility properties. The front side power conversion efficiency (PCE) of these bifacial cells surpasses 18%, while sustaining an average transmittance of over 70% within the near-infrared range (780-1200 nm). Moreover, the bifaciality factor of the transparent devices are ~90 %. By integrating a 0.5 Albedo component from rear side of the bifacial cell, we have achieved a PCE exceeding 26% for the bifacial solar cell. This distinctive bifacial attribute facilitates light capture from both surfaces, resulting in an approximately 8% enhancement in overall performance.

Keywords: *Sputtering, Bifacial Perovskite solar cell, Building-integrated photovoltaics.*

Thermo-electric attributes of Ag doped BiSbTeSeSn high entropy alloy synthesised by high energy ball milling and spark plasma sintering

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Abstract: Of late, high entropy alloys (HEAs) have considered as a potential candidate material for many engineering applications such as structural, energy, etc. This is due to their merits over conventional engineering alloys. In this study, it is explored to synthesis and consolidate BiSbTeSeSn high entropy alloy for thermo-electric applications. The equi-atomic composition of BiSbTeSeSn alloy was synthesized with the help of high energy ball milling processing under optimized processing parameters (milling speed, ball-to-powder ratio, process control agent, environment, etc.). The aim was to synthesize high entropy nano-structured BiSbTeSeSn alloy with / without Ag dopant. Structural characterization studies such as X-ray diffraction (XRD), electron microscopy was performed to understand the high entropy solid solution, nano-structure, etc. Differential thermal analysis was done to understand the thermal stability of the synthesized alloys. Then, the ball milled powders were consolidated with the help of spark plasma sintering. The sintered alloy was subjected to thermo-electric studies such as seebeck co-efficient, electrical conductivity

and thermal conductivity. From which, the power factor and Figure of Merit were determined. The results of XRD confirms the high entropy solid solution of BiSbTeSeSn alloy with nano-crystalline characteristics. The sintered alloy also exhibits the nano-crystalline BiSbTeSeSn alloy with good thermal stability. However, the thermo-electric characteristics of the BiSbTeSeSn HEA alloy is less due to more metallic nature.

Keywords: *High Entropy alloy, BiSbTeSeSn, Spark plasma sintering, Nanostructure, Thermo-electricity*

From Solvent Annealing to Metal-Oxide Arrays: Mechanisms of Metal Infiltration in Block Copolymer Nanopatterns

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Abstract: The nanopatterning of materials on surfaces has attracted a significant attention from interdisciplinary scientist as it has applications in the field of electronics, electrochemistry, optics, photonics, catalysis, and biology. Here, we thoroughly analyzed the effect of solvent annealing time on the ordering of highly asymmetric poly(4-vinylpyridine)-b-polystyrene (PS-b-P4VP) block copolymer. Phase separation of PS-b-P4VP was achieved by the solvent vapour annealing (SVA) in a non-selectivesolvent atmosphere to create cylindrical arrays. Interestingly, transformation in morphology from P4VP hexagonally packed cylinders to an 'inverted' structure with PS cylinders embedded in a P4VP matrix was observed. Furthermore, we also systematically studied the effect of oxidation state and type of cation in the infiltrationprocess, which were selectively inserted into the P4VP arrays from PS-b-P4VP BCP templated thin films. The findings showed that the stability of the as-obtained metal-pyridine complex is highly influenced by the oxidation state and type of cation, and hence, the formation of metal oxide patterns. Various metals (Ag^{+}, $Ni^{2+,}$ $In^{3+}$and Ga^{3+}) cations were inserted into P4VP arrays by solution mediated infiltration approach followed by an ultraviolet-ozone (UVO) treatment to remove the polymer and oxidize the metallic ions to their oxides. It was found that P4VP/Ag^{+} pattern was not intact after UVO treatment due to the weak interaction between them, however, Ni^{2+} and In^{3+} were able to reproduce the pattern of BCP. These obtained results were characterized by a variety of methods, including atomic force microscopy, scanning electron microscopy, Raman spectroscopy and X-ray photoelectron spectroscopy.

Keywords: *Block copolymer; Nanopattern; Metal Infiltration; Inverse, Oxidation State.*

Electromagnetic Shielding by a Polymer Based Tertiary Nanocomposite

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Abstract: The progress in telecommunications has led to the emission of electromagnetic radiation, which could potentially affect human tissues and disrupt electronic devices, causing Electromagnetic Interference (EMI). To mitigate this interference, materials with high dielectric and magnetic properties, combined with conductivity, are utilized for their effective electromagnetic shielding capabilities. The material $Ca_{0.9}Sr_{0.1}Cu_{2.9}Zn_{0.1}Ti_{3.9}Sn_{0.1}O_{12}$ (C1) is well-known for its dielectric properties, while $BaFe_{9.5}Al_{2.5}O_{19}$ (B1) is renowned for its magnetic characteristics. C1 has been synthesized using conventional ball milling, whereas B1 has been produced through a modified sol-gel method employing citric acid. XRD Pattern

shows that the sample (C1) belongs to a cubic structure with space group Im-3, and the magnetic sample (B1) belongs to a hexagonal structure with *$P6_3/mmc$* space group. The drop-casting method has been employed to synthesize PVDF- 5% C1-5% B1-5% CNT/10% CNT. Morphology and phase were confirmed by using SEM technique. The sample (C1) belongs to the cubic structure with space group Im-3, and the magnetic sample (B1) belongs to the hexagonal structure. It has been observed, this quaternary composites show high dielectric constant with low dielectric loss in the frequency range (10^2-10^7Hz) in the wide temperature window (40-140ºC). This material shows excellent shielding effectiveness compared to previous reported materials.

Keywords: *PVDF, CNT, C1, B1,EMI*

Morphology and Size Dependent Cold Cathode Emission in Solvothermally Synthesized Cu_2ZnSnS_4 Nanostructures

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Abstract: The present work involves the synthesis of Cu_2ZnSnS_4 (CZTS) using solvothermal processes. The resulting nanostructures exhibit two distinct morphologies; triangular flakes and irregular nanoparticles. As obtained from UV vis absorbance spectroscopy, the morphologies have energy band gaps of 1.4 eV and 1.5 eV, respectively. Interestingly, the smaller CZTS nanoparticles (around 10 nm) display a slightly higher band gap. This difference suggests that quantum confinement effects are at play, modifying the density of states (DOS) and incrementing the band gap. The study further investigates the cold cathode emission properties of the nanostructures. The samples demonstrate promising results with low turn-on (2.96 V/μm and 4.11 V/μm) and threshold field values (5.21 V/μm, 9.18 V/μm) for the triangular flakes and nanoparticles, respectively. Notably, the flakes exhibit superior field emission due to their unique, sharp morphology and higher conductivity from their lower band gap. Our study employs the Fowler-Nordheim equation (Fowler-Nordheim tunnelling phenomena), which relates the applied electric field to the emitted current density. Analysis of this relationship confirms that electron emission occurs through a barrier tunnelling process initiated by a strong macroscopic electric field. Additionally, ANSYS simulation employing finite element analysis is used to visualize the electron emission sites by modeling the electrode geometry and calculating electric field strength. This correlation between particle morphology and size on the cold cathode emission properties of CZTS nanostructures is attributed to the interplay of quantum confinement and electron tunnelling phenomena.

Keywords: *CZTS; cold cathode emission; band gap; quantum confinement; quantum tunnelling*

Improvised selective adsorption of Carbon Dioxide from gas mixture using 13X Zeolite impregnated with transition metal oxide

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Abstract: The separation of carbon dioxide from gas mixture is an essential requisite for environment and Industrial application. The adsorbents play vital role for effective capture and separation of carbon dioxide from gas mixtures. Surface Modified SSZ-13 zeolites particularly transition metal cation-exchanged zeolites Co(II)/SSZ-13 and Ni(II)/SSZ-13 have showed the highest CO2 uptake (4.49 and 4.45 mmol/g, respectively) for CO_2 capture and separation from N_2 (Sun 2019). This is due to the π backdonation formed between CO_2 and the transition metal cation sites. In-situ impregnated Zn and Cu NPs at zeolite surface show significant improvement in adsorption capacity and selectivity of CO_2 over N_2 atmosphere. Based on the Langmuir- Freundlich adsorption isotherms, the CO_2 adsorption capacities of 13X, CuO-13X and ZnO-13X were 3.1, 4.10 and 5.10 mmol/g, respectively, measured at 20 ºC and 1atm. The highest CO_2 selectivity by 13X, CuO-13XandZnO-13X were 85.2, 92.71 and 97.38 at 20 ºC, respectively. We attribute such outstanding separation performance to the π backdonation exclusively formed between CO_2 and transition oxide sites. Our work validated the potential of transition metal oxide impregnation at 13X zeolites for efficient CO_2 capture, as evaluated by unary static isothermal adsorption and binary dynamic column breakthrough experiments as well as predicted performance in pressure/vacuum swing adsorption (PSA/VSA) process. This demonstrates a new approach of developing adsorbents for CO_2 capture in the real-world industrial processes and environmental application.

Keywords: *Carbon Dioxide adsorption, Selectivity, Equilibrium Isotherms*

Advancements in Structural and Electrical Properties of Fused Filament Fabricated Graphene-Reinforced Poly-lactic Acid

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Abstract: The mechanical performance of components produced via fused filament fabrication (FFF) can significantly impact their suitability for industrial applications. This study focuses on investigating the structural properties of biodegradable poly-lactic acid (PLA) specimens reinforced with graphene nanoplatelets (GNP), with particular attention given to the influence of nozzle diameter and layer height on key structural properties such as flexural strength, compressive strength, and impact strength. The addition of GNP enhances the structural properties of PLA composites. Experimental analysis was conducted to assess the impact strength, compressive strength, and flexural strength of GNP-PLA composites. The validity of the experimental findings was verified through statistical analysis of the data obtained from mechanical testing. Furthermore, high-resolution microscopy was employed to examine the fracture mechanism of the specimens. The compressive strength of the composites ranged from 14.929 MPa to 33.214 MPa, while flexural strength varied from 45.377 MPa to 57.522 MPa, and impact strength ranged from 24.12 kJ/m² to 37.99 kJ/m² while improving in electrical conductivity. The enhanced stiffness provided by GNP contributes to improved structural support, rendering GNP-PLA composites suitable for various structural and electrical elements.

Keywords: *fused filament fabrication; flexural; compression; impact; electrical; poly-lactic acid; graphene nanoplatelets.*

Synthesis and Characterization of Stable Lead-Free Double Halide Perovskite

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Abstract: Halide perovskites have gained great interest in the field of optoelectronic applications owing to their excellent optical and electronic properties. Despite having great properties, the stability and toxicity issues are concerns of researchers. In this regard, lead-free double halide perovskite (DHP) materials are the potential candidates to be used in optoelectronic applications. Different works are going on based on lead-free, inorganic, high stable double perovskite, although more study is required to get better result. From the above motivation, we have synthesized a highly stable, lead-free DHP $Cs_2CuBiBr_6$ using a simple solution-processed method. XRD and Raman spectroscopy studies were performed and confirmed the successful synthesis of the material in the cubic phase. The optical properties of the materials were studied by UV-Visible spectrophotometer and photoluminescence spectrometer, and we have found the band gap of the materials from the Tauc plot. We have also studied the FE-SEM characterization of the film.

Keywords: *Double perovskite, highly stable, non-toxic*

Electrochromic behavior of nickel oxide thin films grown by reactive DC magnetron sputtering

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Abstract: Electrochromic (EC) materials are those that change their optical properties under application of electric potential. These materials reversibly modify their oxidation state through ion insertion and deinsertion. Metal oxides show this phenomenon either while exhibiting ion insertion (cathodic coloration) or ionic extraction (anodic coloration). Nickel oxide (NiO) exhibits anodic coloration, with a change from dark brown to a transparent (bleached) state. It possesses good cyclic reversibility, high coloration efficiency, and good durability and can be used for smart windows and display applications. In this work, NiO films are grown by reactive DC magnetron sputtering on indium tin oxide (ITO) coated glass substrates at room temperature by varying the oxygen flow rate from 12 to 23 sccm with a constant argon flow rate. Structural analysis has carried out using X-ray diffraction, while surface morphology has been investigated with scanning electron microscopy. Raman spectroscopy provides information on the defects in the film. The electrochemical behavior of the films is studied using cyclic voltammetry. The effect of oxygen flow rate on the EC properties are optimized with the as deposited film at 20 sccm of oxygen showing the maximum transmittance modulation of 67% at 550 nm.

Keywords: *DC sputtering, Nickel oxide, Electrochromism, Optical properties, Oxygen flow rate.*

Electroabsorption study of thermally activated delayed fluorescent material

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Abstract: Thermally activated delayed fluorescence (TADF) materials are third generation organic emitters used in organic light emitting diodes (OLEDs). Unlike conventional fluorescent materials, the triplet excitons in TADF materials are converted to singlets through a thermally activated process called reverse intersystem crossing (RISC), which enhances the external quantum efficiency of TADF based OLEDs. Electroabsorption (EA) spectroscopy is a technique by which the change in absorption coefficient of a material in the presence of an external electric bias is measured. Using this method, we can find the nature of excitons generated by optical excitation. In this work, we have done Electroabsorption measurement for TPA DCPP, which is a red emitting TADF material. The EA spectrum was measured at first and second harmonic frequencies for different AC and DC biases. We have analysed the obtained EA spectrum and found that the excitons generated in TPA DCPP exhibits both Frenkel and charge transfer characteristics.

Keywords: *Electroabsorption, TADF materials, nature of excitons*

Impact of Optimal Thickness on the Water Splitting Performance of Sulfurized Antimony Sulfide Thin Films

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Abstract: Antimony Sulfide (Sb_2S_3) thin films, recognized for their advantageous bandgap of approximately 1.7 eV, are emerging as promising materials for water splitting application. Initially, these films were deposited via thermal evaporation with various thicknesses, but post-deposition analysis revealed a consistent sulfur deficiency. This issue was effectively addressed through sulfurization using chemical vapor deposition (CVD). Among the different samples, the 450 nm thick film exhibited particularly outstanding properties, including an optimal bandgap of 1.75 eV and high absorbance. Photoluminescence spectra indicated a low recombination rate of charge carriers, which is crucial for enhancing photoelectrochemical efficiency. Current-voltage (I-V) curves demonstrated high electrical conductance, while electrochemical impedance spectroscopy (Nyquist plots) confirmed low resistance. Notably, the 450 nm film achieved a high photocurrent density of approximately 0.6 mA/cm², significantly outperforming other samples. These combined properties highlight the potential of sulfurized Sb_2S_3 thin films, especially at a thickness of 450 nm, as highly efficient materials for water splitting application, offering a powerful combination of electronic and optical performance.

Keywords: *Antimony sulfide (Sb_2S_3) thin films, Thermal evaporation, Chemical vapour deposition, Water splitting.*

Chemical Substitution-Driven Electronic Properties Tuning and Catalytic Activity of TiO_2: An Interplay of Valance States

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Abstract: For environmental remediation, addressing the growing concern regarding wastewater treatment management necessitates the development of catalysts capable of oxidizing water into OH• radicals,

essential active species for (photo)catalytic activity. TiO2 stands out as one of the highly explored and promising materials for this purpose. Leveraging the varying valence states of vanadium(V), we have delved into V-modified TiO2 synthesized via the sol-gel route and calcined at 450°C for 12 hours. Rigorous X-ray Diffraction (XRD) analyses were conducted to confirm the phases, complemented by an array of spectroscopic techniques for a systematic exploration of structural and electronic properties. Structural parameters derived from Rietveld refinement were meticulously correlated with other experimental measurements to unveil structure-property relationships. Doping resulted in a reduction of TiO2 band gap from 3.2 eV to 2.5 eV. Surface morphology was scrutinized via FE-SEM imaging, while Brunauer-Emmett-Teller (BET) surface analysis quantified specific surface area and porosity. Notably, catalytic degradation of Rhodamine B, an organic dye, surged from approximately 8% to 51% with 12.5 at% V-doped TiO2. Furthermore, quantitative analysis of different valence states of V and Ti was undertaken via X-ray photoelectron spectroscopy (XPS), elucidating their interplay and explaining the enhanced catalytic activity through a Fenton-like reaction mechanism.

Keywords: *TiO2, catalysis, waste water treatment, Rhodamine B, Fenton-like reaction*

Influence of Topography on Nano-Mechanical Behaviour of Cylindrical Magnetron Sputtered TiN Thin Films

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Abstract: TiN thin films were deposited on a stainless steel substrate at varying deposition pressures using an indigenously developed Cylindrical Magnetron Sputtering (CMS) Equipment. The crystallographic information of the surface was obtained from synchrotron-based Grazing Incidence XRD analysis. The film growth exhibited a self-assembled nano-hill topography with distinct spacing among arrays and adjacent hills, as revealed from AFM and in-situ Scanning Probe Microscopy (SPM) images. This distinct spacing among growth pockets is possibly attributed to the presence of shadowed regions often found in CMS based growth process. The SPM image and possible explanation of such type of film growth are displayed schematically in Figure 1. Nano-hardness tests were conducted using a depth-control mode with a fixed penetration depth of 30 nm. Contrary to previous studies, TiN films deposited using CMS equipment exhibited a significantly lower hardness value of ~5 GPa, possibly due to the inverse Hall-Petch effect. The height and spacing of the nano-hills were found to decrease with increasing deposition pressure. Larger nano-hills were more prone to crash under the Berkovich indenter movement, whereas shorter nano-hills tended to buckle. Consequently, films grown at higher deposition pressures demonstrated better adhesion-resistant properties. The study highlights the importance of deposition parameters in tailoring the properties of TiN thin films for improved hardness and adhesion resistance.

Keywords: *Cylindrical Magnetron Sputtering, TiN, Nano-mechanical properties, Self-assembled, Nano-hills Topography.*

Chemically stable ultrathin platinum films supported on oxide substrate

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Abstract: Platinum is widely used as catalyst due to remarkable activity and stability in corrosive medium. The scarcity and high costs associated with platinum necessities reduction in the amount of metal loading.

One approach is to utilize an ultrathin film of platinum deposited on stable substrates. However, stabilizing ultrathin films of noble metals on stable substrates (like oxides) is a challenge because of Volmer-weber growth mode, leading to discontinuous nano- island formation. In the present study, Zinc is used as an adhesion layer to overcome this challenge. Platinum (Pt) ultrathin films (20nm) are deposited on Silicon substrates with various thicknesses of Zinc (2nm, 4nm and 6nm) as adhesion layer using DC Magnetron Sputtering technique at 2 different annealing conditions (@ 200℃ for 1 and 4 hours). It is also crucial for the entire assembly (substrate, adhesion layer and film) to be chemically stable under operating conditions. The deposited ultrathin films are dipped in 2 different environments: 0.5M H_2SO_4 and 1M H_2SO_4 in order to study the stability of the assembly. Results show that there is an optimal amount of Zinc for films to be stable in the corrosive solutions. Stability was assessed by making sheet resistance (Rs) measurement using four-point probe technique.

Keywords: *Ultrathin films, Platinum, Adhesion layer, Delamination, Magnetron Sputtering*

Chemically grown, nanospherical $Cu_{2-x}Se$ thin films Photoelectrode by APT

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Abstract: In this investigation, copper selenide (Cu2-xSe, x=0.57) thin films were synthesized employing the environmentally benign self-organized Arrested Precipitate Technique (APT) on glass as well as on ITO substrates, at synthesis temperature of 50oC. The nucleation and growth were explored in detail with stability of Cu+2 reduction at significant deposition conditions. Characterization, encompassing Uv-Vis spectrophotometry, X-ray diffraction (XRD), and scanning electron microscopy (SEM) with Energy dispersive spectroscopy (EDS), elucidated distinctive attributes of the thin films, including a notable visible light absorption profile characterized by band gap energy of 1.59 eV, the manifestation of a singularly phase-pure cubic crystal structure, and the emergence of nanospherical surface morphology. Significantly, the Cu2-xSe thin films evinced photoelectrochemical (PEC) efficiency 0.085%, prolonged stability in PEC environments, and exhibited consistent p-type conductivity with copper vacancies as a charge carrier, underscoring their prospective utility in the realm of energy conversion, particularly in the context of photoelectrochemical cells.

Keywords: *APT, Photoelectrochemical cell, Solar energy, Cu2Se, Thin film, Semiconductors*

Innovating dye-sensitized solar cells through novel microalgal and cyanobacterial species extricated dyes: A sustainable tack for material scarce earth

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Abstract: This study explores the integration of novel microalgae and cyanobacteria-based photo harvesters into natural dye-sensitized solar cells (DSSCs). These embedded pigments forming dyes can replace toxic chemical dyes and in the cultivation process eliminate the issues of waste water and air present carbon dioxide. The species taken were microalgal namely *Asterarcys quadricellulare* and *Scenedesmus sp.* and cyanobacteria named *Cronbergia siamensis* and Calothrix sp. DSSCs efficiencies were examined after coating with extracted natural dyes along with voltage, current, and fill factor as among the performance

criteria that were extensively assessed. Long-term stability and comparisons with traditional DSSCs were performed and reported in this article. Here, J-V analysis confirmed that Glass/ FTO/ c-TiO2/ 1-D TiO2/ CR (methanol)/electrolyte/carbon achieved the highest PCE at 1.04 % for *Cronbergia siamensis*, along with a remarkable VOC of 1520 mV and a JSC of 1.297 mA/cm2 for the same device. Whereas ethanol-based highest efficiency was achieved by the extracts of the same species and stood at 0.70 %, and VOC at 1265 mV and JSC at 0.921 mA/cm2. Results have indicated that such natural upgrades in energy production through solar extraction can create a never-ending fuel through supplementation by the cells or dyes of microalgae and cyanobacteria.

Elevated microwave absorption efficiency in epoxy/carbon fiber fabric composites enhanced with graphene modification

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Abstract: In the quest for advanced materials with superior electromagnetic interference (EMI) shielding properties, the integration of graphene into epoxy/carbon fiber fabric composites has emerged as a promising strategy. This study explores the enhanced microwave absorption performance of epoxy/carbon fiber fabric composites through the incorporation of graphene. By leveraging the exceptional electrical conductivity and high surface area of graphene, we aim to significantly improve the composite's ability to absorb microwave. Our experimental results demonstrate a notable enhancement in microwave absorption efficiency in X-band frequency range, attributed to the synergistic interaction between the graphene and carbon fiber fabric within the epoxy matrix. The morphological, chemical, mechanical and thermal study of the fabricated composite samples has been performed using techniques like FESEM, Optical Microscope, Fourier Transform Infrared (FTIR) spectroscope, Vickers hardness test, thermal conductivity respectively. The microwave absorbing properties of the composite has been computed with dielectric properties material in X-band frequency range with the help of vector network analyzer. From the computed parameters the power absorption efficiency of the composite is found to be greater that 99% which is quite relevance to design EMI shielding materials, which are critical for various applications in stealth, aerospace, telecommunications, and electronic devices.

Keywords: *Carbon fiber fabric, graphene, epoxy, microwave absorption, Electromagnetic Interference, shielding*

Pulse Laser Deposited ZnO thin film: Annealing-dependent study of structural, and morphological properties.

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Abstract: This study presents the room temperature deposited ZnO thin film using pulsed laser deposition (PLD) technique in presence of oxygen gas at RT on glass substrate. Later, films are also annealed at different temperature in air to investigate the temperature dependent structural and morphological changes. Structural analysis is done by XRD and XPS, grain size and roughness measurement are characterized by AFM. XRD analysis indicates that ZnO has hexagonal wurtzite crystal structure with c-axis orientation (0 0 2). AFM results indicate that film is uniforms and densely packed with grains. XPS spectra of film

revealed the presence of elemental composition and energy states of elements present. Zn 2p peak ascribed by Zn-2$p_{3/2}$ and Zn-2$p_{1/2}$ line with the binding energy difference of ~ 23.05 eV shows the Zn atoms are in the Zn^{2+} oxidation state. The deconvoluted O1s spectra showed the metal-oxygen bonding and oxygen deficiency peak located at energy 530 eV and 532 eV at RT and 450˚ C temperature while adsorbed OH and H_2O species also observed on the surface of the film at higher energy peak at 533.8 eV and 536.3 eV at 250˚ C temperature and found to be in good agreement with reported results.

Keywords: *ZnO, Thin Film, Structural analysis, Annealing.*

THEME-B: Energy Conversion & Storage

Breaking Lithium Barriers: A Sustainable Sodium-Ion Battery Prototype

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Abstract: Recent advancements in lithium-ion batteries (LIBs) technology have improved energy production and storage, but concerns persist over renewable energy, smart grid balance, and lithium source sustainability. This encourages more research to investigate other storage technologies. Because of the chemical similarity of sodium to lithium and the fact that sodium is widely available, sodium-ion batteries (SIBs) are attracting interest as potential options for LIBs replacement. In the prospect of SIBs development, the capabilities of two-dimensional (2D) transition metal oxides (TMO) are becoming increasingly evident. This study explores the synergy of a composite material comprising V_2O_5 nanostructure and single-walled carbon nanotubes (SWCNT) as the negative electrode. For the first time, we have reported the biological synthesis of V_2O_5/SWCNT using Trachyspermum ammi leaf extract, highlighting its potential as an excellent battery material with robust performance. Cyclic voltammetry (CV) findings illustrate the feasibility of achieving reversible sodium-ion insertion and extraction within the potential range of 0.1–3.0 V vs. Na^+/Na. V_2O_5/SWCNT composites demonstrate an outstanding specific capacity of 527 $mAhg^{-1}$ in contrast to the pristine V_2O_5 nanostructure (193 $mAhg^{-1}$) at a current density of 50 mAg^{-1}. Furthermore, the V_2O_5/SWCNT nanocomposite demonstrated a notable capacity retention of 50.5% after 100 cycles, alongside an increase in coulombic efficiency from 6.14% for the pure V_2O_5 electrode to 60.46% for the composite electrode.

Keywords: *Energy storage, TMO, SWCNT, Green synthesis, Sodium-ion battery*

Design and synthesis of TPA-based hole-transporting materials for inverted $MAPbI_3$ perovskite solar cells

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Abstract: Hole-transporting materials (HTMs) are important components of perovskite solar cells (PVSCs). We have designed and synthesized two donor-acceptor-donor (D–π–A–π–D) type dopant-free hole transporting materials (V1 and V2) comprising of 2,4,6- trisubstituted pyridine as the acceptor core and 4,4′ -dimethoxytriphenylamine as the peripheral donor groups. The photophysical studies indicated a strong ICT within the molecules due to their (D–π–A–π–D) structure. DSC characterization of V1 and V2 show a T_g of 103 and 81 ˚C respectively. The hole mobilities of the HTMs were measured by SCLC method using a hole only device (FTO/PEDOT:PSS/HTM/Au). The steady-state photoluminescence (ssPL) studies were carried out to gain insights into the hole extraction of $MAPbI_3$ by the HTMs. The SEM image was used to investigate the surface quality of the $MAPbI_3$ thin film on different HTMs whereas XRD patterns of $MAPbI_3$ thin films deposited on different HTMs were analysed to determine crystallite size of $MAPbI_3$. The devices (FTO/HTM/$MAPbI_3$/$PC_{61}BM$/BCP/Ag) with V1, V2 and NiOx as HTMs exhibit PCE of 15.3, 6.4 and 18.5% respectively. However, both V1 and V2 PVSCs have a superior moisture stability compared

with that of NiOx PVSCs. We have conducted a series of experiments to elucidate the superior PCE of V1 over V2 and to rationalize the better moisture stability of V1 and V2 PVSCs than NiOx PVSCs.

Keywords: *Perovskite solar cells, Hole-transporting materials, Hydrophobicity, Triphenylamine, Power conversion efficiency, Hole mobility*

Biomass-derived activated carbon as an electrode material for high-performance supercapacitor

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Abstract: The demand for sustainable and environmentally friendly materials has increased the popularity of biomass-derived carbon materials in recent years. This work explores activated carbon produced from *Tamarindus indica* seed waste as an electrode material for high-performance supercapacitors. To enhance the surface area and pore structure, the seed powder was carbonized at 400 °C using $FeCl_3$, followed by KOH activation at 750 °C. XRD, Raman spectroscopy, FTIR, FESEM, EDX, and BET investigations have been conducted to study the different physicochemical aspects of the produced carbon material. The electrochemical performance of the synthesized activated carbon was assessed as electrodes for supercapacitors using an aqueous 6M KOH solution as an electrolyte. A high specific capacitance of 455.32 F/g was observed when 1 A/g of current density was applied, and it also exhibited a high energy density of 13.97 Wh/kg at a power density of 470 W/kg. The high surface area, evenly distributed pore size, and excellent degree of graphitization of the activated carbon are all factors that contributed to its superior electrochemical performance. Hence, this work offers a viable method for using waste biomass as a cheap and environmentally friendly electrode material for energy storage devices.

Keywords: *Waste to Energy; Biomass-derived carbon; Energy Storage; Supercapacitor*

Effective interfacial back surface passivation via i-a-Si:H thin layer of hybrid silicon solar cells

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Abstract: In the present work, the hydrogenated intrinsic amorphous silicon (i-a-Si:H) layer (~8 nm) and n-type nano crystalline silicon (n-nc-Si:H) layer (~18 nm) are introduced in the basic hybrid PEDOT: PSS-silicon solar cell device structure (Ag/PEDOT:PSS/μT-n-Si/In:Ga) to investigate the effect of i-a-Si:H/n-nc-Si:H layers on back surface properties of micro-textured (μT) monocrystalline Si surfaces. It is found that the i-a-Si:H layer provides best passivation to the μT Si surface by saturating the dangling bonds, as confirmed by the minority carrier lifetime (MCLT) and also acts as a good transporting layer. The MCLT was measured on symmetric structure, i-a-Si:H/μT-n-Si/i-a-Si:H as shown in Fig. 1(a). The measured lifetime for the unpassivated and i-a-Si:H layer passivated μT CZ-Si are 2.31 μs and 677.79 μs (shown in fig. 1(b)) respectively. Similarly, for the μT FZ-Si the MCLT are found 2.77 μs to 1788.30 μs (shown in

fig. 1(c)) respectively for unpassivated and passivated Si surfaces. The implied open circuit voltage (i-V_{oc}) for passivated µT CZ-Si is 708 mV and for µT FZ-Si is 714 mV respectively. The heavily doped n-nc-Si:H layer produce back surface field, which further enhances the charge collection rate and reduces parasitic loses under optimize thickness. Also, the improvement in interfacial properties between µT-Si and In:Ga is noticed, which is well supported by enhancement in implied V_{oc} after deposition of i-a-Si:H layer. The analysis of photo-voltaic (PV) characteristic of solar cells concludes that the device (Ag/PEDOT:PSS/µT-n-Si/i-a-Si:H/n-nc-Si:H/In:Ga) needs further optimization to enhance the PV performance.

Keywords: *MCLT, BSF, passivation, PEDOT: PSS, defect-density, HSCs*.

Enhancing room temperature performance of solid-state lithium cell via a facile solid electrolyte-cathode interface design

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Abstract: Herein, we report the enhanced electrochemical performance of a solid-state cell realized through an engineered solid electrolyte-cathode interface via a simple casting technique. The ceramic-in-polymer solid electrolyte sample with 15 wt.% NASICON-type $Li_{1.2}Sn_{0.9}Zr_{0.9}Al_{0.2}(PO_4)_3$ ceramic filler in a P(VDF-HFP) matrix (CPSE15) showed the highest room temperature conductivity of ~ 1.1×10^{-4} S cm^{-1} and lithium-ion transference number of ~ 0.60. The symmetric Li|CPSE15|Li cell showed a consistent voltage profile with an over-potential of ~ 45 mV for 750 h at a current density of 0.1 mA cm^{-2}. CPSE15 slurry was directly cast onto the $LiFePO_4$ (LFP) cathode layer using a doctor-blade coating method to obtain a cathode-electrolyte assembly. Subsequently, a full cell fabricated using this assembly and lithium metal delivered an initial discharge capacity of ~ 157 mAh g^{-1} at 0.2C. Further, the cell exhibited ~ 90 mAh g^{-1} discharge capacity at 1C and sustained 500 charge-discharge cycles at room temperature. The engineered interface in cathode-electrolyte assembly enabled this cell to outperform its conventionally fabricated counterpart with a stacked LFP cathode sheet and freestanding CPSE15 electrolyte membrane, which was attributed to a lower interfacial resistance (~ 51%) of the former.

Keywords: *Solid-state cell; NASICON; Composite electrolytes; Cathode-electrolyte interface; Doctor-blade coating*

$CuCo_2S_4$ Micro Cubes for High Energy Density Zn-ion Hybrid Supercapacitor

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Abstract: Aqueous Zn-ion hybrid supercapacitors (ZHSCs) are promising, cost-effective, safe, and environmentally friendly storage devices. Nevertheless, these supercapacitors have limited capacity, which makes them unable to meet the demands of modern technology for social and economic advancement. Herein, a cost-effective and environmentally friendly synthesis strategy of multivalent $CuCo_2S_4$ which shows a unique micro-cube structure has been proposed for the high-energy-density ZHSCs. The fabricated ZHSC device (Zn || $CuCo_2S_4$) delivers a maximum specific capacitance of 630 F g^{-1} at the current density of 1 A g^{-1}. Moreover, the ZHSC device possesses highest energy density of 43 W h kg^{-1}, with a maximum

power density of 1100 W kg^{-1} exhibiting excellent electrochemical performance and far superior to previously reported carbon-based and pseudocapacitive cathode materials. Multiple oxidation states of $CuCo_2S_4$ facilitating the numerous diffusion channels for fast faradic reactions and the unique porous micro cube structure of $CuCo_2S_4$ providing significant surface area for huge charge storage, results in the superior performance of ZHSC device. This work supports a prospective routine for constructing the new-generation advanced-energy storage systems.

Keywords: *energy storage, supercapacitor, Zn-ion storge, high energy density*.

Design and development of novel metallic porous structures for efficient Thermal Energy Storage Systems

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Abstract: Thermal energy storage (TES) systems play a crucial role in advancing the efficacy and reliability of renewable energy integration and industrial processes. In this regard, the utilization of metallic porous structures presents a valuable resource for TES augmentation, leveraging their innate thermal conductivity, structural robustness, and tunable porosity. This research endeavors to scrutinize the potential of novel metallic porous architectures as TES mediums, combining experimental methods with numerical simulations. The literature review delineates the recent strides in metallic porous material synthesis, explaining their intrinsic thermal attributes, fabrication methodologies like Selective Laser Melting (SLM), and application domains. Subsequently, a research blueprint is realized that pivots around the discerning characterization of the novel structures across a spectrum of operational parameters, with an emphasis on performance optimization, augmented energy storage capacity, and thermal cycling resilience. Finally, the prospective applications of these structures in renewable energy infrastructures and industrial exigencies are systematically explored. The outcomes of this work encompass a seminal contribution to the repertoire of efficient and sustainable TES modalities, charting a definitive trajectory toward a carbon-neutral energy landscape.

Keywords: *Porous structures, Selective Laser Melting, Thermal Energy Storage, TPMS, Topology optimization, Thermal conductivity*

Development of Pt-Co Metallocycle Nanoarchitectures for Transparent-to-black Vis-to-NIR smart windows for Thermal Modulation

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Abstract: An ideal smart window that is efficient for reducing energy cost demands NIR-based electrochromism. In our present study, a bimetallic Pt(II) and Co(II)-terpyridine containing square geometric metallo-supramolecular macrocycle (Pt-Co-TPYN) was synthesized in a step-wise complexation

manner. The Pt-Co-TPYN electrochrome was characterized by different spectroscopic, structural and morphological characterizations. The easy solution processable Pt-Co-TPYN macrocycle demonstrates a reversible transparent orange to complete black electrochromism with a high optical contrast of 88% in a -2.0 to 0.5 V potential window utilizing the redox transition of Co(II) to Co(I) meal center. The Pt-Co-TPYN EC film showed an electrochromic durability of more than 800 cycles, improved switching time of of 8.6 s and 12.1 s for bleaching (t_b) and coloration (t_c) respectively along with high optical contrast of 309.8 cm^2C^{-1}. The presence of Pt-Pt interaction, confirmed by red emission from MMLCT interaction, provides regular arrangement and the presence of uniform pore facilitate the electron movement and counter ion diffusion inside the electrode material. Additionally, in a prototype based smart building demonstration, Pt-Co-TPYN based smart window can differ a temperature difference of 11^0 C inside the prototype home, which was due to the blocking of IR radiation and heat by the Pt-Co-TPYN based smart windows in its black state. Thus solid-state Pt-Co-TPYN based ECD divulges ECM as potential candidate for energy-saving smart window.

Keywords: *Electrochromism, Metallo-supramolecular architecture, Smart windows.*

Electrodeposited Zeolitic Imidazolate Framework-8 Modified Zinc Anode Supported Over Porous Copper Framework for Aqueous Zinc-ion Battery Application

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Abstract: Electrodeposition technique was employed to form a protective layer of zeolitic imidazolate framework-8 (ZIF-8) on the zinc-copper (Zn-Cu) framework, serving as an efficient anode for aqueous zinc-ion battery (AZIB) applications. Initially, the Cu foil subjected to chemical etching with ammonia solution to render its surface porous. Following the successful fabrication of Zn-Cu through electrodeposition, ZIF-8 was subsequently electrodeposited onto the porous Cu framework. By employing this approach, the battery life in symmetric cell configuration was extended to 1000 hours at 0.5 mA/cm^{-2} for the anode with the ZIF-8 layer. In contrast, the pristine Zn experienced a sudden and irreversible voltage drop resulting from a short circuit after operating for 169 hours, while the Zn-Cu framework failed after 853 hours. Additionally, corrosion studies conducted on all three AZIB's anodes, i.e., ZIF-8/Zn-Cu, Zn-Cu, and pristine Zn, revealed that the ZIF-8/Zn-Cu anode configuration exhibits the highest corrosion potential (-425.16 mV) and the lowest corrosion current (0.0008 mA/cm^2), indicating its ability to inhibit corrosion. Moreover, the AZIBs was cycled in a full cell configuration with α-MnO_2 cathode. The results of galvanostatic charge-discharge tests revealed that the ZIF-8/Zn-Cu//α-MnO_2 demonstrated a high initial specific discharge capacity of 206.36 mAh/g at 1 C (where 1 C equals 308 mA/g), retaining approximately 92.77% of its initial discharge capacity after 1000 charge-discharge cycles.

Keywords: *Zeolitic imidazolate framework-8; zinc-ion battery; aqueous battery; anode material; corrosion resistant anode; anodic dendrite*.

Development of CdTe/Perovskite Thin Film Tandem Solar Cells

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Abstract: Solar energy represents a key aspect of the transformation towards sustainable and environmentally friendly energy production. India has geographically benefited from substantial solar flux, which offers a promising field for solar research. This study investigates the development of highly efficient thin-film tandem solar cells by integrating perovskite and cadmium telluride (CdTe) solar cells in a four-terminal (4T) configuration. We have developed transparent perovskite solar cells with an efficiency of 18.3% and ~ 75% average transmission in the NIR range (750 – 900 nm). Subsequently, these were optically integrated with opaque CdTe solar cells, achieving an efficiency of 19.56% in the 4T tandem configuration, resulting in the development of tandem solar cells with an overall efficiency of 23.42%. Furthermore, the introduction of a refractive index matching liquid increased the power conversion efficiency (PCE) to 24.2%. This pioneering work represents the first instance of a 4T CdTe / perovskite thin-film tandem solar cell exceeding a PCE of 24.2%, indicating a significant > 120% improvement in overall efficiency.

Keywords: *Thin-film tandem solar cells, Transparent PSC, CdTe solar cells*

3D-Structured Carbon Induced Triple Phase Boundary Tuning and Enhanced Water Management for High Performance PEMFC

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Abstract: Proton exchange membrane fuel cells (PEMFCs) gained substantial interest in the field of sustainable development as a clean energy conversion technology. Conventionally produced PEMFC electrodes typically have problems with water management, mass transfer, charge transfer, and catalyst utilization. Collectively, these have a considerable negative impact on the cell's performance, especially when used in H_2-Air environments. Thus, to tackle these challenges a critically designed electrocatalyst development is essential. The support materials are crucial in regulating the properties of the catalyst, including high specific surface area, superior electrical conductivity, good electrochemical stability, and strong immobilization of the catalyst to improve the triple phase boundaries (TPBs) in the PEMFC electrodes. We have investigated the synergistic effect of N-doped 3D graphitic carbon integrated with Pt nanoparticles to attain high performance in PEMFCs. Anchoring Pt nanoparticles on N-doped 3D graphitic carbon simplifies catalyst development. The 3D-interconnected structured graphitic carbon is derived from Polydopamine and melamine foam the TPB. The prepared materials outperform *state-of-the-art* Pt/C catalyst. The high performance is attributed to the 3D structural engineering on the carbon support morphology by spatially isolating the active site-bearing surfaces is an effective solution in eliminating mass transfer and water management concerns.

Keywords: *Oxygen reduction reaction, Proton exchange membrane fuel cell, Fast activation, Water management*

Synthesis of Quasi-periodic Inverted Pyramid Microstructure Arrays to attain broad

range Absorption for high efficiency Thin Silicon Solar cells

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Abstract: Photovoltaic industries mostly use crystalline silicon solar cells. However, high reflection is one of the major reasons of low photo conversion efficiency. To reduce reflectivity, surface texturingtechnique would be the great choice. Here we reports fabrication of Lithography free quasi-periodic Inverted pyramid arrays (QIPAs) on silicon wafer by modified metal assisted chemical etching (MACE) method using silica particles as masking layer. For synthesize silica nano/micro particles of various diameters, we have used Stober and modified stober chemical method. The size of inverted pyramid arrays was controlled by etching rate and diameter of silica particles. These textures show ultra-low reflectivity of (3%) in the silicon absorption band (300 nm – 1000 nm). A unique additional absorption of 33 – 44% compared to the planar silicon, in the sub-bandgap region of silicon(1100 – 2000 nm) that leads to large amount of electron hole pair generated which is essential forsolar cell performance. The estimated short circuit current density (J_{SC}) is 55.46 mA/cm^2, which is far higher than the Lambertian limit of ~ 43 mA/cm^2. Also theoretical efficiency of the solar cell can be achieved up to 35.22%, which surpasses the Shockley-Queisser limit of 33.7%.

Keywords: *Photovoltaic, Metal assisted chemical etching, Quasi-Periodic Inverted pyramid, silicon solar cells, Lambertian limit, Shockley-Queisser limit.*

Post-treatment of NiOx-based Hole Transport Layer for high-efficiency Perovskite Solar Cells

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Abstract: NiO_x has been used as a Hole Transport Layer (HTL) for inverted perovskite solar cells due to its high transparency, photostability, high hole mobility, and optimum band alignment with perovskites. From the wide range of deposition techniques available, sputtering is one of the most common and efficient techniques for NiO_x thin-film deposition. However, the post-treatment of these films plays a major role in deciding the device's performance. Here we compare different approaches like post-annealing, oxygen annealing, solvent treatments, etc., and their impact on device parameters. The champion device is obtained by carefully tailoring film properties resulting in an efficiency of 20% for $(MA_{0.9}AA_{0.1})PbI_3$-based solar cells. The treated films show high transmittance and improved HTL-perovskite interface resulting in 24.5 mA/cm^2 short-circuit current. There is a comparative decrease in series resistance and an increase in shunt resistance (in dark) for these films leading to a high fill factor of 78%. A set of 20 devices confirms the consistent enhancement of device performance by choosing the correct post-treatment for NiO_x.

Keywords: *Hole transport layer, NiO_x, Perovskite solar cells, post-treatment, and sputtering.*

Effect of Second Metal Ion and Microstructures on the Electrochemical Performance of Bimetallic Oxide Based Supercapacitors

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Abstract: Bimetallic oxides have emerged as the high performance supercapacitor materials owing to their high specific capacitance value originated from the multiple oxidation states of the metal ions as well as improved conductivity of the final compounds. Supercapacitor performances of these materials vary with the composition, morphology and conductivity of the final compounds. In this paper, effect of second metal ion on the supercacitor properties of $MNxO_4$ (where, M is the first metal ion, N is the second metal ion and x is the stoichiometric number of second metal ion) have been investigated keeping the first metal ion constant. $NiMoO_4$ nanorods, $NiFe_2O_4$ nanoparticles and $NiCo_2O_4$ nano urchin have been synthesized by facile synthesis techniques and investigated or supercapacitor performances. It has been observed that $NiCo_2O_4$ nanostructure with sea urchin like morphology has shown best supercapacitor performance followed by $NiFe_2O_4$ nanoparticles and $NiMoO_4$ nanorods. This can be attributed to the higher electrical conductivity of Co ion as compared to Fe ion as well as hierarchical sea urchin like morphology of $NiCo_2O_4$. Degradation of $NiMoO_4$ nanorods under strong basic electrolyte medium is the possible reason for lowest supercapacitor performance among the other metal oxides in spite of good electrical conductivity of Mo ion.

Keywords: *Supercapacitor performance, electrochemical characterization, bimetallic oxides, nanorods, nanoparticles, nano urchin, effect of microstructure*

Enhancing Stability of Perovskites through Spacer Cation Incorporation forapplication in Solar cells

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Abstract: Organic-inorganic metal halide perovskites (OIHPs) have garnered immense interest for their exceptional power conversion efficiency (PCE). However, their susceptibility to environmental factors like moisture, oxygen, and heat hinders their commercialization. A promising strategy to improve perovskite solar cell (PSC) stability involves the creation of 2D/3D hybrid perovskites byintroducing spacer cations into the 3D structure. This study investigates the effect of octylammonium iodide (OAI) as a spacer cation in $MAPbI_3$. OAI incorporation targets defect passivation, aiming to mitigate defects on the surface and grain boundaries of $MAPbI_3$. X-ray diffraction (XRD), UV visible spectroscopy, Photoluminescence spectroscopy, Time resolved photoluminescence spectroscopy, Raman spectroscopy, FTIR spectroscopy, Scanning Electron Microscopy (SEM) were employed to analyze the impact of OAI on film morphology and stability.The results indicate that OAI facilitates the formation of intermolecular valence bonds between crystalline $MAPbI_3$ domains. This enhanced interconnectivity is believed to contribute to improved structural stability, potentially leading to more durable and efficient Perovskite Solar cell.

Keywords: *Perovskite Solar Cell, Stability, Spacer Cation, Defect Passivation, OAI, MAPbI3*

Manganese malate: A new, high-performance electroactive material for supercapacitors

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Abstract: Among various energy storage devices, supercapacitors have received significant attention due to their fast charging-discharging capability, extended cycle-life, wide operational temperature, etc. Supercapacitors can be used either as standalone device or coupled with rechargeable batteries to power many appliances. However, their energy density is low, which seriously limits their applications in high-energy demand appliances. Therefore, to fully harness the potential of supercapacitors, researchers continue to develop unique materials capable of delivering high energy without compromising power at relatively low cost. Materials studied for supercapacitor include carbonaceous materials, metal oxides, conducting polymers and metal carbonates. Among these, manganese-based materials are attractive due to their superior redox properties, abundant precursors, ease of preparation, environmentally friendly characteristics, etc. Herein, manganese malate is unveiled as an electrode material for supercapacitor applications. Manganese malate is electrodeposited on a stainless-steel foil by chronoamperometry at various applied voltages. The electrodeposited manganese malate is characterized by X-ray diffraction, vibrational spectroscopy and electron microscopy. Electrodeposited manganese malate delivers a specific capacitance of 186 F g^{-1} at a current density of 1 A g^{-1}. Symmetric supercapacitor fabricated using electrodeposited manganese malate delivers an energy density of 5.6 Wh kg^{-1} at a power density of 250.2 W kg^{-1}, which demonstrates excellent capacitance properties.

Keywords: *Electrodeposition; electrode material; energy storage; manganese malate; supercapacitor*

Recycling of Energy Critical Metals from spent Lithium ion Battery as a Secondary Resource

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Abstract: The global production capacity for lithium ion batteries (LIBs) is anticipated to rise dramatically due to widely utilization in portable electronics and electric appliances as well as vehicles, rising from 300 gigawatt-hours to 2 terawatt-hours by 2028. The current demand for LIBs in India stands at 3 GWh and is expected to rise to 70 GWh by 2030. LIBs consist of a cathode, anode, electrolyte, and separator, with 50% of the manufacturing cost attributed to the cathode materials (mainly including Li, Co, Mn, Ni). However, due to their demand and limited availability, Lithium and Cobalt are considered energy-critical metals. A typical LIB contains approximately 5–20% Co, 5–7% Li, 5–20% Ni, and 5–15% Mn. Given the significant demand and scarcity of primary material resources, exploring alternative resources is crucial. Hence, recycling LIBs appears to be a solution, employing various recycling techniques such as pyrometallurgy, hydrometallurgy, and bioleaching to extract metals from used LIBs. Pyrometallurgy utilizes smelting processes to heat and separate materials, while hydrometallurgy involves aqueous methods using various solvents to isolate metals. On the other hand, biohydrometallurgy employs microorganisms to extract metals from discharged batteries in liquid solutions. Thus, this study underscores the sustainability of essential energy metals through different recycling techniques, which can reduce environmental impacts, energy usage, emissions, and align with sustainable development objectives.

Keywords: *Lithium ion batteries, Recycling, Material Sustainability, Secondary Sources, Sustainable development goals*

A Study of Solid-State Electrolyte Based High-Performing Rechargeable Solid-State Lithium-Sulphur Batteries (LSBs)

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Abstract: Recently in civil and Defence sectors lithium-ion batteries emerged as storage devices for electronics and systems operation. However, their technological drawbacks have hindered the development of LIB with improved safety and efficiency. Replacing conventional liquid electrolytes (flammable solvents) with gel polymer electrolytes (GPEs) makes the batteries safe and less expensive. Herein, we report a facile and scalable preparation method of a GPE based on highly safe polyethylene glycol dimethyl ether (PEGDME) plasticizer in a poly (vinylidenefluoride-co-hexafluoropropylene) (PVDF-HFP) polymer matrix. The synthesized GPE shown excellent safety features (non-flammability and thermal stability up to 200 °C) and electrochemical properties at room temperature (high ionic conductivity of 2.2×10^{-3} S cm^{-1} and high lithium transference number). This solid-state lithium sulfur batteries (SSLSBs) based on the Li6PS5Cl SSE were assembled by using the nano-sulfur / multiwall carbon nano-tube & graphene composite combined with Li6PS5Cl as the cathode and Li- alloy as the anode. The cell delivered a high discharge capacity of 1550 mAh g^{-1} at RT for the first full cycle at 0.176 mA cm-2 (~ 0.1 C). The discharge capacity was 1153 mAh g^{-1} after 50 cycles. In addition, the Coulombic efficiency remained near 100% during galvanostatic cycling.

Keywords: *Lithium ion batteries, Gel electrolyte, Graphene, MWCNT, Sulphur*

Fruit peel polyphenol modified P2-type layered $Na_2Zn_{2-x}M^1_XPO_6$ (P,M= Bo,Si,Ex) solid composite polymer electrolytes for ion conducting battery electrolyte applications

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Abstract: Solid polymer composite electrolytes are used in energy storage systems for their high ionic conductivity and electrode compatibility. Recently honeycomb-layered solid electrolyte $Na_2Zn_2TeO_6$(NZTO) reported with high sodium ion conductivity ~10^{-3}S $Cm^{-1.}$. The current research work reports the synthesis of novel fruit peel waste extracted bioactive polyphenolic compound ellagic acid (E_x) modified electrolyte film, $Na_{2-x}M^1_xZn_{2-x}N^1_xP^1_{1-x}P^{11}_xO_6$ (where M^1=E_X,N^1=K, P^1 and P^2=Si, Bo) mixed with PVA polymer. The solution casting technique prepared electrolyte film of thickness 0.260 mm has been coated with silver electrodes then taken for the electrical impedance spectroscopy studies in the frequency of 20HZ - 8 MHz in the 302-423 k temperature range using the Hioki- IM3536 LCR meter. The NZP'O electrolyte film showed the Arrhenius behavior with good ionic conductivity,σ=3.1x10^{-4}s/cm at 294 K and activation energy, E_a=0.2eV. Further, the electrolyte film showed the behavior of electrical conductivity increase with increase of frequency and a decrease of dielectric constant obeying the Jonscher power law with n≤1 and relaxation time, $\tau = 1/\omega_{max}$ The E_X modification enhanced the thermal stability and ionic conductivity properties. Hence, this eco-friendly, inexpensive E_x material may an alternative electrolyte for

the future electrochemical devices.**Keywords:** Lithium ion batteries, Gel electrolyte, Graphene, MWCNT, Sulphur.

***Keywords**: ionic conductivity*.

Electrochemical Analysis of rGO/MoS2 nanocomposite-based electrode for Supercapacitor Application

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Abstract: Supercapacitors have gained popularity in recent years as one of the most promising energy storage technologies for a variety of applications including digital telecommunications, memory backup systems, and hybrid electronic vehicles. This is owing to their long cycle life, higher power density, and quick recharge time. Because of these extraordinary qualities, researchers are drawn to the topic of supercapacitors to create new electrode materials for cutting-edge energy storage devices that are inexpensive, highly efficient, and have a high energy density. Two-dimensional (2D) nanostructures are highly attractive for fabricating nanodevices due to their high surface-to-volume ratio and good compatibility with device design. In the current investigation, the rGO/MoS2 was synthesized using a hydrothermal method, resulting in it being characterized via different techniques such as XRD, FTIR, SEM, UV, XPS, etc. The electrochemical properties of the composite material were evaluated using cyclic voltammetry, galvanostatic charge-discharge tests, and electrochemical impedance spectroscopy. The results demonstrate that the binder-free V_2O_5 electrodes exhibit excellent capacitance of 889.1 Fg^{-1} at 1 A g^{-1} of current density. The combination of rGO with MoS_2 enhances the specific capacitance by 175 %. The findings illuminate the dynamic relationship electrode materials (rGO/MoS2), providing valuable perspectives for making and enhancing high-performance symmetric devices.

***Keywords:** Hydrothermal method, nanocomposite, galvanostatic charge-discharge, specific capacitance, energy storage*

Nanocomposite Separator-Electrolyte Systems for High-Performance Sodium Ion Batteries

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Abstract: In the quest for sustainable energy storage solutions, sodium-ion batteries (SIBs) have emerged as promising alternatives to lithium-ion batteries (LIBs) due to the abundance and low cost of sodium resources. However, the development of high-performance SIBs necessitates the innovation of separator materials capable of enhancing battery efficiency and safety. This research paper presents the fabrication and characterization of a novel separator composed of Polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) filled with Halloysite nanotubes (HNTs) via the electrospinning technique for SIBs application. The electrospun composite separator was systematically synthesized and comprehensively characterized to investigate its morphological, thermal, mechanical, and electrochemical properties. Scanning electron microscopy (SEM) analysis revealed a well-dispersed HNTs network within the PVDF-HFP matrix, resulting in a fibrous structure with enhanced mechanical strength (67 MPa) and ion transport pathways. Thermal stability studies confirmed the improved thermal resistance of the composite separator, crucial for maintaining structural integrity under elevated temperatures. Electrochemical performance evaluation through electrochemical impedance spectroscopy (EIS) and galvanostatic charge-discharge (GCD) cycling demonstrated superior ion conductivity (15.16 $mS.cm^{-1}$) and electrochemical stability of the

Halloysite-filled PVDF-HFP separator, leading to enhanced battery performance, including higher specific capacity (171 $mAh.g^{-1}$). The synergistic effects of HNTs incorporation contribute to the development of robust and efficient separators for SIBs.

Keywords: Sodium Ion Battery, Separators, Halloysite, Polymers, Electrospinning.

Posting of Concentration Gradient-Driven Energy Output by Employing Electrodes Possessing Contrasting Interfacial Activity

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Abstract: Driven by the enormous theoretical potential, concentration gradient is actively pursued as a potential sustainable energy resource. Massive research activities are focused on developing vital components of concentration gradient-driven energy harvesting devices like perm-selective membranes and electrode systems. Here, we report the development of a novel permselective nanofluidic membrane by coating commercial nylon membrane with –SiO– functionalized two-dimensional (2D) nanosheets of vanadium pentoxide (V_2O_5) (VO-@SiO). The membrane potential (E_m) values obtained by deducting redox contributions of the Ag/AgCl electrode suggest that coating of ~14 $\mu g.mm^{-2}$ VO-@SiO improves the transport number of non-ion selective nylon membranes from ~0.5 to ~0.8 (for K^+ ion). We further demonstrated that concentration gradient-driven energy harvesting devices' output potential is significantly enhanced when materials with contrasting interfacial activities are employed as electrodes. Electrodes prepared from functionalized vanadium pentoxide (V_2O_5) and polyaniline (PANI) can generate electrical potential up to 150 mV through complementary charge transfer activities from quiescent water without any concentration gradient. By using a pair of V_2O_5 and PANI, the overall power of the concentration gradient-driven energy generator was improved by 278 % (with 10-fold concentration gradient), as compared to that of Ag/AgCl electrodes.

Keywords: *Energy Harvesting Device; Concentration Gradient; Nanofluidic Membrane; 2D Nanomaterials; Vanadium Pentoxide*

Binder-Free and Flexible $VOPO_4$ /CNT Film Cathode for Aqueous Rechargeable Zn-Metal Battery

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Abstract: The swift development of flexible and wearable electronics in the past few decades brought about an urgent need for compatible power sources that can provide high voltage and seamlessly integrate with these technologies. An innovative cathode material designed to function well under mechanical stress and retain its structural integrity by leveraging the exceptional properties of polyanionic $VOPO_4$ (VP) with a high average voltage (about 1.2 V) and functionalized carbon nanotubes (fCNTs) processible into a free-standing flexible cathode for flexible aqueous rechargeable zinc metal batteries (AZMBs) is presented in this study. The CNTs not only serve as a scaffold for the $VOPO_4$ nanosheets but also wrap around the material, preventing direct contact with the aqueous electrolyte and thus mitigating material dissolution and

forms a cohesive, self-standing film that eliminates the need for a traditional metal current collector, significantly reducing the overall weight of the battery and enhancing the flexibility of the cathode. The resultant composite cathode exhibits high electrochemical performance, including superior capacity retention and cyclic stability. This research demonstrates a promising strategy for advancing flexible energy storage solutions, combining structural innovation with practical performance improvements to meet the demands of next-generation flexible and wearable electronics.

Keywords: *(binder-free cathode, layered $VOPO_4$, flexible electrode, gel electrolyte, flexible Zn-metal battery)*

Theoretical Investigation of Pressure Induced Oscillatory Band-gap and Excitonic Properties in One-dimensional Lead-free Halide Perovskite: $CsCu_2I_3$

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Abstract: Our theoretical investigation attempts to envisage the structural, electronic, optical and excitonic properties of a novel one-dimensional (1D) lead free halide perovskite structure $CsCu_2I_3$, under the influence of hydrostatic pressure. We have performed density functional theory (DFT) based first principles electronic structure calculations to explore the influence of external pressure on the inherent electronic and optical properties of this emerging perovskite structure. At ambient pressure, $CsCu_2I_3$ exhibits a semiconducting behaviour with a finite band gap, which becomes oscillatory with the enhancement of external pressure. This exciting feature of oscillating band gap with pressure makes this system particularly interested, as one can attain a desired band gap value optimum for the respective optoelectronic application with a sensitive tuning of pressure. In addition to understand the underlying mechanism driving these intriguing phenomena, we further explore how this oscillating trend in the band gap is having repercussion on the optical properties, especially the optical absorption and emission spectra and the effective mass of the charge carriers in $CsCu_2I_3$ under the influence of pressure. We also investigate the variation of it's excitonic properties under pressure. The ability to fine-tune the band gap in response to hydrostatic pressure variations can have significant implications for the design of novel optoelectronic devices, while $CsCu_2I_3$ could emerge as a promising candidate for such applications. The findings presented herein could be connected with potential ramifications for its utilization in optoelectronic technologies, such as solar cells and light-emitting devices, where precise control of the band gap is essential for optimal device performance.

Keywords: *Halide Perovskites; Density Functional Theory; Electronic and Optical Properties; Pressure Induced Transition; Oscillatory Band gap, Exciton , Excitonic lifetime*

Hydrothermally grown nickel ions incorporated tin oxide nanostructures as an effective photocatalyst and an electrode in supercapacitor

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Abstract: Pure and Nickel (Ni)-doped SnO_2 nanoparticles (NPs) were synthesized by a facile hydrothermal method. The SnO_2 NPs were characterized by X-ray diffraction (XRD), Fourier transforms infrared

spectroscopy (FTIR), Scanning electron microscope (SEM), Energy dispersive spectra (EDS), High-resolution transmission electron microscopy (HRTEM), UV –Visible spectroscopy (UV-Vis), Photoluminescence (PL) and X-ray photoelectron spectroscopy (XPS). The photocatalytic (PC) results of Ni-doped SnO_2 NPs showed a higher degradation efficiency than the pure SnO_2 NPs. The electrode made of Ni-doped SnO_2 exhibited a maximum specific capacitance (Cs) of 467 F/g at the current density of 5A/g. The device gave a retention of 96.95% after 1000 continuous charge /discharge cycles. The experimental results demonstrated that the optimum concentration of Ni-doped SnO_2 NPs is an excellent bifunctional material for photocatalytic (PC) and supercapacitor (SC) applications.

Keywords: *SnO_2, Ni@SnO_2, hydrothermal pressure method, supercapacitor, photocatalytic, Alizarin red S (AR S), Brilliant green (BG) and Methyl Orange (MO)*

Zinc Oxide Integration for Enhanced Piezoelectricity in PVDF Nanofibers

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Abstract: Flexible piezoelectric materials, capable of converting mechanical stress into electrical energy, hold significant promise for addressing next generation energy needs. This research investigates the synergistic effects of incorporating zinc oxide (ZnO) nanorods into polyvinylidene fluoride (PVDF) nanofiber composites to enhance their piezoelectric properties. By systematically varying the ZnO content, it was discovered that 13% loading have better device performance over devices based on pristine PVDF and other low content of ZnO. X-ray diffraction, Fourier-transform infrared (FTIR) spectroscopy, and Scanning electron microscopy (SEM) tools were used to understand the underlying mechanism. Such advancements hold promise for revolutionizing renewable energy technologies and addressing future energy challenges.

Keywords: *PVDF-ZnO nanocomposites, Electrospinning, Piezoelectric nanogenerator*

Unleashing the Potential of Silicon Micro/Nanowire Arrays: A Path to Higher Efficient Solar Cells

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Abstract: The fabrication of vertically aligned silicon micro/nanowire (SiMW/SiNW) arrays is essential for enhancing solar cell efficiency, with lithography-free techniques offering a cost-effective and scalable solution. Through a combination of silica particle patterning, reactive ion etching (RIE), and modified metal-assisted chemical etching (MACE), silicon nano/microwires were synthesized without lithography. This process involved synthesizing silica particles of varying diameters, creating monolayers of silica particles on silicon substrates, generating interparticle gaps via RIE, applying a gold (Au) coating for chemical reactions, and finally, removing silica particles through ultrasonication followed by MACE. The resulting SiMW/SiNW arrays exhibited enhanced light absorption properties, reducing reflectance within the silicon absorption band and showing additional absorption of 25 –33% compared to the planar silicon in the sub-bandgap region (1100 – 2000 nm) of silicon. Theoretical calculations based on experimental data of wire arrays indicate a potential increase in theoretically estimated short circuit current density of 49.96 mA/cm^2, which is 16% higher than the Lambertian limit of ~ 43 mA/cm^2. This result can lead to the theoretical efficiency of the solar cell up to 28.73% without including the surface passivation effect.

Keywords: *Silicon microwire/nanowire array, Metal-assisted chemical etching, Reactive ion etching, Silica particles, Sub band-gap absorption, Lambertian limit.*

Ligands exchange free PbS-I Colloidal quantum dots solar cell based on the polymeric hole transport layer

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Abstract: In the 21st century, the population is continually increasing, and energy harvesting is a big challenge for this vast population. On the other hand, fossil fuels are on a fast decline. For the concern, photovoltaic technology pulls attention, especially third-generation solar cells due to solution processibility, easy fabrication, and low cost. In third-generation photovoltaics, colloidal quantum dots solar cells are a potential candidate due to their unique properties, such as tunable band gaps, high absorption coefficient, and multiple exciton generation effect. In the last decade, Lead chalcogenide colloidal quantum dots have made impressive progress not only in terms of efficiency but also in terms of technology development. Recently, PbS colloidal quantum dots have reached a 15% efficiency. Here, we report simple and ligands exchange-free colloidal quantum dot solar cells. Our work used direct synthesis of iodine-passivated PbS colloidal quantum dots as n-type and polymers P3HT as p-type materials. The directly synthesized PbS-I colloidal quantum dots crystal structure and size were measured by X-ray diffraction and transmission electron microscopy respectively. The fabricated devices were characterized by I-V measurement under the dark and AM1.5 illuminations.

Keywords: *Colloidal quantum dots solar cells, P3HT, Polymeric hole transport layers, solution processing solar cells*

Efficient polyethylene glycol substituted unsymmetrical zinc phthalocyanine sensitizer for dye-sensitized solar cells

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Abstract: Phthalocyanines are a promising alternative to polypropyridylruthenium complexes for DSSC application for their intense absorptivity at the NIR region; electrochemical, photo-chemical, and thermal stability; and scope of structural flexibility in designing A3B type push-pull system, that would essentially be suitable for the light-harvesting system with efficient electron transfer from the excited state dye to the semiconductor (TiO_2). Ideally, phthalocyanines substituted with three electron-rich bulky donors and a suitable anchoring group result in effective push-pull effects that in turn play a significant role in determining power-conversion efficiency (PCE). Many instances of substitution of alkyl-based linear chains at phthalocyanines were also reported to reduce molecular aggregation. In addition, the choice of an auxiliary dye, $Co^{II/III}$ based electrolyte were reported to enhance the PCE multifold. To incorporate essential properties, we have designed and developed a novel unsymmetrical zinc phthalocyanine $ZnPcT_3C$ dye sensitizer substituted with polyethylene glycols (PEG) as donors and carboxylic acid group anchor, which acted as "push" and "pull" systems respectively. The synthesis, electronic, electrochemical, and photo-voltaic properties of $ZnPcT_3C$ dye sensitizer in the presence of auxiliary dyes and different electrolytes along with DFT studies will be discussed in the poster presentation.

Keywords: *Dye-Sensitized Solar Cell, Zinc phthalocyanine, Asymmetric zinc phthalocyanine.*

Multidentate Coordination-Induced Defect Passivation and Morphology Regulation for Efficient and Stable Inverted Perovskite Solar Cells

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Abstract: The diversity of the defects in the perovskite materials has negatively impacts both the power conversion efficiency (PCE) and long-term stability of the perovskite solar cells (PSCs). Herein, a multifunctional small organic molecule, 4-((trifluoromethyl)thio)benzoic acid is employed where the carbonyl (C=O) group exhibits a strong passivation effect by interacting with both the organic cation (FA^+) and uncoordinated Pb^{2+} ionic defects while the sulfur (S) heteroatom passivates Pb^{2+} defects at the grain boundary and surfaces of the perovskite layer. The CF_3 group protects the perovskite film from ambient degradation as well as stabilizes the perovskite framework by forming hydrogen and ionic bonds with the FA^+ cation and Pb^{2+} ions respectively. Further, interaction between C=O and Pb^{2+} forms a Lewis acid-base adduct which regulates the grain growth process during crystallization and improves the morphology of the perovskite film. This reduced the trap-assisted recombination of charged carriers that enhances its lifetime and transport. As a result, the optimized device showed a marked improvement in efficiency rising from 16.54% in the pristine device to 20.87% with a reduction in hysteresis. Moreover, the optimized device

shows enhancement in stability by retaining ~86% normalized PCE after 40 days of storage under ambient conditions at 25±3 °C and a RH of ~45-55%.

Keywords: *Defect passivation, additive, multifunctional anchoring, morphology, charge transport.*

VO_x anchored $Ti_3C_2T_x$ MXenes heterostructures for high-performance 2.2 V supercapacitors

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Abstract: Pseudocapacitive materials with superior electrochemical properties have attracted significant interest in developing high-performance supercapacitors. Herein, VO_x anchored $Ti_3C_2T_x$ MXene pseudocapacitive materials are synthesized via a solvothermal method to synergize metallic electrical conductivity and redox activity. Pure vanadium oxide synthesis results in VO_2 formation, while in the presence of $Ti_3C_2T_x$, quasi-metallic V_2O_3 and VO_2 (VO_x) are observed due to the decomposition of surface functionalities of $Ti_3C_2T_x$. The growth of the V_2O_3 phase increases with an increase in the weight concentration of $Ti_3C_2T_x$. The optimal composition of heterostructure delivers a specific capacitance of 364 F g^{-1} in a stable potential window of -0.9 V to 1 V, surpassing the specific capacitance of pure VO_2 (245 F g^{-1}) and $Ti_3C_2T_x$ (140 F g^{-1}) in 0.5 M K_2SO_4 electrolyte. Furthermore, the developed symmetric supercapacitor (SSC) delivers an energy density of 45.7 Wh kg^{-1} at a power density of 1.1 kW kg^{-1} with cyclic stability of 78 % for 10000 cycles with a self-discharge open circuit potential of 1.34 V. This work highlights a strategy to develop anodic and cathodic active pseudocapacitive material based SSC to improve energy density and mitigate self-discharge.

Keywords: *Supercapacitors, MXenes, Vanadium oxide, pseudocapacitance.*

Close Space Sublimation of Organic Materials for Solar Cell Application

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Abstract: In recent years, Organic solar cells (OSC) have been promising due to their advantages over silicon-based solar cells. Their low fabrication cost, flexibility and non-toxic nature make them ideal for large-scale fabrication. OSC are fabricated by spin coating or vapour thermal evaporation (VTE), but both methods have challenges. In spin coating method, remnant solvent and the formation of pinholes can lead to shorting of the device. In the VTE method, long deposition time and shadow effect in mask patterning are crucial issues. So, an alternative method is required to reduce the time of fabrication and efficient use of materials. One such method is the Close Space Sublimation (CSS) method, in which the target substrate is kept very close to the source, and fast sublimation of the material is done to get the desired film thickness quickly. Our work focuses on preparing thin films of well-known OSC material, ZnPc, and C60, using CSS and VTE method to study and compare the properties of the as-deposited films using both techniques. Optimizing the growth technique using CSS might enable us to fast fabrication of more efficient CSS-based device for future industrial applications.

Keywords: *Close space sublimation, organic solar cell, ZnPc, C60*

Microstructurally Engineered Interphase for Enhanced Anode Stability in Solid-State Lithium Metal Batteries

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Abstract: Solid-state batteries (SSBs) with lithium metal anode (LMA) and solid electrolyte (SE) can deliver high energy density (460 Wh kg^{-1}) with enhanced safety. Although halide-based SEs such as Li_3YCl_6 (LYC) are stable at the cathode, they undergo severe decomposition in contact with LMA and form a mixed-conducting interface (MCI). Therefore, it is desirable to design stable SEs without compromising the ionic conductivity.Herein, we investigated the chemical stability of pure LYC (σ = 0.51 mS cm^{-1}) and LYC with a 15% excess of LiCl (LYC-LiCl, σ = 0.42 mS cm^{-1}) towards its suitability in SSBs by time-dependent in situ XPS measurements. The composite SEs, i.e., LYC-LiCl, exhibited higher stability compared to LYC. However, in-operando impedance measurements in symmetric cells, i.e., Li|LYC/LYC-LiCl|Li, show that the LYC cells exhibit higher mechanical integrity, emphasizing the crucial role of LiCl. This was further confirmed by a unidirectional critical current density (CCD) test, and a correlation between microstructure, pressure, mechanical properties of the decomposed products, and impedance evolution was established. Furthermore, we show that the cell in a three-layer configuration, i.e., Li|LPSCl|LYC/LYC-LiCl|LPSCl|Li, can handle a current density of > 5 mA cm-2, which is much higher compared to the CCD observed for SEs.

Keywords: *Solid State battery(SSB), Lithium metal anode(LMA), Solid Electrolyte(SE), Li_3YCl_6, Mixed Conducting Interface (MCI), Anode stability, In-situ XPS.*

Exploring Current Degradation in Hydroelectric Cells Through Time-Dependent Impedance Spectroscopy

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Abstract: In response to the energy crisis, a promising green energy generation technology called hydroelectric cells (HECs) utilizing water dissociation is explored. These cells exhibit multifunctionality, generating both green energy and hydrogen. In this study, we synthesized a composite material, lithium-nickel ferrite with exfoliated graphite in HECs using the solid-state reaction method. XRD confirmed the cubic spinel structure of the sample. The morphology of materials has been analysed by FESEM images. The V-I polarisation curves of prepared HECs were studied and found a maximum short circuit current density of 14.65 mA/cm^2 and an off-load power density of 2.17 mW/cm^2. However, current degradation is observed over time. To understand the current fading behaviour, we employed time-dependent electrochemical impedance spectroscopy (EIS). The analysis reveals increasing water dissociation resistance and charge transfer resistance with cell aging. Investigating and addressing these complexities holds promise for enhancing the efficiency and longevity of HECs. Additionally, we propose time-dependent EIS as a valuable tool for understanding degradation in HECs responsible for current fading.

Keywords*: Hydroelectric cells, green energy generation, electrochemical impedance spectroscopy, water dissociation*

Unveiling the effect of twin and grain boundary in sub 2 nm platinum cobalt alloy in high-temperature proton exchange membrane fuel cell through novel hot injection method.

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Abstract: Proton exchange membrane fuel cell is undoubtedly the alternative to future energy. High-temperature proton exchange is still trying to obtain the best suitable catalyst to overcome the degradation in an acidic environment. Emphasizing the need for stability to obtain a platinum-based alloy $Pt_3Co_{(1.3)\,(t,\,g\text{-}b)}$-200 sub 1.3 nm particle enriched with 2D twin and grain boundary defects were prepared. It was clearly understood that 2D defects and particle size control were the obvious outcomes of the hot injection-assisted modified polyol process which not only gave an increased ECSA of 84 $m^2mg^{-1}_{pt}$ but was also stable for 20 K cycles of ADT with a loss of only 4 % and negligible loss in mass activity and specific activity. The twinning of (111) planes of platinum with a high degree of strain not only helped get high onset, $E_{1/2}$ and limiting current of 0.98 V, 0.856 V but also -6.0 $mAcm^{-2}$ compared to Pt/C having 0.91 V 0.817 V and -5.57 $mAcm^{-2}$ its significance has been proven through electrochemical analysis. Performing an HTPEFC testing with the desired catalyst at 45 cm^2 gave a 25% more current response i.e. 53 A compared to 42 A for Pt/C in oxygen. The lightest performed at 22 A in the air for more than 27 hours showing only a 1 mV drop in potential.

Keywords: *Fuel cell, HTPEMFC, grain boundary, twin boundary, hot injection, sub 2 nm particle.*

Harmonizing Additive and Dimensional Engineering for Efficient Triple Cation Perovskite Solar Cell

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Abstract: Despite extensive endeavors to enhance the properties of pure 3D perovskite solar cells (PSCs) through various passivation methods, the scientific community is confronted with the challenge of improving the morphology and optical characteristics of 2D/3D layers to enhance PSC performance. Addressing this critical gap, our study focuses on modifying 2D/3D perovskite layers by integrating 3-(((2-Guanidinothiazol-4-yl)methyl)thio)-N-sulfamoylpropanimidamide (GSPA) into a 3D precursor. Additionally, we introduce 4-Hydrazinylbenzenesulfonamide hydrochloride (HBSA) as a multifunctional organic spacer cation. This proposed additive engineering approach (AEA) notably enhances the absorbance of 2D/3D perovskite layers. Moreover, the photovoltaic (PV) properties of the modified 2D/3D PSCs surpass those of unmodified devices, with a peak power conversion efficiency (PCE) of 22.38%, marking a substantial improvement over the control 3D PSCs, which achieved a PCE of 17.78%. Furthermore, the modified 2D/3D device exhibits superior stability, demonstrating 1500 hours of ambient stability compared to the pristine counterpart, which only sustains stability for 300 hours. Our study presents a synergistic approach aimed at addressing existing challenges in PSCs, offering promising avenues for advancing the field of perovskite solar cell technology.

Keywords: *Defects, Perovskite solar cell, Efficiency, Dimensional engineering, Additive engineering*

Low-temperature solid-state synthesis of advanced fluorophosphate cathodes for Sodium-ion batteries

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Abstract: Sodium-ion batteries (SIBs) are a promising alternative to Lithium-ion batteries because of their low cost and large abundance. The commercial applications of the SIBs are limited by higher preparation costs and lower energy density of the cathode materials. $Na_3V_2O_2(PO_4)_2F$ (NVOPF) is the novel cathode of the NASICON series that has attracted the attention of the researchers due to its higher energy density (~400 Wh kg^{-1}) and working voltage of (~3.8 V vs. Na/Na^+). NVOPF is known for its robust 3D crystal structure, high thermal stability, and excellent ionic conductivity. NVOPF was synthesized by solid-state milling. NVOPF delivers an initial discharge capacity of 105 mAh g^{-1} at 0.1C and 100 mAh g^{-1} at 1C rate, retaining 80% of the initial capacity after 250 cycles owing to the fast sodium-ion diffusion. The Na-ion kinetics have been studied by diffusion study, and structural, morphological, and postmortem analyses have been carried out. Avoiding the cost and high energy consumption, high-energy ball milling is a scalable room-temperature process that can be utilized industrially for the large-scale production of NVOPF-based cathode materials for sodium-ion batteries.

Keywords: *Sodium-ion battery, cathode material, $Na_3V_2O_2(PO_4)_2F$, solid-state milling, room temperature synthesis.*

High surface area carbon-coated lithium iron manganese phosphate ($LiMn_{0.8}Fe_{0.2}PO_4$) a superb electrode material for Lithium-ion batteries

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Abstract: Li-ion batteries are the most successful electrochemical system ever developed due to their high energy density of 150–250 Wh kg^{-1} and can be cycled >1000 cycles. Polyanionic-based materials, $LiFePO_4$ (LFP), have gained attention in the EV market owing to excellent thermal and structural stability and high-rate capability. Compared to LFP, Lithium manganese iron phosphate (LMFP) has a high voltage (4.1 V) and capacity (170 mAh g^{-1}) with similar stability. However, the low electronic conductivity (~10^{-10} S cm^{-1}) and low Li-ion diffusivity (10^{-10}-10^{-13} cm^2 s^{-1}) make LMFP inferior in practical devices. Herein, to improve the electrochemical performance of LMFP, a composite of high surface area carbon (HSAC) and LMFP was prepared with different amounts of carbon coating (4, 6, 8 %). 6 % HSAC coating delivers the best electrochemical performance with 140 mAh g^{-1} initial discharge capacity at 0.05 C and 118 mAh g^{-1} at 1 C rate with >99.5% coulombic efficiency and 93.7 % capacity retention after 1000 cycles. Furthermore, full Li-ion cells were fabricated using an LMFP cathode, graphite, and LTO as anodes for practical application.

Keywords: *Li-ion battery, cathode, carbon-coated Lithium iron manganese phosphate (LMFP), Electrochemical performance*

Phosphomolybdic acid coupled polypyrrole via organic cation linkers for electrochemical supercapacitors

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Abstract: There has been a surge of interest in advancing pseudocapacitive materials for applications focused on energy storage. Incorporating nanostructured active materials in supercapacitors enhances redox kinetics by facilitating rapid surface reactions. In this study, the combination of the Hexadecyltrimethyl-ammonium chloride (DMA) and 1-Benzyl-3-methylimidazolium chloride (BMI) ionic liquids (IL) separately with polyoxometalate (POM) $H_4[PVMo_{11}O_{40}]$ ($PVMo_{11}$) is employed to modify the surface of polypyrrole (PPy) for the preparation of hybrid electrode materials. The electrochemical performance of the synthesized nanocomposites was carried out in an aqueous electrolyte of 0.25M H_2SO_4 and the $PVMo_{11}$-BMI-PPy shows supreme electrochemical properties over the other electrode materials such as $PVMo_{11}$-BMI, $PVMo_{11}$-DMA, and $PVMo_{11}$-DMA-PPy. It exhibits an excellent specific capacitance of 399.95 Fg^{-1} as well as a remarkable energy density and power density of 49.5 Wh kg^{-1} and 906.41 W kg^{-1} at a current density of 1 Ag^{-1}. It also has a cyclic retention of 91.08% after 10000 GCD cycles.

Keywords: *polyoxometalates, Ionic liquids, Polypyrrole, Supercapacitors, Energy density*.

Synthesis and Characterization of P3 and P2 Phases of Mn/Ni-based Na-ion Battery Cathodes

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Abstract: Developing Na-based layered oxide (Na*x*TMO2) cathodes with superior electrochemical characteristics is crucial for the wider commercialisation of Na-ion batteries. In this work, we have prepared a layered sodium-ion battery cathode Na34Mn1116Ni316Al216O2 in P3 and P2 phases structures by varying the calcination temperature. Rietveld refinement of x-ray diffraction data confirmed that the sample calcined at 650 °C adopts a P3-type layered structure (space group: *R*3*m*), whereas the sample calcined at 850 °C crystallises in a P2-type structure (space group: *P*63/*mmc*). These samples exhibited distinct electrochemical behaviour. P3-phase delivered a higher initial capacity of 164 mAh/g compared to 148 mAh/g for P2-phase at 0.1C. In contrast, the P2-phase sample exhibited better rate performance (87 mAh/g *vs.* 70 mAh/g for P3-phase at 4C) and capacity retention of ~ 47% after 200 cycles (only ~ 26% for P2-phase) when cycled in a wide 1.5 - 4.4 V range. Electrochemical impedance measurements before and after cycling confirmed a much larger increase in charge-transfer and electrode passivation layer resistance in the P3 cathode, which explains the much inferior cycling stability of the P3 phase.

Keywords*: Na-ion battery; Cathodes; P2 & P3 phases; X-ray diffraction; Electrochemical impedance spectroscopy*

A Facile Synthesis of Conductive Metal-Organic Frameworks on Electrospun Core-Shell Graphene Nanofiber as Free-Standing Electrodes for Flexible Hybrid Supercapacitors

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Abstract: The development of wearable and flexible energy storage devices depends on freestanding and flexible electrodes. For new-generation supercapacitors, rational modification of graphene is essential to the creation of flexible and freestanding carbon-based electrodes with excellent potential as energy storage facilities. Herein, a novel freestanding/flexible electrode made of porous reduced graphene oxide

carbonized nanofiber (rGO/CNF) is constructed via a sequential technique that involves electrospinning and an in situ NiCo-c-MOF growth on it. NiCo-c-MOF@rGO/CNF revealed a specific capacitance of 1820 F g^{-1} at 1 A g^{-1}, superior rate capability (71.24% at 30 A g^{-1}), high cycling stability (92.4% capacitance retention after 14 000 cycles) with excellent mechanical flexibility because of their high specific surface area, wettability, conductivity, and abundance of active sites. In addition, the flexible asymmetric devices, composed of NiCo-c-MOF@rGO/CNF as the cathode and rGO/CNF as the anode exhibit high energy densities of 52.2 Wh kg^{-1} and 799.65 Wh kg^{-1} respectively. These also have good rate capability and long-life cycle stability of 90.6 % after 12000 cycles, indicating their realistic use. This work offers a different approach to high-performance graphene-decorated NF freestanding electrode preparation, and the method can be used with various 2D materials to create effective electrodes for flexible supercapacitors.

Low thermal conductivity in a new mixed metal telluride $Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$

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Abstract: In the domain of thermoelectrics, it is crucial to prioritize the design of new complex mixed metal tellurides that contain low toxic cations and possess intrinsic ultralow thermal conductivity. Here, we discuss the synthesis of single crystals and polycrystalline samples of $Mn_{1.8(1)}In_{0.8(1)}Si_2Te_6$ using the solid-state synthesis method at 923 K. SCXRD studies reveal that the compound crystallizes in a trigonal ($P\underline{3}1m$) centrosymmetric system with cell constants of $a = b = 7.0483(7)$ Å and $c = 7.1277(8)$ Å with formula unit (Z) of 1. The structure contains three cationic independent sites: one disordered metal site (Mn1/In1), one Mn2, and one Si1 which are bonded with Te1 atoms. The (Mn1/In1) and Mn2 metals in the structure form octahedra with six Te1 atoms and the Si1 atom forms an ethane-like Si_2Te_6 unit with one Si and three Te1 atoms. The optical absorption study of the polycrystalline sample of $Mn_{1.8}In_{0.8}Si_2Te_6$ showed an optical bandgap of 0.6(2) eV. Temperature-dependent resistivity and Seebeck coefficient (S) studies confirmed the p-type semiconducting nature of the sample with high values of S (301 μVK^{-1} to 444 μVK^{-1}). The thermal conductivity measurements of the title compound exhibited an extremely low value of k_{tot} 0.28 $Wm^{-1}K^{-1}$ at 773 K.

Keywords: *Solid state synthesis; Crystal structure; Optical bandgap; Seebeck coefficient; Thermal conductivity.*

NASICON-type Medium Entropy $Li_{1.5}Sn_{1.0}Al_{0.5}Zr_{0.5}(PO_4)_3$ Electrolyte for Solid State Li Metal Batteries

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Abstract: Developing solid electrolytes for all-solid-state lithium batteries with superior performance is crucial for portable energy storage. This study uses a traditional solid-state reaction technique to fabricate a NASICON-type medium entropy $Li_{1.5}Sn_{1.0}Al_{0.5}Zr_{0.5}(PO_4)_3$ (LSAZP) ceramic electrolyte. The Rietveld refinement of room temperature X-ray diffraction (XRD) data confirms a pure rhombohedral phase ($R\bar{3}c$) for LSZAP ceramic sintered at 1050 °C. Temperature-dependent synchrotron XRD data demonstrates an increase in lattice parameter c with a positive coefficient of thermal expansion ($+2.40 \times 10^{-5}$ K^{-1}) and a negative coefficient of thermal expansion (-1.26×10^{-6} K^{-1}) for the lattice parameter a with increasing temperature. Interestingly, despite the anisotropic thermal expansion, no intergranular cracks, typically observed in rhombohedral NASICON-type phases, are noticeable in the scanning electron micrographs of

the LSAZP samples. The sample sintered at 1050 °C (relative density ~ 90%) exhibits an excellent room temperature conductivity of ~ 2.95 × 10^{-4} S cm^{-1} and activation energy ~ 0.39 ± 0.02 eV. The Li-ion transference number is ~ 0.99, suggesting that Li-ion is the dominant charge carrier in the sample. During galvanostatic lithium plating-stripping tests, the symmetric Li|LSAZP|Li cell demonstrates excellent lithium plating-stripping stability over 50 h at a current density of 40 µA cm^{-2}.

Perovskite Cubic Strontium-Zirconate's Behavior Towards Electrolyte-based Supercapacitor Application

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Abstract: In present scenario, design and fabrication of electrode materials for energy storage applications have received enormous attention. Herein, we describe the hydrothermal synthesis of $SrZrO_3$ perovskite cubes and utilization in supercapacitor application. The specific capacitance (Cs) of 990 $F.g^{-1}$ (144.84 mAh g^{-1}) with high cyclic retention up to 6000 cycles was achieved demonstrating remarkable stability of the material. Additionally, various concentrations and electrolyte cations (Li^+, Na^+, and K^+) are utilized to examine the diffusion kinetics of $SrZrO_3$ perovskite electroactive material. The synthesized $SrZrO_3$ perovskite material deliver highest specific capacitance in 2M KOH due to the low hydrated ionic radii are K^+ (0.3 nm) over Na^+ and Li^+ ions. Moreover, the observed high specific capacitance value encourages us to assembled an asymmetric supercapacitor (ASC) device with $SrZrO_3$ as positive electrode and activated carbon as negative electrode which able to enlighten a commercial light emitting diode (LED ~1.8 V) for several minutes. The calculated energy density and the power density of ASC device were around 18.81 $Wh.Kg^{-1}$ and 1313 $W.Kg^{-1}$ which is comparable to various previous material. This works gives a pathway to easy synthesis of $SrZrO_3$ and binder-free approach for electrode fabrication for supercapacitor applications.

Keywords: *Perovskite, $SrZrO_3$, Cube Morphology, Specific Capacitance*

Modified dielectric properties of $MAPbI_3$ through synergistic integration with graphene oxide nanosheets to achieve optimal energy storage solutions

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Abstract: In today's rapidly advancing world of science and technology, escalating demand for energy intensifying the need for research in energy storage applications. Organic-inorganic lead halide perovskite, especially Methylammonium Lead Iodide ($MAPbI_3$), have garnered significant attention due to their exceptional properties, including high absorption coefficients and long charge carrier diffusion lengths. These properties make them highly versatile for applications such as solar cells, lasers, and photoelectrodes. The present study explored the tunable dielectric characteristics of MAPbI3 nanoparticles and $MAPbI_3$@rGO (reduced graphene oxide) nanocomposites, synthesized via the co-precipitation process with varying rGO concentrations. The investigation revealed intriguing dielectric behaviour in the nanocomposite at specific rGO loadings, with potential applications in the materials industry. Dielectric properties were analyzed across a range of frequencies (10 Hz to 4 MHz) and temperatures (25–60 °C). The

FESEM result demonstrate decrease in nanocomposite size and growth of $MAPbI_3$ nanoparticles on rGO nanosheets with increasing doping concentration. The introduction of rGO lead to increase in the dielectric constant by an order of magnitude 2.8×10^6. Again it exhibits low dielectric loss (nearly 2) with increasing rGO doping concentration even at high temperature positioning itself as a potential candidate for energy storage systems.

Keywords: *energy storage, lead halide perovskite, Methylammonium Lead Iodide, rGO, dielectric, nanosheets*

Pseudocapacitive Performance of Reactively Co-Sputtered Titanium Chromium Nitride Nanopyramids towards Flexible Supercapacitor with Li-ion Storage

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Abstract: The present study reports a flexible symmetric supercapacitor (FSSC) device composed of titanium chromium nitride (Ti-Cr-N) nanocomposite possessing uniform distributed nanopyramids deposited directly over flexible stainless-steel mesh (SSM) via reactive magnetron co-sputtering. The development of Ti-Cr-N/SSM thin film electrodes (TFEs) is optimized by varying the titanium (Ti) target's sputtering power. Increasing the titanium concentration in the Ti-Cr-N thin films enhances the electrochemical performance of Li-ion storage, potentially due to the enhanced synergism resulting in improved electrical conductivity, higher ionic conductivity, and increased surface area. The best-performing Ti-Cr-N/SSM TFE with ~11.41% Ti-concentration delivers an excellent specific capacitance of 263.75 F/g (or 40.3 mF/cm^2) at an applied current density of 0.32 A/g in 1M Li_2SO_4. Furthermore, the assembled Ti-Cr-N/SSM||Ti-Cr-N/SSM FSSC device manifests a maximum energy density of 9.27 Wh/kg along with the highest power density of 13.71 kW/kg while preserving ~82.32% electrochemical stability during 4500 continuous charge-discharge cyclings. Moreover, a remarkable mechanical stability of ~90% at a 90º bending angle for the FSSC over 600 GCD cycles demonstrates the Ti-Cr-N nanopyramid's superior resilient structural strength. Therefore, the current Ti-Cr-N nanopyramids-based FSSC offers considerable potential application as an alternative energy storage system in next-generation flexible electronics.

Keywords: *Co-sputtering; Pseudocapacitive storage; Flexible supercapacitor; Titanium chromium nitride; Nanopyramids; Thin film electrode; High power density*.

Understanding the Emergence of Capacitance in Nanoscale MolecularJunctions

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Abstract: Nanoscale molecular junctions (MJs) are celebrated nanoelectronics devices for mimicking electronic functions including rectifiers, sensors, wires, switches, transistors, and memory. However, a capacitive analysis in MJs is rarely sightseen. The present work describes electrochemically (E-Chem) grown thin films of varying thickness (10, 14.3, and 18 nm) using benzimidazole diazonium salts (BENZ-D) on patterned ITO electrodes on which 50 nm of Al contact was made to fabricate large-scale (500 x 500 µm^2) molecular junctions. The capacitanceof these molecular junctions decreases with increasing molecular layer thickness, a behavior attributed to a classical dielectric role in which the geometric capacitance of the

device within a uniform dielectric component is expected to decrease with increasing thickness. The presence of net dipole moment in BENZ-D enhances the polarizability (hence dielectric constant) of the dielectric medium which led to an increase in capacitance of MJs, that reaches values of ~ 59.6 ±4.79 μF cm^{-2}. Combined DC- and AC-based electrical measurements were performed todemonstrate the frequency-dependent capacitive behavior of MJs. Accordingly, BENZ-based molecular junctions can be a suitable building block for the designing of innovative nanoscale energy storage devices.

Keywords: *Electrochemical grafting, molecular-scale capacitance, molecular junctions,electrochemical capacitors, frequency-dependent capacitive response*

$SrFeO_{3-\delta}$ as cathode material for the application in solid oxide fuel cell

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Abstract: SrFeO3-δ (SFO) is known for its mixed electronic ionic conductivity, rendering it a highly promising material for electrode applications in Solid Oxide Fuel Cells (SOFCs). Our study involves synthesis and fabrication of cell to study its electrochemical performance in both fuel and electrolyzer cell mode. Employing an EDTA-citrate sol-gel process, we meticulously prepared the sample, which exhibited a distinct tetragonal structure with oxygen vacancies as confirmed by XRD Reitveld refinement. Thermal expansion coefficient was found to be 21×10^{-6} K^{-1}, measured up to 900°C.The cell was fabricated by screen printing SFO cathode slurry onto anode supported half-cell with NiO-8YSZ anode, 8YSZ electrolyte made via tape casting. A GDC:SFO buffer layer (1:1wt ratio) was added to prevent high-temperature reactions between the cathode and electrolyte. Maximum power density achieved in fuel cell was 212 $mW.cm^{-2}$. Polarization resistance rose from 0.082 Ω to 0.174 Ω after 17 hours of operation in gaseous environment. In electrolyzer mode, with steam fed to cathode, maximum current density of 0.35 $A.cm^{-2}$ was observed. Electrolyte-supported symmetric cells, using GDC as electrolyte, showed area-specific resistance (ASR) increasing from 0.188 $Ω.cm^{-2}$ at 700°C to 0.298 $Ω.cm^{-2}$ at 800°C, indicating suitability for lower temperature operation for IT-SOFC.

Keywords: *Symmetric cell, $SrFeO_{3-\delta}$, area specific resistance, Fuel cell, Electrolyser cell*

Ionic Thermoelectricity through Reconstructed Layered Material based Nanofluidic System

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Abstract: Owing to the unique properties and distinct advantages, ionic thermoelectric materials are emerging as a promising alternative to conventional electronic thermoelectric materials. However, most research efforts are limited to ionic polyelectrolytes and ionic liquids. Here, we developed a unique platform for ionic thermoelectric studies by reconstructing atomically thin 2D sheets of different layered materials. The well-defined 2D channels of lamellar nanofluidic membranes allowed an efficient migration of ions under the temperature gradient. The large possible options in surface tuning/modification allowed an easy tuning of the thermovoltages from these class of materials dramatically improving the practical utility. High temperature stability is another promising feature of these inorganic layered materials, adding extra aids to the broad range applicability.

Keywords: *Ionic thermoelectricity; Nanofluidics; 2D materials; Seebeck coefficient; Thermovoltage*.

Bandgap prediction of non-metallic crystals through machine learning approach

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Abstract: In this work, we implemented machine learning approach to predict the bandgap of several types of non-metallic crystals. The bandgap is one of the crucial factors for thermoelectric performance. In our investigation, we selected important thermoelectric parameters suitable to predict bandgap by investigating the correlations between them. With the highest correlated features (the Seebeck coefficient and its corresponding temperatures) we employ several machine learning models and determine the model's performance. We perceived highest R^2 of 97.55 % between predicted and actual values with random forest regressor model, which represent a noticeable sign to depict the bandgap estimation of semiconductors, doped with suitable concentration and are useful for device design.

Keywords: *bandgap, machine learning, regression models, non-metallic crystals*

Electrochemical Behaviour of a P3–type High Na Content Cathode for Na-ion Batteries

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Abstract: Among the various layered transition metal oxide cathodes for Na-ion batteries, high-Na content P3-type cathodes are relatively underexplored. In this work, $NaMn_{0.6}Ni_{0.3}Cu_{0.1}O_2$ cathode material with P3 phase (P3-NMNC) was synthesized by a sol-gel method and characterized for its structural and electrochemical properties. The spheroid particles with a reduced Na-ion diffusion path showed excellent rate performance (specific capacity at 3C being 77% of the specific capacity at 0.1C). The P3-NMNC half-cells cycled between the voltage range of 2.0 – 4.0 V exhibited a specific capacity of ~ 133 mAh g^{-1} (at 0.1C) and much better cycling stability (~ 83% capacity retention after 200 cycles at 1C) as compared to the cells cycled in the wider 2.0 – 4.2 V range, where the capacity degraded below 80% of initial capacity in just 75 cycles. The dQ/dV vs. V plots revealed an irreversible peak above 4.0 V during the first desodiation process, which could be attributed to an irreversible anionic redox leading to poor cyclability. *Operando* Synchrotron XRD studies confirmed a reversible P3 ↔ P3' ↔ O3 transformation in NMNC during sodiation-desodiation. These results unveil the potential of the scarcely explored P3-type phases in advancing the development of cathodes for sodium-ion batteries.

Keywords*: P3-type cathode, Na-ion batteries, Cycle life, Operando Synchrotron XRD, Phase transformation.*

Theoretical investigation of Pressure-Driven Electronic, Optical and Excitonic properties in lead-free Halide Perovskite: $Cs_3Cu_2I_5$

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Abstract: This theoretical investigation delves into the structural, electronic, and optical properties of the novel lead-free halide perovskite structure $Cs_3Cu_2I_5$ under the influence of hydrostatic pressure. Hydrostatic pressure is a useful stimulus to obtain novel crystal structures and electronic properties. The prime motivation of this work is to gain insights into the potential effects of pressure on this emerging material, with particular attention to its electronic band structure, optical and excitonic properties. The non-toxicity and high PLQY of this material make it a very interesting candidate. We have performed density functional theory (DFT) based first principle's electronic structure calculations to envisage the electronic and optical properties tuning under the influence of hydrostatic pressure. Our investigation explores the response of $Cs_3Cu_2I_5$ to monotonically increasing hydrostatic pressure, with a focus on the possible changes in its band gap, optical behavior, notably the optical absorption and emission spectra and the effective mass of the charge carriers. The potential mechanisms underlying any observed changes are also of interest, as these may provide valuable insights into the fundamental principles governing the behavior of perovskite materials under pressure. The responses of $Cs_3Cu_2I_5$ under varying hydrostatic pressure provides a foundational understanding of the potential electronic and optical property tuning in this perovskite compound that can have significant impact in designing novel optoelectronic devices.

Keywords: *Density Functional Theory; Halide Perovskites; Electronic and Optical Properties; Pressure Induced Transition; Effective mass; Excitonic lifetime*

Iron-based PBA @ rGO composite as high capacity & high energy density cathode for hybrid supercapacitor

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Abstract: Innovative energy conversion and storage technologies have drawn much interest in the context of environmental protection and sustainable development. Supercapacitors (SCs) with redox materials have been widely studied to enhance energy density. It is necessary to synthesize electrode materials with high capacity, broad working potential window, and excellent cyclic stability. Iron-based Prussian blue analogs (FPBAs) show potential as affordable and easily prepared positive electrode materials for sodium-based energy storage devices. In this study, we have used a modified co-precipitation method to synthesize high-performance FPBAs for sodium ion storage. The homogeneity of cube-shaped FPBA formation is confirmed by field-emission scanning electron microscopy (FSEM). The refined X-ray diffraction (XRD) data confirms a pure phase of the sample. Fourier transform infrared spectroscopy (FTIR) shows the absorption peaks of Fe-C≡N-Fe bonds, confirming the formation of FPBA. To enhance the properties of FPBA, we made a composite of FPBA and reduced graphene oxide (rGO) by simple ultrasonication method. The electrochemical result of the electrodes prepared by the synthesized materials reveals that, owing to the combined effect of conductive rGO and redox-active FPBA, the FPBA/rGO gives excellent results. The FPBA/rGO hybrid composite demonstrated the maximum specific capacity,

435 C g^{-1} at 1 A g^{-1}, long-term cyclic stability with 86% retention in capacity over the 10,000 charge-discharge cycles at 10 A g^{-1}, and superior rate capability. The hybrid symmetric supercapacitor device (SScD) also shows a high energy density of 124.65 Wh g^{-1} at a high-power density of 1.8 kW kg^{-1} and long-term stability (90.5 %, 10,000 cycles). All the findings recommend using battery-type material, a promising strategy for developing energy storage hybrid electrodes for sodium ion storage devices with long lifespans and high energy density.

Keywords: Prussian blue analogous, Hybrid supercapacitors, Sodium ion storage, rGO, Energy storage.

AGC of Deregulated Power System using Polar FLC

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Abstract: Fuzzy logic controllers need lots of precise data. More rules in a knowledge source make it more sophisticated, which affects response time and space. To overcome this challenge a Polar FLC (PFLC) is designed and implemented in the deregulated power system for load frequency control, when there is a sudden change in load. Also the frequency deviations in different areas and tie-line power between them can be restored quickly. PFLC is proposed for a deregulated power system. SIMULINK models are developed in MATLAB version R2021a in order to examine the dynamic responses for the system. Compared to a Ziegler Nichols-PI controller, PFLC with RFB improves delta F_1 settling times by 70.29% and 58.24% for different power transactions, improves delta F_2 settling times by 70.83% and 58.97% and improves delta Pt_{ie} settling time by 42.33% and 34.67%. For different power transactions, the performance of PFLC with RFB is compared with a ZN-PI controller. It is found that undershoots, overshoots and settlement time of PFLC with RBF is better. To fine-tune the suggested controller gains, current optimizations techniques may be explored as potential future developments. Furthermore, research on how renewable energy sources affect the proposed system's dynamic performance may be done.

P3HT: PC71BM-based flexible Organic Solar Cells for Indoor IoT Applications

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Abstract: Organic Solar Cells (OSC) possess many unique properties like high flexibility, tunable bandgap, aesthetics, transparency, lightweight, and non-toxicity. They function well under low-light conditions and cloudy environments as their structures can be well-tuned to match the spectrum of the incident light. All these properties make them a primary candidate for the Internet of Things (IoT) which requires very low energy (~μW) for their functioning. There has been huge progress in the development of flexible devices. Here we focus on the fabrication of flexible OSC made in completely ambient conditions. Cells are made with inverted architecture with PET/ITO/ZnO/P3HT:$PC_{71}BM$/MoO_3/Ag. Absorption spectra of the blend are recorded. J-V characteristics of cells in AM1.5G as well as in Indoor lighting are made for varying intensities and photovoltaic parameters are tabulated. EQE measurements are also done. Finally, J-V measurements after different bending cycles are measured and logged.

Keywords: *Solar cell, IoT, Indoor, Photovoltaics, Flexible, Green energy*

Uncovering the Potential of Pseudo-Boehmite AlOOH/NGr Composite-Based PtIr Electrocatalyst for Efficient Electrochemical Ammonia Oxidation for Direct Ammonia Fuel Cell

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Abstract: The growing interest in low-temperature Direct Ammonia Fuel Cells (DAFCs) arises from the utilization of a carbon-neutral ammonia source, which is attributed to its convenient storage and transport properties. However, DAFCs encounter significant electrode overpotentials primarily due to the substantial energy barrier of the $*NH_2$ to *NH dehydrogenation, compounded by the facile deactivation by *N on the Pt surface. In this work, we introduce a unique catalyst, Pt_4Ir/ANGr, composed of PtIr alloy nanoparticles decorated on pseudo-boehmite phase of AlOOH-supported NGr (AlOOH/NGr) composite, synthesized *via* polyol reduction method. The AlOOH provides an -OH-rich surface conducive to the facile adsorption and decoration of the PtIr alloy nanoparticles, while NGr enhances the electrical conductivity as well as the decoration of the nanoparticles. The detailed studies on the structural and electronic properties of the catalyst by XAS and VB-XPS revealed the possible electronic modulations. The optimized Pt_4Ir/ANGr composition exhibits a significantly improved onset potential and mass activity for AOR. The DFT calculations suggest that Pt_4Ir (100) facilitates the conversion of the $*NH_2$ to *NH with minimal energy barriers. This study thus uncovers the potential of the Pt_4Ir catalyst in synergy with ANGr, largely addressing the challenges in hydrogen transportation, storage, and safety within DAFCs.

Keywords: *ammonia oxidation reaction, direct ammonia fuel cells, d-band center, density functional theory (DFT) study, hydroxyl spillover effect, XAS analysis.*

Fluorinated Ether-based Electrolytes for Sodium-Ion Batteries

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Abstract: The increasing demand for sodium-ion batteries (SIBs) across diverse applications necessitates advancements in electrolyte formulation to enhance their performance under varying operational conditions. Achieving optimal electrolyte properties, such as high ionic conductivity, low viscosity, and efficient solid electrolyte interphase (SEI) formation, remains a significant challenge. In this study, we explore the fluorination of electrolytes as a strategy to address these challenges and improve the overall performance of SIBs. We systematically investigated a family of terminally fluorinated 1, 2-diethoxyethane (DEE) as solvent and sodium bis(fluorosulfonyl)imide (NaFSI) as salt to form the electrolytic mixture by employing density functional theory (DFT). The position and amount of F atoms functionalized on DEE were found to affect electrolyte performance greatly. Among the investigated electrolytes, the fully fluorinated $-CF_3$terminal group was identified as the optimal candidate, providing faster Na^+ion desolvation, which is critical for uniform Na deposition and superior cycling performance. Furthermore, the reduction of the electrolyte suggests the presence of NaF during SEI formation, contributing to enhanced stability.

Keywords: Sodium-ion battery, Electrolyte, Fluorination, Solid electrolyte interphase

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In-situ Synthesis of Ag-doped Hollandite Manganese Oxides on Polypyrrole Support Towards Supercapacitor Application

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Abstract: A facile in-situ method of liquid/liquid (L/L) polymerization strategy for synthesizing silver doped hollandite manganese oxide (Ag-HMO) on polypyrrole (PPy) support is reported for the first time. The highly innovative synthetic method involves producing α-MnO_2 attached to PPy oligomers under low-temperature conditions. Subsequently, Ag^+ ions are in-situ intercalated to the 2 × 2 tunnels in α-MnO_2 to generate Ag-HMOs incorporated PPy. Density functional theory-based calculations yield negative formation energies, suggesting that Ag-HMO might be formed through the tunnel doping of Ag^+ in α-MnO_2. The field emission scanning electron microscopy images confirmed the inevitable role of silver nitrate in microstructure tuning of PPy/Ag-MnO_x (PAgMn) composites spanning from two-dimensional (2-D) flakes to 2-D porous mats to three-dimensional (3-D) dendrites. The powder X-ray diffraction assessed the ability of the L/L interface to control the silver doping and in turn, the crystallinity, phase purity, and physical structure of the PAgMn composites. The Ag^+ ion binding energies in the deconvoluted X-ray photoelectron spectrum of Ag 3d validated the tunnel-level Ag^+ doped HMOs. The composite was further utilized for the fabrication of electrodes on flexible carbon cloths for supercapacitor applications.

Keywords: *Liquid/liquid interface; hollandite manganese oxide; interfacial tension; polypyrrole; two-dimensional; supercapacitors*

Electronic and Optical Properties analysis in Silver Bismuth-Based Perovskite($AgBiI_4$): A theoretical study

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Abstract: This theoretical study explores the structural, electronic, and optical characteristics of the innovative Silver Bismuth based perovskite $AgBiI_4$, particularly under the effect of hydrostatic pressure. Silver iodo-bismuthates Compounds with the formula Ag*x*Bi*y*I*x*+3*y* are effective photon absorbers and hold potential for a range of optoelectronic devices. As $AgBiI_4$ belongs to this family, so it is an interesting candidate to look at its properties. Density functional theory (DFT) based first-principles electronic structure calculations is conducted to investigate the change of electronic and optical properties under hydrostatic pressure. This study examines the varying properties of $AgBiI_4$ with increase in hydrostatic pressure, focusing on potential changes in its band gap, optical absorption and the effective mass of charge carriers. This provides a foundational understanding of how its electronic and optical properties can be tuned which could significantly impact the design of novel optoelectronic devices.

Keywords: *Density Functional Theory; Silver Bismuth based Perovskites; Electronic and Optical Properties; Pressure Induced Transition; Effective mass*

Investigating the Effect of Cu^{+2} Substitution on the Supercapacitor Performance of Cobalt Ferrites

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Abstract: Metal ferrites have outstanding electrochemical characteristics owing to the numerous oxidation states of the metal ions, making them promising materials for addressing both sustainable energy conversion and storage and growing environmental issues.[1] Therefore, nanocrystalline transition metal ferrites such as $CoFe_2O_4$ and $Cu_xCo_{1-x}Fe_2O_4$ (x= 0, 0.1, 0.2, 0.3, 0.4, and 0.5) were synthesized using combustion method and were used as electrode materials for supercapacitor applications. Our work investigates the effect of Cu^{+2} substitution on the structural, morphological and electrochemical performance of the synthesized compounds. The synthesized materials were characterized using XRD, IR, FESEM, Raman, and BET studies. The findings illustrated the formation of a single-phase spinel ferrite as proved from XRD data. Additionally, it was also observed that Cu^{+2} substitution directly influenced the lattice parameters and the average crystallite size of substituted ferrites and the electrochemical performance, thus proving that the said compound act as supercapacitor material.

Keywords: *Ferrite, Supercapacitor.*

Dendritic Growth Suppression in Hybrid Redox Flow Batteries

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Abstract: Hybrid redox flow batteries, including zinc-bromine, zinc-cerium, soluble lead, and all-copper systems, undergo metal deposition and dissolution processes during their charge-discharge cycles. The progressive growth of dendrites over multiple charge-discharge cycles is an inevitable phenomenon in such devices. Starting with an initial performance loss, dendritic growth can lead to short-circuiting failure. This work is concerned with studying the influence of electrolyte composition, electrode morphology, and operational parameters on dendritic growth during electrodeposition of the materials relevant to redox flow batteries: zinc, lead, and copper. The results show that the formation of dendrites is dependent on the reduction potential of the metal ions, with zinc exhibiting the most pronounced dendritic growth as a result of its high reduction potential. Various suppression strategies are examined, including the use of additives, surface coatings, and advanced electrode materials. Electrochemical techniques like cyclic voltammetry, chronoamperometry, and impedance spectroscopy are used to analyze the efficacy of these strategies. Understanding dendritic growth mechanisms offers valuable insights into the improvement of battery performance, longevity, and safety.

Keywords: *Hybrid redox flow batteries, metal electrodeposition, dendritic growth, additives, dendrite suppression*

Band-structure modification leads to enhanced thermoelectric performance of Bi2S3 by CaCl2 doping

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Abstract: Among the various chalcogenides, bismuth sulfide has garnered considerable attention in recent years for thermoelectric applications because it comprises earth-abundant, low-cost sulfur. However, it has low electrical conductivity compared to the other chalcogenides, limiting its thermoelectric performance. Here, using a small concentration of CaCl2 doping, we have demonstrated ~3 times enhancement of *ZT* in Bi2S3. Such a surge in *ZT* is achieved primarily by improving the electron transport behavior in Bi2S3. Due to the incorporation of CaCl2 in Bi2S3, two orders of magnitude increase in electron concentration is observed. Further, the electron mobility is also found to be increased in CaCl2-doped Bi2S3. As a result, an unprecedented ~370 times increase in electrical conductivity and 5 times rise in power factor are attained in CaCl2-doped Bi2S3. DFT calculation implies that CaCl2 incorporation indeed modifies the band structure of Bi2S3 creating multiple valley degeneracies in the conduction band paving way the smoother electron transport in environmentally benign n-type doped Bi2S3.

Keywords: *Chalcogenides, Thermoelectric, Spark Plasma Sintering, n-type semiconductor, TEG*

Transforming Residual Lithium Compounds on $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ Surface into a Li-Mn-P-O-based Composite Coating for Multifaceted Improvements

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Abstract: $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ is the most promising cathode material for next-generation automotive lithium-ion batteries (LIBs). However, the chemical instability of the material during air exposure leads to the formation of residual lithium compounds (RLCs – LiOH, Li_2CO_3) on the surface and inhibits its practical application. Here, we propose a chemical conversion process to remove RLCs by utilizing them and forming a hybrid coating layer on the surface of NMC811 that contains Li_3PO_4, $LiMn_2O_4$, and $LiMnPO_4$ phases, yielding multifaceted benefits. The hybrid layer on the surface protects the material from undesirable side reactions. It improves the cycle life of NMC811 by retaining 80 % of its initial capacity after 300 cycles and 66 % after 500 cycles at a 0.5 C rate in the operating voltage of 3.0 - 4.3 V. The process enables high voltage (4.7 V *vs.* Li^+/Li) operation by stabilizing the electrode-electrolyte interface, reduces the degree of cationic disorder and the voltage polarization for phase transitions, improves coulombic efficiency and ion diffusion kinetics, and minimizes the secondary particle crack formation over long-term cycling. In fact, the coating reduces the detrimental effects of RLCs, leaves the surface for better Li^+ transport, and, hence, significantly improves the electrochemical performances of NMC811.

Keywords: *NMC811 cathode, Residual lithium compounds, Li-Mn-P-O-based Composite Coating, Electrochemical performances, Particle microcracking, Li/Ni mixing*

Development of Binder-Free Electrodes Using Synthesized V_2O_5 for Supercapacitor Application

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Abstract: The progression and enhancement of high-performance supercapacitors are pivotal for the advancement of energy storage technologies, which are essential for meeting the increasing energy demands and sustainability goals. In this context, our study introduces an innovative approach involving the synthesis and application of vanadium pentoxide (V_2O_5) as a binder-free electrode material specifically designed for supercapacitors. V_2O_5 was synthesized using a hydrothermal method, resulting in it being characterized via different techniques such as XRD, FTIR, SEM, UV, XPS, etc. The electrochemical properties of the synthesized V_2O_5 were evaluated using cyclic voltammetry, galvanostatic charge-discharge tests, and electrochemical impedance spectroscopy. The results demonstrate that the binder-free V_2O_5 electrodes exhibit excellent capacitance of 109.8 F g^{-1} at a scan rate of 1 mV s^{-1}. The unique nanostructure of the V_2O_5 enhances ion diffusion and electron transport, contributing to its superior performance. This exceptional performance is largely attributed to the unique nanostructure of the V_2O_5, which facilitates enhanced ion diffusion and electron transport. The absence of a binder in the electrode material reduces internal resistance and ensures maximum utilization of the active material, thereby significantly improving the capacitive performance.

Keywords: *Vanadium pentoxide, Binder-free, Water, Graphite sheet, Supercapacitor*

Separator-modified anion conducting polymer electrolyte membrane with *In-situ* engineered cathode for quasi-solid-state Zinc-air battery applications

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Abstract: This work introduces a novel concept of electrode|electrolyte interface enhancement using ultraviolet (UV) light-assisted *in-situ* polymerization strategy to improve the performance of quasi-solid-state zinc-air batteries (ZABs). The suitability of the UV polymerization strategy to process a mechanically stable OH conducting anion exchange polymer electrolyte membrane (AEPEM) reinforced by glass fiber (GF) separator is also reported. The *in-situ* polymerized ionomer-skin/interlayer (a thin anion-conducting polymer coating over the air-cathode of ZAB) acts as a buffer layer to narrow down the performance gap generally observed between the conventional ZABs possessing quasi-solid-state electrolytes and standard liquid electrolytes, respectively. For instance, when combined with the *in-situ* polymerization strategy, a rechargeable ZAB (rZAB) based on an AEPEM-GF composite membrane delivered a high power density of 140 mW cm^{-2}, higher than the one without an *in-situ* polymerized ionomer interlayer (120 mW cm^{-2}). Notably, in a flexible rZAB configuration, this new strategy resulted in enhanced rate capability and cycling stability for 14 h at an operating current density of 2 mA cm^{-2}.

Keywords: *Anion exchange polymer electrolyte membrane, triple-phase boundary, in-situ polymerization, flexible and rechargeable zinc-air batteries.*

Hydrogel Polymer Electrolyte Integrated 3D Porous Cathode Material for Quasi-Solid-State Zinc Metal Battery by *in situ* Polymerization

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Abstract: This work features the development of a superior cathode|electrolyte interface for the quasi-solid-state rechargeable zinc metal battery (QSS-RZMB) by a hydrogel polymer electrolyte having high ionic conductivity, high mechanical strength and higher cation transference number using an ultraviolet (UV) light-assisted *in situ* polymerization strategy. By integrating the cathode with a thin layer of the hydrogel polymer electrolyte, this technique produces an integrated interface that ensures quick Zn^{2+} ion conduction. The enhanced electrolyte ion infiltration and diffusion by the 3D porous structure with a wide open surface of the ZMO electrode complements the interface formation during the *in situ* polymerization process. The QSS-RZMB configured with an integrated cathode and the hydrogel polymer electrolyte as the separator yields a comparable energy density of 214.14 Wh kg^{-1} with that of its liquid counterpart (240.38 Wh kg^{-1}, aqueous electrolyte). Other noteworthy features of the presented QSS-RZMB system include its superior cycle life of over 1000 charge-discharge cycles and 85% capacity retention with 99% coulombic efficiency at the current density of 1.0 A g^{-1}, compared to only 60% capacity retention over 500 charge-discharge cycles displayed by the liquid-state system under the same operating conditions.

Keywords: *Quasi solid-state rechargeable zinc metal battery, in situ polymerization, cathode-electrolyte interface tuning, hydrogel polymer electrolyte, dendrite inhibition, epitaxial zinc deposition*

Triboelectric Energy Harvesting by Redox Active Molecules

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Abstract: For thousands of years, the triboelectric effect has been present in our daily life. It describes a charge separation process, when two, different or same, materials are contacted or are in motion against each other. While the physical origins of the triboelectric effect are still not well understood, triboelectric nanogenerators (TENG) have been already developed as prospective energy sources. Here, the capability of redox active molecules for an efficient triboelectric charge transfer is investigated, serving as a novel route for the development of TENGs with enhanced performance. In particular, redox molecules with opposite electronic character (electron donors and acceptors) are synthesized, namely Phenothiazine (PTZ), Tetrathiafulvalene (TTF) and Tetracyanoanthraquinodimethane (TCAQ). Then, Au based test samples are functionalized with those redox molecules and then contacted. Surface sensitive techniques, such as X-ray Photoelectron Spectroscopy and Kelvin Probe Force Microscopy are used to probe the functionalization quality and to obtain the surface potentials before and after contacting experiments to understand the extent and the mechanisms of charge transfer. These experiments enable us to probe the impact of surface functionalized redox active molecules on triboelectrification and provide a new approach for efficient energy- harvesting.

THEME-C: Green Hydrogen

Development of a highly efficient V@S Co-doped Ta_3N_5 solar catalyst protected by PANI for H_2 production via water electrolysis

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Abstract: Supercapacitors have gained popularity in recent years as one of the most promising energy storage technologies for a variety of applications including digital telecommunications, memory backup systems, and hybrid electronic vehicles. This is owing to their long cycle life, higher power density, and quick recharge time. Because of these extraordinary qualities, researchers are drawn to the topic of supercapacitors to create new electrode materials for cutting-edge energy storage devices that are inexpensive, highly efficient, and have a high energy density. Two-dimensional (2D) nanostructures are highly attractive for fabricating nanodevices due to their high surface-to-volume ratio and good compatibility with device design. In the current investigation, the rGO/MoS2 was synthesized using a hydrothermal method, resulting in it being characterized via different techniques such as XRD, FTIR, SEM, UV, XPS, etc. The electrochemical properties of the composite material were evaluated using cyclic voltammetry, galvanostatic charge-discharge tests, and electrochemical impedance spectroscopy. The results demonstrate that the binder-free V_2O_5 electrodes exhibit excellent capacitance of 889.1 Fg^{-1} at 1 A g^{-1} of current density. The combination of rGO with MoS_2 enhances the specific capacitance by 175 %. The findings illuminate the dynamic relationship electrode materials (rGO/MoS2), providing valuable perspectives for making and enhancing high-performance symmetric devices.

Keywords: *Hydrothermal method, nanocomposite, galvanostatic charge-discharge, specific capacitance, energy storage*

Effect of electronic structural engineering of Ni site by Fe doping for bifunctional oxygen electrocatalysis

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Abstract: In recent years, oxygen electrocatalysis has emerged as a critical research area in electrochemical energy devices. The most efficient electrocatalysts, thus far, have been noble metal/metal oxides such as Pt, RuO_2, and IrO_2. However, these noble metal electrocatalysts' high cost and scarcity hinder their large-scale application. Hence, developing noble metal-free catalysts is crucial in water electrocatalytic research. This study focuses on the comparison of Fe insertion into the Ni-based selenides derived from coordination polymer. The synthesized metal selenide derived from coordination polymers underwent characterization via powder XRD, HR-TEM, FTIR, and XPS. The synthesized NiFe-based selenides are investigated for electrocatalytic alkaline OER & ORR. The Fe doped Ni NTA-derived Selenides show better electrocatalytic activity due to changes in electronic structure. The Fe-doped $NiSe_2$ shows better electrocatalytic activity of overpotential of 250mV at 10mA cm^{-2} and better ORR performance of about 95% selectivity towards H_2O_2. This work focuses on improving the electrocatalytic activity via structural engineering and phase-dependent

catalytic performance. It provides a strategy to rationally design and fabricate, which can extend to prepare other non-precious electrocatalysts with high efficiency and long-term stability.

Keywords: *Non-noble metal, coordination polymer, OER, ORR*

Tuning the Electronic Structure of Controlled 1T-MoS_2 for Hydrogen Evolution

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Abstract: Hydrogen is emerging as an alternative green fuel due to its highest gravimetric energy density and zero-pollutant emission to replace traditional fossil fuel and reduce environmental issues. MoS_2 shows efficient HER performance comparable to that of Pt for their unique layered structure and electronic property. The edge site 'S' atoms in MoS_2 are found to be the catalytic active sites, on the other hand basal plane 'S' atoms are inert. The metastable 1T MoS_2 reveals 10^7 times greater electronic conductivity than that of semiconductor 2H MoS_2, occurring fast charge transfer for HER. Due to its' metastable nature, the synthesis of high purity and stable 1T MoS_2 remains a great challenge. Herein, we report that 80% pure 1T MoS_2 (M3) is synthesized by hydrothermal method which exhibits an overpotential 230 mV at 10 mA/cm^{-2} current density and Tafel slope 51 mV dec^{-1} with excellent stability in acidic media. The core level XPS analysis shows that there is no Mo^{+6}, sulfite ($[SO_3]^{-2}$) and sulfate ($[SO_4]^{-2}$) group in M3. The oxidation states of Mo^{+4} and S^{-2} play an important role towards HER for M3.

Keywords: *1T MoS_2, HER, core level, XPS analysis, overpotential and Tafel slope.*

Charge transfer kinetics of Zn_2SnO_4 Nanorods grown on ZnO seed layer for photoelectrochemical water splitting

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Abstract: Growth of Zn_2SnO_4 nanorods on two differently prepared ZnO seed layers is demonstrated using hydrothermal approach. The ZnO seed layers are prepared using dip-coating and electrodeposition techniques. The grown Zn_2SnO_4 nanorods are in cubic phase. However, the different seed layer results alternation in the diameter of grown Zn_2SnO_4 nanorods. The Zn_2SnO_4 nanorods grown on electrodeposited ZnO seed layer shows around 4.5 times higher photocurrent than the Zn_2SnO_4 grown on dip-coated ZnO seed layer. The Nyquist plots of Zn_2SnO_4 nanorods on electrodeposited ZnO seed layer result in lower charge transfer resistance (R_{ct} = 37.7 Ω) and lower bulk resistance (R_{bulk} = 64 KΩ), boosting charge transport properties. The change in diameter of Zn_2SnO_4 nanorods significantly alter the charge transfer behavior. The calculated charge injection efficiency did not exhibit a significant change. However, there was a 1.6-fold enhancement observed in charge separation efficiency for Zn_2SnO_4 when grown on electrodeposited seed layer.

Keywords: *Green hydrogen, Zinc tin oxide (Zn_2SnO_4), ZnO seed layer, Charge transfer kinetics, Photoelectrochemical Water splitting*

Aluminium, Nitrogen-Dual-Doped Reduced Graphene Oxide Co-Existing with Cobalt-Encapsulated Graphitic Carbon Nanotube as an Activity Modulated Electrocatalyst for Oxygen Electrocatalyst for Oxygen Electrochemistry Applications

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Abstract: There is a rising need to create high-performing, affordable electrocatalysts in the new field of oxygen electrochemistry. Here, a cost-effective, activity-modulated electrocatalyst with the capacity to trigger both the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) in an alkaline environment is presented. The catalyst (Al, Co/N-rGCNT) is made up of aluminium, nitrogen-dual-doped reduced graphene oxide sheets co-existing with cobalt-encapsulated carbon nanotube units. Based on X-ray Absorption Spectroscopy (XAS) studies, it is established that the superior reaction kinetics in Al, Co/N-rGCNT over their bulk counterparts can be attributed to their electronic regulation. The Al, Co/N-rGCNT performs as a versatile bifunctional electrocatalyst for zinc-air battery (ZAB), delivering an open circuit potential ≈1.35 V and peak power density of 106.3 $mWcm^{-2}$, which are comparable to the system based on Pt/C. The Al, Co/N-rGCNT-based system showed a specific capacity of 737 mAh $g_{Zn^{-1}}$ compared to 696 mAh $g_{Zn^{-1}}$ delivered by the system based on Pt/C. The DFT calculations indicate that the adsorption of Co in the presence of Al doping in NGr improves the electronic properties favoring ORR. Thus, the Al, Co/N-rGCNT-based rechargeable ZAB (RZAB) emerges as a highly viable and affordable option for the development of RZAB for practical applications.

Keywords: *Al, bifunctional catalyst, DFT study, encapsulated structure, N-dual doping, oxygen evolution reaction, oxygen reduction reaction, rechargeable zinc-air battery, X-ray absorption spectroscopy*

Electrodeposited manganese carbonate as an electrocatalyst for hydrogen evolution reaction in acidic medium

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Abstract: Fossil fuel, a primary energy source, on combustion releases pollutants and greenhouse gases that are incompatible with a sustainable society. To reduce our dependency on fossil fuels, there is a growing need to develop alternative, environmentally friendly energy sources. Among the alternatives, hydrogen emerges as a promising candidate as the combustion of hydrogen produces water. A spectrum of processes is used to produce hydrogen wherein, water electrolysis emerges as a standout method, while also acknowledging the challenges posed by the high overpotential of electrochemical reactions, necessitating the use of electrocatalysts. Traditionally, Pt has been employed as an electrocatalyst, but its limitations in terms of scarcity and cost are acknowledged. Manganese-based compounds are attractive options owing to earth-abundant precursors, environmental friendliness and good electrochemical properties. Herein, manganese carbonate is electrodeposited onto pencil graphite substrate by chronoamperometric method and the same was confirmed by XRD, vibrational, and microscopic studies. $MnCO_3$ electrodeposited for 15 mins at 2 V demonstrates a good HER (overpotential of 127 mV to reach 10 mA cm^{-2}) activity in 0.5 M

H_2SO_4 with a Tafel slope of 79 mV dec^{-1}. In addition, the electrocatalyst showed good stability (over 3000 cycles and 14 hours of continuous operation).

Keywords: *Electrocatalyst; Electrodeposition; HER; Manganese carbonate; Pencil graphite; Water splitting*

Enhancing the efficiency of water splitting through spin-filtering anodic current using chiral transition metal-based 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. 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. In this study, we demonstrate the enhancement of oxygen evolution reaction kinetics by spin filtering the anodic current by using electrochemically deposited chiral transition metal-based oxide. The overpotential for the OER process is revealed to be smaller for the chiral oxide with respect to the achiral metal 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 higher electrochemical potential is reduced while using chiral oxide as an anode. This observation is attributed to the formation of spin-polarized intermediates which help in promoting the oxygen evolution reaction and accounting for the observed outcomes.

Keywords: *Electrodeposition, Chiral Induced Spin Selectivity effect, Oxygen evolution reaction, Transition metal oxide thin film, Spin filtering.*

Single Crystalline α-Fe_2O_3 Nanosheets with Improved PEC Performance for Water Splitting

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Abstract: We report photoelectrochemical (PEC) performance of densely grown single crystalline hematite (α-Fe_2O_3) nanosheet photoanode for water splitting. Unlike expensive ITO/FTO substrates, the sheets were grown on a piece of pure Fe through controlled thermal oxidation method. The sheets grow with widest surface parallel to basal plane (0001). Iron oxide formed on Fe consists of layer structure α-Fe_2O_3–Fe_3O_4–Fe is elucidated from GIXRD and correlated to spectral features observed in Raman and UV-Vis. spectroscopy. The top α-Fe_2O_3 nanosheet layer serves as photoanode whereas the conducting Fe_3O_4 layer helps to transport photogenerated electrons to counter electrode through its back contact. Compared to thin film of α-Fe_2O_3 grown on FTO substrate, ~ 3 times higher photocurrent density (0.33 $mAcm^{-2}$ at

1.23 V_{RHE}) was achieved in the nanosheets sample. The sample shows bandgap of 2.1 eV and *n*-type conductivity with carrier density 9.59×10^{17} cm^{-3}. Electrochemical impedance spectroscopy (EIS) measurements reveal enhanced charge transport properties. Anodic shift of flat band potential, delayed electron-hole recombination, growth direction parallel to highly conducting basal plane (0001) are contributing factors to the higher photocurrent observed in the NS photoanode are discussed. Characterizations carried out before and after PEC reaction show excellent stability of the nanosheets in alkaline electrochemical environment.

Keywords: *Hematite, Magnetite, Nanosheet, Photocurrent, PEC water splitting.*

Exploring Electrocatalytic Decamethylferrocene-mediated Hydrazine Oxidation in Organic medium

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Abstract: Hydrazine oxidation reaction (HzOR) offers energy-saving alternatives to oxygen evolution reaction (OER), producing carbon-free products and reducing catalyst poisoning. The oxidation of hydrazine has been studied extensively in aqueous media but not as much in organic ones This study explores the oxidation of hydrazine in acetonitrile medium using decamethylferrocene, a derivative of ferrocene known for its stability-enhanced electron-donating property. The current research aimed at studying reaction kinetics to establish rate law, which showed first-order dependence on both concentrations of decamethylferrocene and hydrazine. Further effect of pyridine-derived bases on the HzOR has been studied. Insights of mechanism for HzOR will be established. Additionally, temperature-dependent studies revealed 12.02 kJ/mol activation barrier for HzOR. The overpotential for HzOR in organic medium has been established by measuring open circuit potential (OCP). Chronoamperometry and Gas Chromatographic studies has been carried out to quantitatively measure the yield of hydrogen and nitrogen. Consequently, vital data regarding HzOR in organic medium has been contributed towards the existing data of literature.

Keywords: *Decamethylferrocene, Hydrazine Oxidation, Organic medium, Overpotential, Reaction kinetics*

Simulation of Proton Exchange Membrane Electrolyzer for HydrogenProduction: A Broader View on Electrochemical Aspects

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Abstract: The world has made a shift to the use of green hydrogen to put a check on the immense quantity of carbon-based pollutants. The energy generated from the renewable resources have also found an easier alternative to be transported and stored. Electrolyzers have given a very promising reasonand result for the shift because of their ability to generate hydrogen on a very vast extent. With this advancement made, different parameters like temperature, voltage, transport mechanisms to obtain the perfect combinations for maximum production were put to the upfront. The electrochemical aspects of PEM electrolyzers have always been an important aspect for their modeling. The variation of overpotential with current and its further study has opened insights onthe working parameters (Alhassan Salami Tijani, 2019). Along with

this arose the concerns and sparked debate relating to the modeling of PEM with the appropriate choice of electrodes and materials, which was studied and found that different metals have different bond strengths to pairwith and the existing catalysts were tested and they were replaced in hopes of a better economic match (Pham, 2021). Thus, in our research work rigorous study and different parameters will be optimized to obtain the ideal conditions.

Keywords: PEM Electrolyzers, Green fuel, Temperature, Butler volmer equation, Porous electrode, Electrochemical species transport

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Effect of Potential on Ni-Co-Fe Alloy Electrodeposition for Hydrogen Evolution Reaction

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Abstract: Efficient electrocatalysts are pivotal for hydrogen production via electrocatalysis. We investigate Ni-Co-Fe alloy films, synthesized via chronoamperometric electrodeposition on stainless steel substrate. Varying deposition potentials impact the structure and electrochemical performance of the Ni-Co-Fe alloy films. Nickel, cobalt, and iron synergy yields superior electrocatalytic activity and stability for the hydrogen evolution reaction (HER) in alkaline solutions. All deposited alloys exhibited a face-centered cubic (fcc) crystal structure. However, higher potentials yield thicker films with increased electroactive sites. Notably, the Ni-Co-Fe/SS electrode deposited at -1.4 V exhibits the lowest overpotential (87 mV) and (377 mV) for achieving -10 $mAcm^{-2}$ and -100 $mAcm^{-2}$ of current density respectively, alongside the lowest Tafel slope (159 mV/dec) and the highest exchange current density (2.57 $mAcm^{-2}$). Electrochemical impedance spectroscopy (EIS) during HER demonstrates that the Ni-Co-Fe/SS electrode at -1.4 V displays the lowest charge transfer resistance (1.31 Ω) in 1M KOH, outperforming other samples. Moreover, this electrode maintains stability over a 2-hour chronopotentiometry test at -10 mA/cm², confirming its suitability for alkaline water electrolysis.

Keywords: *Alkaline water electrolysis, Electrocatalyst, Ni-Co-Fe alloy films, hydrogen evolution reaction, Chronoamperometric electrodeposition.*

A Nickel-Doped Two-Dimensional Covalent Organic Polymer (2D-COP) for Electrocatalytic Hydrogen Evolution Reaction

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Abstract: A special class of porous polymers called two-dimensional covalent organic polymers (2D COPs) are formed by the linkage of covalently organic building monomers through noncovalent interactions. In this work, we have prepared nickel-doped 2D COP (Ni@COP) from a synthesized COP and used it for the electrochemical hydrogen evolution reaction (HER). Ni@COP has exhibited better HER activity in

comparison to $Ni(NO_3)_2 \cdot 6H_2O$ and COP. In a solution of 0.5 M H_2SO_4, the HER activities are measured. An overpotential of 290 mV and a Tafel slope of 112 mV dec^{-1} were obtained for Ni@COP. The 112 mV dec^{-1} value suggests that Ni@COP followed the Volmer–Heyrovsky pathway for the acid-catalyzed HER. The stability and catalytic effectiveness of the materials are solely dependent on COP. It is interesting to note that Ni@COP functions as a model electrocatalyst when employed as a solid cathodic electrode over the surface of carbon paper electrodes. Ni@COP for the HER exhibits exceptional activity and stability, highlighting its enormous potential for diverse energy transformation applications.

Keywords: *two-dimensional covalent organic polymer (2DCOP), electrocatalyst, hydrogen evolution reaction (HER).*

Biogenic Fe-Cu-Mo Salts for Electrochemical Total Water Splitting and CO_2RR: Excellent Durability & Low Overpotential

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Abstract: Increased emission of anthropogenic CO_2 contributes to climate change and thus there is a global effort to replace fossil-fuel derived products. Development of technologies for Green Hydrogen production and Carbon-Capture Utilization and Storage (CCUS) are becoming need of the hour. Durable and affordable catalysts for electrochemical water splitting and CO_2 reduction at low over potential with high Faradaic Efficiency remain the bottleneck in these scaling up processes. We have developed a biogenic Fe-Cu-Mo Salts electrocatalyst and deposited it on nickel foam via solvothermal process. These metal salts are highly abundant in nature and thus highly economical. FeCuMo/NF catalyst demonstrates outstanding electrochemical water splitting in alkaline medium (1M KOH) with low overpotentials of 85mV and 90mV for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at 10mAcm^{-2} respectively. The catalyst is highly durable, more than 500 hours at 200 mAcm^{-2} for total water splitting. The salt composition, primarily Copper loading is varied to augment its activity of CO_2 reduction to methanol. The catalyst shows impressive faradaic efficiency >80% for CO_2RR to methanol.

Keywords: *Biohybrid electrocatalyst, low overpotential, durability, selectivity*

MXenes as a component of electrocatalysts for Oxygen Evolution Reaction

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Abstract: Electrochemical water splitting presents a promising aspect for both mitigating fossil fuel use and storing energy from renewable sources in the form of hydrogen fuel. However, the four electron transfer process, OER, remains a bottlencek, as, even with catalysts, the overpotential is quite high(around 300mV). Iridium and Rubidium oxide are proved to be good electrocatalysts but are very costly. Now the aim is to synthesize an electrocatalyst to achieve a low overpotential at a feasible cost. Mxenes are known to have a high surface area, high electroconductivity and are extremely hydrophilic, which makes them quite a promising component of electrocatalysts for OER. Electrochemical measurements can provide insight into the electronic interaction, stability and structural change in different MXene based catalysts.

Keywords: *MXene, Oxygen Evolution Reaction, OER, Electrocatalysts*

Metal-free Electrocatalytic Valorization of PET Plastic Waste with Co-generation of Hydrogen

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Abstract: Plastic waste generates numerous environmental and ecosystem disruptions.Click or tap here to enter text. The electrochemical transformation of polyethylene terephthalate (PET) waste into valuable commodity chemicals offers a sustainable solution, potentially advancing a circular plastic economy. Despite this, a significant obstacle in converting PET waste into beneficial C2 products is the absence of a cost-effective and selective electrocatalyst to guide the oxidation process. In the current study, we have investigated the use of metal-free (2,2,6,6-tetramethyl-1-piperidin-1-yl)oxyl (TEMPO) for its ability to promote the electrochemical conversion of PET hydrolysate into glycolate. TEMPO operates at a low onset potential of 1.19 V *vs.* RHE and achieves notable faradaic efficiency over a variety of pH levels and applied potentials, along with hydrogen production at the cathode. Using chronoamperometry at a constant potential of 1.53 V *vs.* RHE, the conversion resulted in 42.50% and 42.88% glycolate from ethylene glycol and PET hydrolysate oxidation, respectively, at pH 10 with TEMPO. The mechanism was further understood by identifying intermediate products such as glycolate, oxalate, and formate formed during the oxidation of ethylene glycol. This research offers a model for developing PET upcycling technologies with high selectivity for glycolate.

Keywords: *Metal-free Catalyst, PET Plastic Waste, Glycolate, Hydrogen production*

Towards Enhanced Efficiency in Electrocatalytic Hybrid Water Splitting: A Comparative Study of Manganese, Iron, and Nickel-Based Metal-Organic Framework Catalysts

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Abstract: Hybrid water electrolysis can act as a source of renewable hydrogen instead of conventional water electrolysis due to kinetically sluggish, and energy-inefficient anodic oxygen evolution reaction (OER). Hybrid water electrolysis offers enhanced flexibility, value addition, and energy efficiency. This study explores the synthesis, characterization, and electrochemical activity comparison of different nonnoble transition metal-based MOF catalysts grown on Ni foam (M BDC/ Ni foam), where M = Manganese, Iron, and Nickel, BDC = Benzene dicarboxylic acid. The catalytic activity of these catalysts towards both water oxidation and substrate oxidation was investigated. Results reveal that the Mn BDC catalyst exhibits exceptional activity while the Fe BDC lacks efficacy for substrate oxidation whereas the Fe BDC catalyst shows excellent activity and the Mn BDC underperforms in water oxidation. The underlying mechanism for the observed trend will be further investigated.

Keywords: *Electrocatalysis, Water Splitting, Metal-Organic Framework Catalysts, Oxygen Evolution Reaction, Substrate Oxidation*

Modeling and Synthesis of High-Pressure Proton Exchange Membrane Electrolyzer: A Special Focus on Safety and Modulating the Efficiency of Hydrogen Production and Storage

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Abstract: Green hydrogen production from water and intermittent renewable energy is most promising with Proton Exchange Membrane water electrolysis. These PEM electrolyzers have the benefit of generating fast load response time, compact design, high current density (>2 A/cm), producing ultrapure hydrogen, low operating temperature (30°C–80°C) and capability of operating at extremely high pressure (Mohd Nur Ikhmal Salehmin, 2022). High-pressure PEM electrolyzers, which do not require external compression for storage, are proving to be a promising technique for producing hydrogen which results in minimal energy consumption and hence reduces the cost. However, the challenges encompass operational concerns, issues of integrating high pressure- PEMWE with renewable energy, and constraints of decoupling HP-PEMWE from gas compressors. Also, in PEM electrolyzers under high differential pressures, hydrogen back-diffusion strongly decreases Faradaic efficiency and increases hydrogen concentration on the anode side, which reduces stack component lifespan and poses safety risks (Maximilian Schalenbach, 2013). An electrochemical model is used to study hydrogen generation issues in these electrolyzers by modifying design parameters and material properties. This computational tool optimizes operating pressure efficiency, and decreases hydrogen storage limitations.

Keywords: *Hydrogen Production, Water Electrolysis, High-Pressure PEM Water Electrolyzer, Storage, Safety issues*

Ti-doped $B_{12}C_6N_6$ nanocages for hydrogen storage: DFT study

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Abstract: The level of carbon dioxide (CO_2), a significant greenhouse gas, has almost hit 412 parts per million (ppm) due to the energy demands in various sectors. This is a 47 percent rise since the start of the Industrial Age, when CO_2 level was about 280 ppm, and an 11 percent jump since the year 2000, when it was close to 370 ppm. Green energy is one of the solutions suggested to lower atmospheric CO_2 levels. Hydrogen gas (H_2) stands out for its unique properties, offering potential as a clean energy source. If hydrogen is used as a fuel, the only byproduct it produces is water. The most significant obstacle to achieving the vision of green energy is the storage of hydrogen. Adsorption on a solid substrate is a viable solution for hydrogen storage. The search for new hydrogen storage materials is an ongoing endeavor in the scientific community. In our research we have investigated hydrogen adsorption properties of Ti-doped $B_{12}C_6N_6$ nanocage using density functional theory with wB97XD functional. Various parameters were evaluated, including binding energy calculation, density of states (DOS), projected density of states (PDOS), natural bond orbital (NBO) charge analysis, desorption energy and temperature.

Keywords: *density functional theory, B12C6N6 nanocage, DOS, hydrogen storage, adsorption energy*.

C_{20} nanocage and Its Derivatives for hydrogen storage: A DFT investigation

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Abstract: Energy issues, highlighted by increasing concern about climate change and the necessity for long-term solutions, have prompted a shift towards cleaner and more efficient energy sources. Hydrogen has emerged as a promising solution in this scenario due to its versatility and environmental benefits. However, one of the critical challenges in utilizing hydrogen lies in its storage and transportation. Storing hydrogen in gaseous and liquid forms raises safety concerns, prompting a shift towards solid-state storage. Adsorption on solid substrates holds promise in this regard, driving ongoing efforts within the scientific community to discover novel storage materials. Our research focuses on investigating the hydrogen adsorption properties of nanoclusters using density functional theory. We have designed and assessed the hydrogen storage properties of a single Ti-doped C_{20} nanocage and its derivatives with the help of the density functional theory approach. In total, 15 structures are designed by substituting heteroatoms, boron and nitrogen, and out of these, only 8 structures are suitable for Ti doping and H_2 adsorption viz. C_{20}, $C_{12}N_8$, $C_{12}B_8$, $C_{12}B_4N_4$, $C_{10}B_5N_5$, $C_{10}B_{10}$, $B_{10}C_{10}$ and $B_{10}N_{10}$. The obtained H_2 adsorption energy for all the structures falls within the range of 0.2 to 0.7 eV, which is conducive to reversible hydrogen storage.

Keywords: hydrogen storage, DFT, C_{20} derivatives, heteroatom substitution, metal decoration, H_2 adsorption.

Metal-functionalized supramolecular hydrogels as efficient electrocatalysts for HER and OER

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Abstract: The rapid depletion of fossil fuels and environmental deterioration is an urgent call for developing clean and renewable energy technologies and materials. Therefore, we have prepared sonication-induced peptide bolaamphiphile anchored self-assembled cobalt-based coordination polymeric hydrogel. We employed the organic molecule (FF-AdiA-FF) with $CoCl_2.6H_2O$, $Co(OAc)_2.4H_2O$, $CoSO_4.6H_2O$, and $Co(NO_3)_2.6H_2O$ metal salts for the gelation and we noticed that the gelation is counter anion specific. The FF-AdiA-FF forms the hydrogel in presence of metal salts $CoCl_2.6H_2O$ (gel-1) and $Co(OAc)_2.4H_2O$ (gel-2). However, the gelation was not observed with $CoSO_4.6H_2O$ (non-gel-1) and $Co(NO_3)_2.6H_2O$ (non-gel-2) metal salts. We used SEM, TEM, CSLM, AFM, FTIR, BET, rheology and XPS analysis to examine the morphological and spectroscopic characterizations. The xerogels of all the electrocatalysts have been used to fabricate the electrodes and utilized in energy conversion. HER performances of gel-1 and gel-2 exhibit ultralow Tafel slope 107 mV dec^{-1} and 110 mV dec^{-1} respectively and very low overpotential 110 mV and 118 mV at -10 mA cm^{-2} current density in 0.5 M H_2SO_4 electrolyte than the non-gel electrocatalyst under same experimental conditions. Similarly, the OER activities of gel-1 and gel-2 are higher than non-gel electrocatalysts with a small overpotential of 151 mV and 159 mV along with the ultralow Tafel slope of 62 mV dec^{-1} and 67 mV dec^{-1} respectively to reach 10 mA cm^{-2} current density in 1 M KOH. The higher-order self-assembled structure of the hydrogel is beneficial for the smooth transport and intercalation/deintercalation of the electrolyte ions to enhance the activity of the catalyst. Furthermore, the gel-1 and gel-2 are witnessed as highly stable electrocatalysts during chronopotentiometry performance for 50 h in acidic and alkaline electrolyte. Hence, biomolecule-assisted electrocatalytic results

open a new route to design efficient electrocatalysts for the significant implications in green energy conversion.

Keywords: *peptide bolaamphiphile; self-assembly; coordination polymeric hydrogel; electrocatalysis; Oxygen Evolution Reaction (OER); Hydrogen Evolution Reaction (HER)*

Insight into the active key species of Mo_2C and Mo/Mo_2C systems in unstable alkaline hydrogen evolution reaction

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Abstract: MoO_x has been identified as a dynamic active species in Mo based alkaline HER. Mo_2C is an attractive non-noble electrocatalyst for alkaline hydrogen evolution reaction. Recent studies have shown that Mo/Mo_2C heterostructures are highly active for HER due to the enhanced electron transfer of metallic Mo to Mo_2CClick or tap here to enter text.. However, an Pourbaix diagram of Mo_2C reveals that in an unstable alkaline media Mo_2C undergo corrosion and dissolves as MoO_4^{2-} speciesClick or tap here to enter text.. So, understanding the activity and stability of Mo_2C is very important in recent scenario. In our work, we have synthesized Mo_2C and Mo/Mo_2C with different Mo to C ratio and observe their local environment reconstruction through in-situ X-ray absorption spectroscopy (XAS) and in-situ Raman spectroscopy. Post characterization and in-situ characterization of the catalysts has revealed that best active catalyst Mo_2C is prone is form defective MoO_x species under alkaline environment.

Keywords: *Mo_2C, MoO_x, XAS, alkaline HER, electrocatalyst*

Exfoliated Cobalt-Doped Manganese Oxide Nanosheets: An Efficient and Stable Electrocatalyst for Hydrogen Evolution Reaction in an Alkaline Medium

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Abstract: Research and development are still ongoing to create an electrocatalyst for the hydrogen evolution reaction (HER) that is non-noble metal-based, long-lasting, efficient, and simple to use. Two-dimensional transition metal oxide nanosheets (NSs) are leading the way due to their large lateral size relative to thickness. These NSs possess unique electronic and physicochemical properties, making them promising catalytic centres for HER. In this study, chemical exfoliation was used to synthesise co-doped MnO_2 [$Mn_{1-x}Co_xO_2$, x = 0.0−0.5] NSs. The electrochemical measurements for hydrogen evolution reaction (HER) were done in 1M KOH solution by drop casting the NS dispersion on Ti foil, where the exfoliated samples outperformed bulk samples for HER. Notably, 20% Co-doped MnO_2 exhibited the best performance, with an overpotential of 218 mV at 10 mA cm^{-2} and a Tafel slope of 122 mV dec^{-1}. It shows a stable current density of ~10 mA cm^{-2} for ~12 hours. Enhanced performance attributes to larger oxygen vacancies, preferential water molecule adsorption, higher conductivity, and rapid charge transfer. Remarkably, electrode preparation using this NS dispersion required no binder or conductive carbon, offering a promising, cost-effective, and scalable electrocatalyst for HER applications.

Keywords: *Nanosheet, Doping, Hydrogen Evolution Reaction, Electrocatalyst, Hydrogen energy*

Hydrogen storage properties of Ti doped [1,1,1,1] paracyclophane and its derivatives: A DFT study

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Abstract: The prominence of hydrogen energy is rapidly growing within the energy sector. It's believed that hydrogen holds the potential to mitigate issues such as fossil fuel depletion, global warming, and pollution. However, the transition towards sustainable hydrogen energy encounters obstacles, particularly concerning storage. Storing hydrogen in gaseous and liquid forms raises safety concerns, prompting a shift towards solid-state storage. Utilizing adsorption on solid substrates is viewed as a promising solution for hydrogen storage. The quest for novel materials for hydrogen storage is an ongoing endeavor in the scientific community. Our research focuses on investigating the hydrogen adsorption properties of nanoclusters using density functional theory. We have designed Ti-doped [1,1,1,1] paracyclophane (PCP) and its derivatives by incorporating heteroatoms like boron and nitrogen, and examined their hydrogen storage capabilities. The substitution of heteroatoms in PCP influences H_2 uptake capacity, Ti binding energy, and H_2 adsorption energy. The boron-doped structures considered in our study exhibit the necessary H_2 uptake capacity, appropriate adsorption energy within the range of 0.2-0.7 eV to facilitate quicker adsorption and desorption kinetics, thermodynamically favorable H_2 adsorption under ambient conditions, moderate desorption temperatures required for practical use, and strong binding of Ti atoms both before and after H_2 adsorption.

Keywords: *hydrogen storage, DFT, paracyclophane, heteroatom substitution, metal decoration, H_2 adsorption*.

$MoSe_2$ nanosheets anchored phosphorous doped rGO as an efficient electrocatalyst for overall water splitting

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Abstract: One effective way to achieve the bifunctionality of nanocatalysts is to construct a heterogeneous interface utilising distinct components; additionally, the electrocatalytic performance can be further optimised by synergistic interactions between the multiple compounds. In this work, we tried to create effective and long-lasting $MoSe_2$ nanosheets grown on reduced graphene oxide doped with heteroatoms, specifically phosphorus (P-rGO). This P-rGO/$MoSe_2$ nanocomposite, which has well-intercalated nanosheets and a clearly defined interface, is made using a straightforward hydrothermal process. Using X-ray diffraction analysis, the hexagonal phase of the $MoSe_2$ layered structure anchored on P-rGO ultrathin nanosheets is identified. Further the P-rGO nanocomposite with $MoSe_2$ is confirmed due to the presence of two bands, D (defects) and G (graphitic) in the Raman spectra. Field emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM) were used for the morphological investigation. The electrocatalytic Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER) capabilities were investigated using a three-electrode electrochemical cell. The remarkable electrocatalytic OER and HER results of P-rGO/$MoSe_2$ are attributed to their synergistic effect, of abundant active sites, and this

unique nanocomposition. P-rGO/$MoSe_2$ nanocomposite requires 437 mV and 369 mV overpotentials with 126 mV/dec and 147 mV/dec Tafel slopes, respectively, to achieve 10 mA/cm^2 current density for OER and HER, and it also exhibited exceptional stability over a 24-hour period. Cyclic Voltammetry (CV) was also used to evaluate the electrocatalytic active surface area (ECSA) of P-rGO/$MoSe_2$ in the non-faradic regions. In order to simulate the actual overall water splitting (OWS), the prepared nanocomposite was assembled into a P-rGO/$MoSe_2$ || P-rGO/$MoSe_2$ modified two-electrode system, which delivers 10 mA/cm^2 with a low cell voltage of only 1.57 V in alkaline medium. These findings demonstrate the sensible design of building electrocatalytic bifunctional materials based on carbon-supported transition metal selenides for useful water splitting systems.

Keywords: *$MoSe_2$, reduced graphene oxide (rGO), nanosheets, OER, HER and electrocatalytic overall water splitting.*

Controlled growth of Cu_2ZnSnS_4 (CZTS) quantum dots for photoelectrochemical water splitting

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Abstract: Efficient photocathodes for solar-driven water splitting to produce hydrogen are crucial to address the global energy demand. P-type Cu_2ZnSnS_4 (CZTS) is a material having high absorption properties, earth-abundant constituents, and environmental friendliness making it a suitable candidate to act as a photocathode. In this study, we have synthesized the Cu_2ZnSnS_4 (CZTS) quantum dots by Hot injection route. The controlled growth of the CZTS QDs has been achieved by varying the amine to the precursor molar ratio. Further, CZTS QDs coated on FTO with the help of the dip coating method to prepare the thin films. XRD analysis revealed the formation of the pure Kesterite phase and tetragonal crystal structure of the CZTS QDs. Spherical and aggregated particles have been observed by the FESEM study. Additionally, EDX analysis has been in good agreement with the CZTS compositions. Moreover, the UV–vis spectroscopy showed high optical absorption in the visible region, and the obtained bandgap is in the range of 2 to 2.5 eV for as-synthesized CZTS QDs. Further, the prepared CZTS QDs@FTO thin films were utilized as photocathodes for photoelectrochemical water-splitting. The CZTS QDs@FTO with a 0.6:1 ratio of precursor to amine demonstrated the highest photocurrent density compared to other ratios tested.

Keywords: *CZTS, photocathode, photoelectrochemical water splitting.*

Solar Alchemy: Rejigging Green Hydrogen Production Through Photoelectrochemical Water Splitting (PEC).

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Abstract: This study probes the promising realm of green hydrogen production through photoelectrochemical (PEC) water splitting, positioning it as a supercilious alternative to blue hydrogen procured from fossil fuels with carbon capture and storage (CCS). Getting a bead on, this research aims to identify and address the critical challenges in maximizing the efficacy and robustness of PEC water splitting. Utilizing state-of-the-art semiconductor materials and innovative catalytic systems, the PEC process leverages solar energy to achieve direct water dissociation into hydrogen and oxygen. As revealed in preparatory results, solar-to-hydrogen (STH) efficiency is 18.5% for the PEC process, loftier than conventional electrolysis and blue hydrogen production methods. Financial analysis evinces levelized cost of hydrogen (LCOH) at $2.30/kg, undercutting the $4.50/kg cost of blue hydrogen. Environmental assessments further highlight the benefits, with PEC-based green hydrogen exhibiting a minimal carbon footprint of 12 kg CO2 per MWh, compared to 70 kg CO2 per MWh for blue hydrogen. In defiance of promising upshots, significant challenges remain in scaling up PEC technology for commercial use. Designing a lucrative and productive PEC water splitting system, we approach to develop new semiconductor materials and catalyst configurations augmenting adeptness thus serving the ultimate purpose of sustainability.

Keywords: *Green hydrogen, Photoelectrochemical water splitting, Sustainability, Semiconductor materials, Carbon footprint.*

Fe-$NiCo_2O_4$@S, N-rGO nanocomposite for improved water electrocatalysis

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Abstract: Electrocatalysis is crucial in advancing renewable energy technologies, such as green hydrogen production by electrochemical water splitting. Non-precious metal-based electrocatalysts have garnered significant attention due to their cost-effectiveness and abundance compared to precious metal counterparts. Similarly, heteroatom-doped nanocarbons show excellent stability with activity. In the present work, we have synthesized Fe-$NiCo_2O_4$ nanomaterial on S, N-rGO to create effective electrocatalysts. The hydrothermal route was followed by calcination to prepare Fe-$NiCo_2O_4$ nanomaterial, and then ultrasonication was used to prepare the final nanocomposite. X-ray diffraction (XRD) analysis confirmed the prepared material's crystal structure, and the nanoparticles agglomerated to nanorod-like surface morphology was verified by Field emission scanning electron microscopy (FESEM). The hydrogen and oxygen evolution performances were recorded in a standard three-electrode electrochemical cell. This nanocomposite showed excellent water-splitting performance, resulting from the highly exposed surface area due to the amalgamation of nanoparticle and nanorod structure. The effect of compositionally engineered $NiCo_2O_4$ crystal by Fe-doping and the additional contribution from the highly conductive S, N-rGO nanosheets enhanced the electrocatalytic performance. The modulated electronic environment, rough surface, and conductivity of the prepared nanocomposite increase the active site concentration and help this nanocomposite exhibit excellent electrocatalytic performance for overall water splitting.

Keywords: *Green energy, H_2 production, electrochemical water splitting, nanomaterial, electrocatalysts.*

THEME-D: Environmental Monitoring & Remediation

Investigation on the Effectiveness of Eggshell Biowaste for Multi-stage Water Purification

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Abstract: Urbanization and anthropogenic activities have substantially impacted the environment and human health through heavy metal contaminants. Adsorption is one of the most versatile methods for heavy metal-contaminated water purification. Although the choice of adsorbents is innumerable, they should be cost-effective, practical, and sustainable. Eggshell (ES) is one such bio-adsorbent that is naturally available, low-cost, and economically viable. These rules out the possibility of landfilling, further reducing the pollution caused by ES. However, the poor kinetics and limited adsorption capacity of ES toward water contaminant removal may impede the choice of it as an alternative adsorbent compared to the widely used charcoal filters. On the contrary, charcoal adsorbent has very poor selectivity for specific water contaminants. To this endeavor, an alternative strategy for effective purification technology shall be developed for heavy metal-contaminated water. Porous Organic Polymers (POPs) have gained tremendous attention and have shown excellent potential as adsorbents due to their high surface area, tunable functionality, selective adsorption sites, high stability, and tailorable porosity. Herein, we will report on integrating the POPs and eggshell biowaste and their usage in heavy metal-contaminated water purification (Scheme a and b). This method showcases a viable approach for effective use of eggshell biowaste in a double-stage water purification system.

Keywords: *Eggshell; Porous Organic Polymers; Heavy metals; Water purification; Multi-stage*

Pivotal role of CuS nanoflowers on the performance of CuS/rGO/GCN heterojunction photocatalyst against Industrial Dyes

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Abstract: Herein, nanostructures of CuS, CuS/GCN, CuS/rGO were synthesized using the hydrothermal method. CuS and Graphitic Carbon Nitride (GCN) have been anchored onto the Reduced Graphene Oxide (rGO) surface to fabricate ternary CuS/rGO/GCN nanocomposites for photocatalytic application. The synthesized nanostructures are characterized by XRD, FTIR, SEM, and UV-Vis spectroscopy. Visible light Photocatalysis of Malachite Green (MG) and Indigo Carmine (IC) dyes was investigated using synthesized materials. The ternary composite CuS/rGO/GCN showed 97.05 % and 80.9 % degradation for MG and IC dyes within 70 min of the timeframe. Further to understand the catalytic behavior, impedance and PL spectroscopy were used. The ternary composite has shown low charge transfer resistance in impedance studies and lower intensity in the PL spectra compared to other samples. When visible light is irradiated on CuS/rGO/GCN, the electrons from the valance band of GCN can migrate directly to the CuS nanostructures, which serve as a co-catalyst. The introduction of CuS, helps in improving the photocatalytic properties of ternary composites. These results suggest that the synthesized nanostructures shows an outstanding photocatalytic reaction on degrading MG and IC dyes.

Keywords: *CuS nanoflowers, hydrothermal technique, CuS/rGO/GCN ternary composites, industrial dyes, photocatalysis, degradation mechanism.*

Integrated Batch-type Fenton-Electrocoagulation-Adsorption Processes for the Treatment of Tannery Wastewater and Chromium Recovery

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Abstract: The leather industry consumes significant amounts of chemicals including chromium based tanning agents for leather production that generates vast quantities of wastewater which are detrimental to the environment. Similarly, the coconut processing industry generates huge quantity of coir pith (CP) waste comprised of high lignin (30-40%), cellulose (40-50%), hemicelluloses (15-35%) content, and carbon-nitrogen ratio (112:1) that resist its natural biological decomposition. Therefore, the activated carbon/Fe_3O_4 based Fenton catalysts was successfully developed from CP waste by simple KOH activation and precipitation methods. The tannery wastewater underwent aeration for 4 days followed by integrated batch treatment processes including Fenton oxidation, electrocoagulation, and adsorption. The treatment efficiency was calculated by the reduction of chemical oxygen demand (COD) and chromium values. The initial COD and chromium concentration of raw wastewater was 4000 mg/L and 119 mg/L which was reduced to 576 mg/L and 0.215 mg/L after the integrated processes. These findings recommend that the integrated processes are effective in the treatment of tannery wastewater as compared to individual processes. Thus, the utilization of waste material for the treatment of wastewater could be a sustainable solid and liquid waste management process.

Keywords: *Leather industry, Tannery wastewater, Integrated Processes, Fenton oxidation, Electrocoagulation, Adsorption, Chromium recovery*.

Hydroxyapatite nanoparticles decorated with metal–organic framework, Co-Cu/ZIF@HAp, and evaluation of photocatalytic performance of the prepared nanocomposite towards the degradation of organic pollutants

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Abstract: In this research, a novel hydroxyapatite (HAp)-based composite, Co-Cu/ZIF@- HAp, was constructed through in situ growth and simultaneous sonication followed by magnetic string. Herein, the HAp-based nanocomposite was obtained in which HAp was coated with cobalt–copper bimetallic zeolitic imidazolate framework (ZIF) in one-pot synthesis method. The as-synthesized composite was characterized by PXRD, FTIR, FE-SEM, EDS, HR-TEM, TGA-DTG, XPS, BET, and UV-DRS techniques, which suggested that HAp was well coated with bimetallic ZIF. The prepared composite was utilized as a catalyst in degradation of organic pollutants. Removal of organic pollutants such as organic dyes has become indispensable due to their higher stability, toxicity, and mutagenic nature. Two commonly found organic dyes, namely, Eosin Yellow (EY) and Brilliant Green (BG), were chosen for the investigation of photocatalytic activity of the as-prepared catalyst. The degradation process was carried out under solar radiation, and there was no utilization of any oxidizing and reducing agent. Several parameters such as amount of catalyst dose, initial concentration of the dye solution, and effect of different pH conditions were evaluated for better understanding of photocatalytic performance of Co-Cu/ ZIF@HAp composite. Both EY and BG dyes were almost degraded up to 98.3% and 99.5%, respectively, within 50 min by the as-

prepared nanocomposite. Also, quenching test was performed that confirmed the formation of superoxide radicals (O2.) as reactive oxygen species (ROS) in the photodegradation process. The as-synthesized catalyst was repeatedly used for five times to ascertain the stability and reusability of catalyst.

Keywords: *Hydroxyapatite, Metal Organic Frameworks, Nanocomposite Photocatalysis, Environmental Remediation.*

Synthesis of Layered Double Hydroxide supported Metal-organic framework composites for the adsorptive removal of anionic dyes in wastewater treatment.

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Abstract: Industrial wastewater containing huge loads of organic dyes, released into the water poses a serious environmental threat as they are toxic and carcinogenic in nature. These dyes are persistent pollutants and cannot be removed completely by conventional water treatment techniques. Adsorption has been found to be effective for the complete removal of these dyes from water. Thus, developing efficient/sustainable adsorbent materials to remove these dyes is challenging. Layered double hydroxides (LDH) are synthetic clay materials containing divalent and trivalent metal ions with exchangeable interlayer anions. Zeolitic imidazolate frameworks (ZIF) are a subclass of nano-porous metal-organic frameworks (MOF) with caged structures and inorganic zeolites-like functionality. The composite material obtained by combining MOFs and LDH could significantly enhance the surface area, porosity and hence the adsorption properties. The present research aimed to develop LDH-based composite adsorbents to efficiently remove dyes/colorants from water/wastewater. With this objective, Mg/Fe LDH-ZIF-8 composites were synthesized, characterized, and applied to remove cationic and anionic dyes from water. The composite showed a dye removal percentage of over 95% for the Acid orange 7 and 9.2% for the Rhodamine B dye. The adsorption equilibrium, kinetics, and the influence of water pH on the adsorption were also discussed. The developed Mg/Fe LDH-ZIF-8 composite showed promising adsorbent for water/wastewater treatment, thus opening a new area of advanced adsorbent material for removing both anionic and cationic dyes from water.

Keywords: *Layered double hydroxide, Adsorption, Water/wastewater, Dye removal, Zeolitic Imidazolate Framework,*

An Overview of AI/ML Techniques in Environment Conservation: Biodiversity and Forest Management

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Abstract: In today's Era, maintaining sustainable development in an environment, tackling the global warming issues and conservation of biodiversity is a critical task to handle. To be alive in an Earth, maintaining ecological balance is essential because it directly or indirectly affects the life .This paper explores the blooming role of artificial intelligence in biodiversity conservation and forest management efforts. Artificial intelligence is one of the swiftest growing techniques to tackle the global environmental crisis. Through a detailed analysis of various AI applications, from remote sensing and wildlife protection to climate change prediction, forest management and biodiversity conservation, AI can revolutionize our

approach to safeguarding the environment. It discusses the various applications of AI technologies, such as data analysis, species identification, predictive modeling, and optimization strategies, in addressing the complex challenges facing biodiversity and environmental conservation. The aim of writing this paper is to present a comprehensive review of how Artificial intelligence and machine learning algorithms are utilized in the development of sustainable environment in the sector of forest management and biodiversity conservation in all over the world. The paper also examines the potential advantages, opportunities, challenges, and ethical concerns associated with the use of AI in conservation tactics. Machine learning, in which computer systems learn to improve their accuracy and efficiency without human interference, is leading these developments. Now, this technology is transfiguring conservation endeavor in very excited and fascinating ways.

Keywords: *Artificial Intelligence, Machine Learning, Environment, Biodiversity, Conservation, Remote Sensing, Wildlife Protection, Climate Change, Natural Resources*

Metal-Doped Laser-Induced Graphene Electrodes and Filters for Electrochemical Disinfection of Enteric Viruses from Wastewater

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Abstract: Pathogenic enteric viruses prevalent in wastewater have detrimental health impacts and thus, their removal is crucial to provide safe drinking water. Conventional disinfection techniques including chlorination, UV, and ozone face disadvantages of disinfection byproducts formation, and high energy consumption. This led to emergence of alternate disinfection techniques like electrochemical disinfection, which utilizes efficient electrodes for water treatment. Laser-induced graphene (LIG) has garnered widespread interest as electrodes due to its single-step, facile synthesis method, and unique electrical, thermal, and mechanical properties. Thus, in this study, titanium suboxide-doped LIG surfaces were fabricated in a single step as electrodes and filters for the electrochemical inactivation of enteric viruses. Three model enteric virus surrogates such as bacteriophages MS2, T4, and Phi6 were employed. An enhanced virus inactivation was achieved which was functional to the increasing doping concentration and applied voltage in the batch mode. In the flow-through condition, complete inactivation of MS2 was achieved at 2.5 V, and for T4 and Phi6 at 10 V. Additionally, the varying resistance incurred by these enteric viruses to disinfection was examined and the mechanism of inactivation was explored with the LIG-based systems. Thus, the present work would be empirical to develop disinfection-based systems for wastewater treatment.

Keywords: *Virus Disinfection, Laser-Induced Graphene, Inactivation Mechanism, Virus Susceptibility, Electrochemical Processes*

Stabilization of *Candida ruogsa* lipase for optimized production of biodiesel

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Abstract: The application of fatty acid methyl esters (FAME, also called biodiesel) as an alternative fuel for diesel, is a global practice. Enzymatic biodiesel synthesis using lipase has advantages of clean, green and room-temperature process without using corrosive catalysts. However, methanol, one of the substrates, denatures lipase and reduces FAME yield. Using reaction medium engineering, glycine betaine has been shown to protect lipase, improving FAME yield [1]. In this work, Taguchi methodology was used to improve the yield further, by optimizing reaction parameters. The FAME synthesized from kitchen waste oil, soybean acid waste oil was characterized using tests recommended by ASTM D6751. Furthermore, reusability of *Candida rugosa* lipase (CRL) was improved by immobilizing it on suitable support matrix. Graphite coated glass cloth, a high hydrophobic (contact angle 127°), easily available and economical support matrix can bind CRL in suitable quantities (binds 6.5 units of 12.5U CRL on 4 cm^2 matrix). The free and enzyme-bound matrices were characterized by SEM indicating bound protein. The biochemical analysis of free-CRL (K_m 4.95) and bound-CRL (K_m 1.92), using sunflower oil indicated bound-CRL was relatively more thermostable (upto 50°C) and reusable upto 6 times while retaining >80% of its original enzyme activity. These results conclude that graphite coated glass cloth can be a suitable matrix for CRL immobilization for improving FAME production.

Keywords: *Biodiesel, reaction medium engineering, glycine betaine, immobilization, graphite coated glass cloth, reusability.*

Analyzing the Effect of Cottonseed Biodiesel Blend Produced from Heterogeneous Catalyst and n-Butanol on Reactivity Controlled Compression Ignition (RCCI) Engine

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Abstract: Depleting trends in the availability of fossil fuels has become a significant threat to many of the automobile industries. An alternative to conventional diesel and gasoline is the top priority for most automobile users. Increasing emissions from diesel and petrol is another major threat on the list. RCCI (Reactive controlled compression ignition engine) enhances the in-cylinder combustion process, reducing most harmful emissions such as NO_x and smoke. The effect of n-butanol and cotton seed biodiesel over RCCI engine using split injection strategies by varying the ratios (10%, 20%, and 30%) of n-Butanol is investigated in this study. Cottonseed biodiesel is used as pilot fuel, and n-Butanol as primary fuel was investigated in the RCCI engine. The performance, combustion and emissions characteristics at various loads are studied and analysed. It was concluded that the BTE increases and SFC decreases while increased load, for CSB + 30% n-Butanol than diesel. NO_x emissions have a decreasing trend in usage of CSB + 30% n-butanol blend ratio. Overall, the CSB + 30% n-butanol blend is the best alternative for increasing engine performance and decreasing NOx emissions by 33.15%.

Keywords: *Cotton seed biodiesel; n-Butanol; RCCI Engine parameters; Spilt injection; Characterization of biodiesel*

Transition Metal-doping Optimisation for Laser-Induced Graphene (LIG) Composite Electrodes and Filters for Enhanced Disinfection

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Abstract: Waterborne pathogens pose a significant threat to public health, often leading to severe diseases. Consequently, the development of reliable disinfection systems with state-of-the-art electrode material is paramount. Laser-induced graphene (LIG) presents a promising solution, being a graphene material fabricated in a facile step using a carbon dioxide laser. Its remarkable conductive and electrochemical characteristics make it effective in microbial eradication. However, LIG's antimicrobial activity relies solely upon electrical treatment. Thus, there's a need for modifications to enable its efficacy even in the absence of electricity. In this study, we explored the integration of copper nanoparticles with LIG at various concentrations, aiming to optimize their synergistic disinfection performance. Through meticulous dosage optimization, we sought to enhance LIG's electrochemical properties with minimal copper concentration, thereby enabling it to function effectively both with and without electrical treatment. The research indicates that incorporating a 1% concentration of copper nanoparticles enhances the electrochemical disinfection capabilities against a mixed bacterial culture and bacteriophage MS2. Moreover, the investigation extends to the development of electroconductive membrane filters. These filters exhibit complete inactivation, removing 6-logs of both bacteria and virus at 2.5 V, particularly at a high flux of approximately 500 Lm^2h^{-1}. The straightforward preparation of these electrode materials offers a promising path for simplified fabrication processes, reduced energy consumption, and potential avenues for commercialization.

Keywords: *Copper-doped LIG, Electroconductive Surface, Metal-doping optimization, Electrochemical Disinfection, Electrode Material*

Au nanoparticles modified $KCa_2Nb_3O_{10}$/g-C_3N_4 Nanosheets Heterojunctions for Photocatalytic CO_2 Reduction

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Abstract: Increased human activity, pollution, dependence on fossil fuels for industrial growth, increased energy consumption have depleted non-renewable energy sources that are limited on Earth. To overcome these problems, CO_2 photoreduction into fuels and value-added chemicals is now attracting immense attention. But, low surface area, fast recombination of charge carriers and low selectivity of catalysts are still significant challenges for CO_2 photoreduction. Therefore, 2D niobate nanosheet materials are being investigated for CO_2 photoreduction. But, due to its wide band gap, it can only respond to UV light irradiation. Therefore, increasing its light response range and lifetime of charge carriers is important to achieve a high activity in photocatalytic applications. Among various 2D nanosheets, g-C_3N_4 is gaining attention due to its easy preparation, excellent chemical stability and visible light response owing to its

narrow band gap (2.7eV). In this work, a visible light driven 2D hybrid system is constructed by 2D g-C_3N_4 and exfoliated calcium niobate nanosheets. This heterojunction is decorated by the Au nanoparticles with different methods. The photocatalytic performance of Au nanoparticles modified $KCa_2Nb_3O_{10}$/g-C_3N_4 2D-2D nanosheet heterojunction is evaluated by way of photocatalytic reduction of CO_2 under solar light irradiation. The structural, chemical and optical properties of $KCa_2Nb_3O_{10}$/g-C_3N_4 2D-2D nanosheets are evaluated by P-XRD, FE-SEM, EDS, XPS, BET, TGA, TEM, HR-TEM and UV-Vis spectroscopy.

Keywords: *Photocatalysis, CO_2 photoreduction, perovskite nanosheets, g-C_3N_4, heterojunction.*

Electrochemical Investigation of Polyoxometalate to Understand PCET

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Abstract: Polyoxometalates (POMs) are complex molecules with multiple clusters undergoing several redox reactions. They have utility in electrochemical energy storage (redox flow batteries, electrocatalysis, and supercapacitors) owing to their high rate coefficients and capability to extract multiple electrons per molecule. Another unique property of POMs is the proton-coupled electron-transfer (PCET) i.e. simultaneous exchange of proton and electrons in a molecule. Thus, POMs release H_2 gas while oxidizing in the presence of electrocatalysts like Pt or C. To understand the redox reactions and PCET in POMs, $Li_6[P_2W_{18}O_{62}]$ (P_2W_{18}) is chosen for investigation. Synthesized P_2W_{18} is electrochemically investigated by recording voltammograms and validated from the literature. It is observed that the electrode surface is modified on repeated oxidation and reduction of P_2W_{18}. The rate of increase in HER (hydrogen evolution reaction) current with each cycle in the blank electrolyte increases significantly. It can be attributed to the adsorption of P_2W_{18} which increases the H^+ ion concentration on an electrode surface. The hypothesis is supported by the increase in reduction current at low pH and after a number of voltammograms are recorded. Further investigation is required to obtain firm conclusions so that the observations can be applied to study the HER in POMs.

Keywords: *Polyoxometalates (POMs), proton-coupled electron-transfer (PCET), P_2W_{18}, HER Current, Hydrogen Storage*

Remote Sensing based Water Quality Monitoring of Indian Ramsar Wetlands

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Abstract: There are eighty Ramsar wetlands sites present across India across different climatic and topographical conditions. Among them, forty wetland sites are urban wetlands that are present in the city, making the water quality of the sites vulnerable due to the presence of the dense urban population and cropland in their catchment area. Therefore, we conducted a remote sensing-based assessment of the water quality using Sentinel 2 datasets for computing the NDCI, NDMI, NDTI, and NDWI indices from 2019 to 2023. These indices used to monitor the chlorophyll, moisture, turbidity, and water content of these sites assist us in monitoring the site area that is available with clear water content for the maximum period. Therefore, our study provides the site-specific outcomes for threats to the regional water quality of wetlands and changes required to restore the regional hydrological cycle and conserve regional biodiversity.

Keywords: *Water Quality, Ramsar Wetlands, Remote Sensing, Sentinel 2*

Enhancing faecal sludge treatment: study on effects of mixing and inoculation on organic matter degradation

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Abstract: The management of faecal sludge in India's urban areas without sewerage systems faces challenges due to rapid urbanization and population growth, impacting approximately 40% of the urban population. Faecal sludge, containing organic matter, nutrients, and pathogens, poses significant environmental and public health risks. This study conducted anaerobic experiments using fresh faecal sludge, assessing conditions such as "with mixing with inoculum" and "with mixing without inoculum." Initial characterization revealed total ammonia at 145.6 mg/L, total phosphates at 10.62 mg/L, total Kjeldahl nitrogen at 160.44 mg/L, pH at 7.69, volatile suspended solids at 266.34 mg/L, total suspended solids at 153.84 mg/L, total dissolved solids at 350.0 mg/L, and chemical oxygen demand at 1019.2 mg/L. These findings indicate substantial organic and nutrient loads, necessitating advanced treatment. The study explored onsite anaerobic digestion with active digested inoculum as a potential solution for managing faecal sludge, enhancing the breakdown of organic matter. Results showed higher organic matter removal efficiency in setups involving both mixing and inoculum, emphasizing their importance in improving treatment effectiveness. This highlights the need to incorporate mixing and inoculation in designing anaerobic bioprocesses for faecal sludge treatment in urban areas without sewerage infrastructure. The study supports anaerobic digestion as a sustainable and health-promoting approach for managing urban faecal sludge in India.

Keywords: *Faecal sludge, Chemical oxygen demand(COD), Inoculum, Anaerobic digestion, Mixing.*

Investigating microbial diversity and antimicrobial resistance properties of faecal sludge before and after various treatment processes

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Abstract: Untreated faecal sludge disposal spreads waterborne diseases due to its content of pathogens, helminth eggs, high organic matter, and heavy metals. Therefore, its treatment and resource recovery are crucial for disease prevention. Fresh faecal matter samples were collected from CSIR NIIST residential apartments. Treatment methods included bottle scale analysis (with aid of mixing and inoculum), bio-methanation using multiple substrates, and treatment using natural media in a reactor with an attached growth process. Microbial presence, including *E. coli*, *Salmonella*, *Shigella*, *Staphylococcus*, *Pseudomonas*, and *Vibrio* species, was examined using spread and streak plating techniques. Next-Generation Sequencing (NGS) assessed microbial diversity on a broader scale. NGS using Illumina (Novaseq 6000), 150PE identified *Proteobacteria*, *Firmicutes*, and *Euryarchaeota* as the dominant phyla. Spread and streak plating showed abundant *E. coli*, *Staphylococcus*, and *Salmonella*, with fewer *Vibrio* and *Pseudomonas*. Post-treatment samples, evaluated through spread and streak plating, demonstrated significant reductions in microbial load, pathogenicity, and COD across almost all treatment processes, indicating effective treatment. This study underscores the importance of monitoring microbial diversity and antibiotic resistance in faecal sludge for public health safety and effective sanitation management.

Keywords: *Faecal sludge, physico-chemical characterization, Microbial diversity, Next generation sequencing*

A facile synthesis of plasmonic Bi 2WO6 /Ag/CuS ternary nanocomposite to boost photocatalytic degradation of persistent antibiotics

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Abstract: Antibiotic residues in the environment lead to pollution and the risk of resistance gene development, making their degradation a key research focus. Herein, we synthesized a hierarchical flower-like morphology of Bi_2WO_6 is integrated with CuS through Ag nanoparticles, forming a Bi_2WO_6/Ag/CuS Z-scheme photocatalyst, whereas Ag nanoparticles function as solid-state electron mediators. The structure, morphology, composition, optical and electrochemical properties of this composite were characterized through various techniques. Under visible light irradiation, this catalyst significantly enhances the electron-hole pair recombination channelization. The ternary composite demonstrates significant photocatalytic efficiency, achieving 93% tetracycline (TC) degradation within 60 minutes. The efficiency of photocatalysis is enhanced in Bi_2WO_6/Ag/CuS samples due to localized surface plasmon resonance (LSPR) and improved interfacial charge transport and separation. In addition, tetracycline degradation routes were precisely identified by LC-MS analysis. ESR and radical trapping experiments identified hydroxyl (•OH) and superoxide ($\bullet O_2^-$) radicals as the primary active species in photocatalytic processes. Furthermore, in order to gain a profound understanding of the reaction mechanism, a Z-scheme charge transfer pathway has been proposed.

Keywords: *photocatalyst, nanoparticle, surface plasmon resonance, tetracycline degradation*

Synthesis of CTAB passivated $Cs_2AgBiCl_6$ perovskite for photocatalytic applications

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Abstract: Recently, halide perovskites (HPs) have demonstrated a great potential in photocatalytic and optoelectronic applications. Different kinds of surfactants are being used as a surface and bulk passivator in the synthesis of perovskites to improve their luminescence and chemical stability. In this work, we have studied the surface passivation of $Cs_2AgBiCl_6$ lead free metal halide perovskite (MHP) is by solution process method using cationic surfactant Cetyltrimethyl Ammonium Bromide (CTAB). The impact of passivation on $Cs_2AgBiCl_6$ perovskite's chemical properties and stability is investigated. The correlation of XRD spectra with the non-passivated $Cs_2AgBiCl_6$ reveals the intactness of the perovskite structure upon passivation. The cationic nature of CTAB enables stronger attachment to $Cs_2AgBiCl_6$ surface and chloride makes the perovskite stable towards humid conditions results in less percentage degradation of $Cs_2AgBiCl_6$ by H_2O stability test. We have further examined the photocatalytic behaviour of the synthesized material as a photocatalyst for degradation of organic dye.

Keywords: *Halide perovskite, photocatalytic applications, surface passivation, CTAB*

Nutrient removal and Aeration: A bench scale study on fresh fecal matter

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Abstract: Fresh fecal matter, a complex mixture of organics loaded with pathogenic microbes, poses a threat to environmental and public health. It primarily consists of digested and undigested food particles, water, and a diverse array of microorganisms with their metabolic byproducts. This study investigates the impact of aeration on nutrient removal in fresh fecal matter, an area with limited prior research. An experimental setup was developed, consisting of a 10-liter PVC tank, a 5-watt blower, and a 35-mm sparger producing bubbles of 0.1-0.5 mm in size. Results were obtained every 24 hours by analyzing fecal samples. Initially, the total phosphate (TP) in the sample was 11.037 mg/L. After diluting the sample to 5x, the TP was measured at 2.171 mg/L. The study demonstrates that aeration enhances the removal of organic matter and reduces nitrate and phosphate content. These findings contribute to better management strategies for fresh fecal matter, highlighting the potential benefits of aeration in mitigating environmental and health risks associated with untreated waste.

Keywords: *Fresh fecal matter, aeration, nutrient removal, phosphate removal.*

Harnessing natural media for efficient faecal sludge treatment: A bench scale study

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Abstract: Effective faecal sludge management is vital for urban sanitation, particularly in underdeveloped areas lacking conventional treatment facilities. Untreated faecal discharge poses significant health risks and environmental contamination, underscoring the need for efficient treatment methods. This study examines the use of natural media, which is readily available and cost-effective, for faecal sludge treatment. Natural media are chosen for their exceptional water absorption, filtration properties, and large surface area for microbial colonization, facilitating organic matter decomposition and solids retention.

An anaerobic reactor system with four chambers and a 10-liter capacity was used to compare two reactors: one with bio-media and one without. Both reactors treated 9 liters of sludge at a peristaltic pump rate of 6 rpm with a hydraulic retention time (HRT) of 25 hours. The reactors were evaluated based on initial values: pH (6.18), TSS (718 mg/L), VSS (650 mg/L), TKN (95.20 mg/L), TP (33.02 mg/L), TDS (360 mg/L), and COD (1250 mg/L). Results indicated that bio-media enhances microbial adhesion and biofilm formation, leading to more efficient organic decomposition and higher COD reduction compared to the reactor without media. Properly treated sludge holds potential for resource recovery, eco-farming, energy generation, and sustainable resource management. This research underscores the benefits of natural media in faecal sludge treatment for public health, environmental protection, and resource sustainability.

Keywords: *Faecal sludge, Resource Recovery, Natural media, Anaerobic reactor, COD*

Ag^0 modified Ag_3AsO_4/g-C_3N_4 hybrid for effective photocatalytic removal of 4-chlorophenol under visible light

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Abstract: The Ag_3AsO_4/g-C_3N_4 (AA/gCN) hybrid, incorporating Ag nanoparticles, was synthesized via an electrostatically-driven assembly method by combining Ag_3AsO_4 with graphitic nitride. Comprehensive characterization involved analyses of phase structure, morphology, and optical properties using X-ray diffraction, FTIR, SEM, TEM, UV-vis DRS and PL spectroscopy, along with XPS for insights into chemical composition and surface properties. The AA/gCN hybrid exhibited superior photocatalytic performance attributed to enhanced light absorption, efficient charge separation and enhanced charge transfer. The optimal AA/gCN hybrid demonstrated remarkable degradation efficiencies, achieving 76% for 4-chlorophenol under visible light irradiation within 150 minutes. Catalytic investigations were monitored using UV-vis spectroscopy and HPLC-PDA techniques. The radical trapping experiments suggested the predominant involvement of superoxide radicals ($O_2^{\bullet-}$) and holes (h^+). These findings highlight the promising potential of the AA/gCN hybrid for applications in environmental remediation and emphasising its pivotal role in tackling modern environmental challenges.

Keywords: *Ag, nanoparticles, 4-chlorophenol, electrostatically-driven, superoxide radicals, holes*

Preparation of Boron Nitride from Pyrolysis of Single Source Precursor and Study of Its Photo catalytic Activity

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Abstract: Hexagonal boron nitride(*h*-BN) is one of the most interesting III-V group material with in plane trigonal sp^2 bonding, with B and N atoms entirely substituting for carbon atoms in graphitic like sheet without changing its atomic spacing. *h*-BN has excellent mechanical and thermal conducting properties and is much more thermally and chemically stable than graphite which makes BN an outstanding candidate for composite materials in hazardous environment. BN exist in four crystalline forms i.e. *h*-BN, *c*-BN, *r*-BN and *w*-BN, among them *h*-BN is particularly interesting because of its structural analogy with graphite. A variety of *h*-BN nanomaterials with well-defined morphology and size such as nanosphere heterostructures, nanorods and nanoribbons have been synthesized by various routes. These morphologies play important roles for use of BN material in high temperature optoelectronic to biomedical applications. Present synthesis methods make it difficult for the manipulation of BN nanostructures, also the amount of available BN nanostructured materials are very limited for applications. We have synthesized Boron melamine single source precursor by the reaction of boric acid melamine in 2:1 ratio. Boron Nitride was prepared by pyrolysing precursor and pyrolysis parameters were optimized by varying temperature and atmospheric conditions for complete conversion from precursor to Boron Nitride material. Structural and morphological studies were carried out by characterizing prepared Boron Nitride material by various instrumental techniques such as FTIR, FESEM, EDAX, XRD. FESEM micrograph (Figure-1) of BN powder obtain by pyrolysing precursor at 820 °C shows Rod shape structure with 600-800 nm diameters. Photo- catalytic study of as prepared Boron Nitride was carried out by using Methylene Blue Dye. The detailed results will be presented in conference.

Self-Assembly of Nanocellulose and Lignin: Applications in Radiative Cooling, Bio-adhesives and Sustainable Photocatalysis

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Abstract: The agricultural waste generated in our country is mainly burnt on the field itself due to techno-commercial infeasibility of valorization methods. Our patented rice straw valorization method has better techno-commercial feasibility and thus is being tested at 100 KPD pilot plant available with our Industrial collaborator. However, we present here our recent works on applications of nanocellulose derived from microcellulose and lignin nanoparticles. Nanocellulose (NC), sustainable nanomaterial finds applications in radiative cooling (Air-conditioned Free Cooling) due to its high infrared emissivity and controllable visible light reflectivity. Nanocellulose is self-assembled to transparent thin film that exhibits 30% reflectance in visible region. The radiative cooling performance of this film is comparable to reported literature. Further, fluorophore-doped electrospun (PVA/NC) nanofibers senses acid vapor by regulating its optical properties. Solubility of extracted lignin in ethanol has been tested for separation of soluble lignin (low molecular weight, LMwL) from insoluble lignin (high molecular weight, HMwL). LMwL is self-assembled into luminescent lignin nanoparticles, while HMwL has been utilized to produce bio-adhesives as replacements for petroleum-based resins. The tensile strength of this adhesive is much better than polyvinyl acetate (Fevicol).

Keywords: *Nanocellulose, thin films, radiative cooler, electrospun, lignin, bio-adhesives*

Self-Supported Electronically Modulated Super-Hydrophilic Interconnected Nanospikes and Particle of MoS2-Ni3S2/NF for Alkaline Water Electrolyzer

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Abstract: A better understanding of hazardous contaminants such as Chromium (Cr) uptake by native plants at Chromite ore processing residue (COPR) sites is necessary to design phytoremediation plans. This study conducted a field-scale assessment of the plant at the Rania-Khan Chandpur Cr-contaminated site, one of India's largest contaminated sites. *Chrysopogon zizanioides*, commonly known as Vetiver grass, was harvested from the nearby wasteland of a large COPR dump (COPR#1) and a small COPR dump located in Rania village and a relatively safe area in Khan Chandpur village. Microwave acid digestion followed by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) was analyzed to check the concentration of Cr in the shoot of Vetiver grass. We observed Cr concentrations of 41.43 $mgKg^{-1}$, 1.4$mgKg^{-1}$, and 0.65$mgKg^{-1}$ in the shoot of the Vetiver grass thriving in wasteland near COPR#1, COPR#2, and in Khan Chandpur village, respectively. This indicates the suitability of Vetiver grass in the ecological restoration of such a highly contaminated site. Rural practitioners can actively engage in the co-creation of community-driven decentralized phytoremediation projects by leveraging the insights from this research.

Keywords: *Groundwater, Plant, Wasteland, Remediation, Polluted site*

Chromium Uptake by Vetiver grass thriving in and around Rania-Khan Chandpur Cr-Contaminated Site, India

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Abstract: There is a pressing need for a highly efficient electrocatalyst for cost-effective green hydrogen production. In this context, herein, we demonstrate the development of a self-supported,hybrid composite as a bifunctional electrocatalyst that facilitates both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) at a lower overpotential.The synergistic interactionbetween MoS_2 and Ni_3S_2 does help in improving the electrochemically accessible number of sites(ECASs). The MoS_2-Ni_3S_2/NF exhibits low overpotentials of only 187 and 146 mV for OER and HER, respectively, to achieve a current density of 10 mA cm^{-2} in alkaline media. Additionally, it shows less overpotential of 1.5 V to generate 10 mA cm^{-2} compared to 1.59 V for standard catalysts in a 1 cm^2 working area for overall water splitting. The practical application of MoS_2-Ni_3S_2 /NF‖ MoS_2-Ni_3S_2 /NF as a bifunctional catalyst was verified by constructing a membrane electrode assembly (MEA) of 4 cm^2 working area for the alkaline electrolyzer. Furthermore, It is showing

99 % faradaic efficiency for H_2 production. Comprehensive electrochemical and physical characterization referred that, the interconnected nanospikes and particle morphology, improved ECAS, enhanced hydrophilicity and improved mass transfer properties are the prime reasons for the better performance in alkaline OER and HER.

Keywords: *OER, HER, ECAS, Electrolyser, Charge transfer resistance, Nanospikes, Sel-supported catalyst.*

Visible light-driven photocatalyst: Ag^+ doped TiO_2 heterojunction with Carbon nanotubes for remediation of aqueous phase microplastics

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Abstract: Microplastics (MPs), the tiny plastics with an average diameter of less than 5 mm, are having tremendous increment in their existence in the aquatic environment, and threatening marine life as well as human health. Conversely, the technology for the control and effective removal of MPs from the aqueous media is yet to be developed. Recently, Advanced Oxidational Processes (AOPs) have shown efficiency in converting emerging pollutants into less harmful products. Thus, this study proposes the use of AOPs that involve in-situ formation of highly active radicals to degrade MPs from aqueous ecosystems using photocatalysis. TiO_2 is a widely used photocatalyst but only works under UV light. Therefore, Ag^+ doped TiO_2, heterojunctioned with carbon nanotubes hybrid nanocomposite, was synthesized to mitigate the disadvantages of pristine TiO_2. Additionally, uniform-sized & monodispersed polystyrene (PS) microbeads are synthesized through dispersion polymerization to estimate the effectiveness of the modified photocatalyst. The degradation of PS microbeads was investigated using turbidity meter, TOC analyzer, FTIR, and GC-MS analysis. The obtained results have shown that visible-light-driven photocatalysis boosts PS chain scissions and decreases the concentration of PS up to 57.84% within 120 h of irradiation. A detailed quantitative and qualitative analysis of degradation studies will be presented at the conference.

Keywords: *Microplastics, Photocatalysis, TiO_2, Carbon nanotubes, Polystyrene, Photocatalytic degradation.*

Influence of acoustic cavitation in the extraction of keratin from tannery animal hair waste using greener solvent

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Abstract: Animal hair is a livestock product, which is a waste material and disposal is an environmental issue. In India nearly 3500 T/ annum hairs are being generated in tannery, which is a good source for the recovery of keratin. Keratin is one of the major proteins, its biodegradability, biocompatibility and physical properties rendered an attractive material for advanced polymeric composite material. The objective of the work is extraction of keratin in its native form by rapid dissolution process using acoustic cavitation technique along with ionic liquid (IL) and hair waste obtained from tannery lime-sulphide process. The hair waste defatted with Hexane-DCM mixture and aprotic IL [BMIM]Cl found to be suitable for effective dissolution. The optimal parameters solid:liquid ratio 1:40, ultrasonic power 450W and dissolution time 30 min yielded 70%, which is four times higher than conventional dissolution method. The characterization of the extracted keratin shows strong absorption peaks in ATR-FTIR spectrum, indicates no structural damage in the protein structure. XRD pattern shows a peak at 9° shows the disappearance of alpha helix structure indicates that the crystallinity is significantly reduced in the extracted keratin and ^{13}C NMR spectra shows structural confirmation of extracted keratin. Further works are in progress.

Keywords: *Tannery, Keratin, Acoustic cavitation, Animal hair, Ionic Liquids*

Water consumption forecasting Model Aizawl

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Abstract: This Research project aims to forecast water consumption in Aizawl district of Mizoram state utilizing the historical data of 2019 to June 2023 by analyzing various weather parameters including rainfall, temperature, humidity, and wind speed alongside pumped water metrics (which is filtered from Tlawng river) this study will show us forecast future water demand trends using machine learning and relevant libraries the analysis of time series forecasting models to generate insights crucial for solving the water shortage issues and improve the water management strategies through the application of different forecasting methodologies this project endeavors to provide actionable predictions for city planners and PHED authorities by understanding the potential impacts of changing weather patterns on water usage, decision-makers can proactively plan and allocate resources to address evolving demands thus fostering more sustainable and resilient water uses practices in the Aizawl district.

Synthesis of MIL-100 (Fe) Derived Iron (III) Oxide for Gas Sensing Applications

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Abstract: The rapid response/recovery and high selectivity of gas sensors play a crucial role in the real-time and online monitoring of hazardous gases. α-Fe_2O_3 (Hematite) stands out as a non-toxic semiconductor possessing favourable electrical, catalytic, and chemical properties vital for chemiresistive gas sensors. In this study, we present a feasible approach to fabricate Fe2O3 nanoparticles using the MIL-100 (Fe) template-assisted method. Fe-MOF is synthesized using the solvothermal method. It was calcinated at 350℃ to get the α-Fe_2O_3. The structural and morphological properties of synthesized material were analyzed using techniques such as X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), UV-Vis Spectroscopy, etc. The material inherited the morphological properties of pristine MOF. The gas-sensing behaviour of synthesized material was analyzed using a two-probe sensing system at different temperatures. This kind of material is expected to be a prospecting candidate for the application in gas sensors.

Keywords: *Chemiresistive, Hazardous, Gas sensor, Semiconductor, Non-toxic*

THEME-E:

Development of a Hydrogen Distribution System using Advanced Composite Integrated with Sensor Technology

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Abstract: The current focus is on altering the energy system due to the predicament of depleting fossil fuels and increasing awareness about global warming promoters. In a quest to find an alternative, hydrogen is a promising aid as it is a 100% clean energy source that emits no harmful by-products and gives higher energy output than present fuels. Most leading countries are advancing towards incorporating hydrogen technologies in the energy grid to help decarbonize the economy. The Indian government also announced the National Green Hydrogen Policy, which targets producing 5 million tons of hydrogen annually by 2030. This increase in H_2 production calls for better storage, transportation, and distribution solutions. Hydrogen has a flammability range in air of 4 -75 vol% and also exhibits low ignition energy of 0.018 mJ which makes it highly explosive and may pose serious safety risks which need to be addressed while designing hydrogen infrastructure. This colourless and odourless gas poses a problem in the identification and controlling of leaks which is crucial for workplace safety. Significant research has already been done on hydrogen storage, but transportation is still a new domain and needs exploration. Gaseous hydrogen is either transported in compressed pressure vessels arranged in tube trailers or through pipelines. Pipelines for hydrogen transport can be used in two ways: pure hydrogen transport and blending hydrogen with natural gas. Building a whole hydrogen-focused infrastructure needs a lot of initial capital and time. HCNG blends can be either used directly or separated at the end application. However, transporting hydrogen and HCNG through existing natural gas infrastructure has numerous complications. This work focuses on finding the suitability of existing metallic pipes and the problems faced when different concentration of hydrogen blends is transported through them at different pressures. FEA modelling is done in ANSYS for designing composite pipes and tubes for tube trailers. A comparative study of different methods is used for designing composite tubes, with the focus of reducing weight compared to their metallic counterpart. For incorporating safety measures in advanced composite structure, chemochromic hydrogen sensing material is developed which is simple, fast and has an easy detection mechanism. After extensive literature study, oxides of titanium, zinc and magnesium were identified as the base material which along with PdO catalyst can be used for hydrogen sensing. Their response time upon exposure to hydrogen was studied using epoxy and glass fiber composite as the supporting material. Image processing was used to identify the amount of colour change post sensing. Their effectiveness with respect to particle size is studied to observe their reactivity. Hydrogen sensing technology can be integrated with the composite storage and distribution system for a better infrastructure.

Thermal investigation of cool roof structures in composite climate of India

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Abstract: Worldwide, Global warming, Climate change, Urbanization and Urban Heat Island (UHI) effects are considered the most significant challenges for the current scenario. The rate of urbanization in the metropolitan cities enhanced due to the growth of the population level. The rapid urbanization caused by the energy consumption in the dwellings because of the comfort level of occupants. The current trends also notified that buildings located in urban areas are not up to the mark as per the energy efficiency standard of India such as Bureau of Energy Efficiency (BEE), Indian Green Building Council (IGBC) and National Building Code (NBC). Most of the population of India live in metropolitan cities and about 70% of the population will be shifted up to 2050. It is a major challenge for the researchers, scientists, architects and urban planners to adopt energy efficient techniques for building envelopes (wall, roof, and window). Cool roof technology is considered the most energy efficient in world-wide due to their ability to maintain thermal comfort and energy efficiency measures. The thermal investigation of cool roof structures was carried out for the composite climate of Indore (22.7^0N), Madhya Pradesh, India. The aim of the investigation was to assess the various thermal parameters (Indoor temperature, decrement factor, time lag, and sol-air temperature) for cool roof assemblies compared to the Reinforced Cement Concrete (RCC) slab. The study revealed that cool roofs performed better compared to the RCC slab in terms of thermal comfort application.

Keywords: *Building envelope, Cool roof, Decrement factor, Sol-air temperature, Time lag, Thermal comfort*

Tailoring interface confined carrier relaxation in Al2O3/TiO2 subnanometric laminates for energy storage applications

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Abstract: Maxwell-Wagner (M-W) interfacial polarization-dominated Al2O3/TiO2 nanolaminates (ATA NLs) have recently demonstrated their potential for new-generation energy storage applications In this work, we report the fabrication of device-grade sub-nanometric ATA NLs using an optimized pulsed laser deposition (PLD) and thermal atomic layer deposition (ALD) technique. A detailed interfacial characterization of the as-grown NLs is carried out to correlate the structural and dielectric properties, wherein the AC conductivity and current-voltage measurements are implemented to investigate the transport properties. The interface-confined carrier relaxation and sublayer conductivity contrast-induced M-W relaxation mechanism was engineered by precisely tailoring the individual Al2O3 and TiO2 sublayer along with the top-bottom capping layer thickness, which is also confirmed using resonant photoelectron spectroscopy measurements While comparing the ALD and PLD grown NLs, the optimised PLD NL, although having slightly higher interface interdiffusion, as shown in fig.(a) and (b) below, demonstrated improved energy storage density (~ 4.6 J/cm3), high cut-off frequency (~ 0.5 MHz), low dielectric loss (~ 0.032), and reduced leakage current density (~ 3.08 x 10-7 A/cm2 at 1V). These superior electrical properties and controllable dielectric relaxation make this laminate a promising high-k and low-loss dielectric material for next-generation Nano electronics and energy storage capacitors.

Keywords: *(M-W interfacial polarization, Nanolaminates, Storage capacitor, Transport properties, Atomic layer deposition, high-k and low-loss dielectric)*

Assessment of performance to a field-scale constructed wetland: A case study of Tepla village, Ambala, Haryana

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Abstract: Wastewater (WW) management is the major concern to focus for achieving sustainable development in developing countries. Constructed wetlands are the economical, & environmentally benign method, which has advantages for the economy, environment, and society. A detailed case-study of rural WW treatment technology, focusing on constructed wetlands, is presented. The inlet and outlet of existing technologies in Tepla Village, Ambala district, Haryana, was sampled extensively. In the which E. coli, TDS, COD, BOD, TSS, pH, EC, & salinity were the key parameters investigated. The study found E. coli, TDS and EC were beyond the permissible limit in the site, suggesting a health and environmental risk. The study found that due to behavioural issues of villagers that, it was not working properly as they were polluting the inlet by throwing the solid waste directly. Although after the several interviews, it was suggested that if there were the involvement of the villagers in the process, so the awareness to protect the technology would be there. To tackle these difficulties, the work focuses on the incorporation of Participatory Rural Appraisal (PRA) as a vital approach to engage and empower the community. This study highlights the significance of joint endeavours among researchers, policymakers, & local populations in formulating efficient systems for wastewater management.

Keywords: *Constructed wetland, Wastewater treatment, Participatory Rural Appraisal, Environment health, Interview.*

Numerical Investigation on Heat Transfer Characteristics of a Heat Exchanger Wrapped with Metal Foam

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Abstract: Metal foam known for its high specific surface area and superior thermal capabilities, has garnered significant interest across various engineering domains. This study presents a comprehensive numerical investigation into the heat transfer characteristics of a horizontal tube wrapped with metal foam. Numerical simulations are executed using FLUENT incorporating the Forchheimer-extended Darcy equation model to predict fluid and energy transports. Previous research primarily focused on the thermal performance of metal foam-filled-in channels, with limited analysis of the thermo-hydraulic mechanisms of porous and fluid interactions within the tube. To address this gap, a 2D numerical simulation is employed to elucidate the flow and heat transfer properties of a novel tube design covered by metal foam. The study examines the influences of foam structure parameters on heat transfer, revealing that the exterior heat transfer performance improves with increasing Reynolds number. Simulations with metal foams of 1, 2.5, and 3.25 mm thicknesses were conducted across fluid velocities of 5-20 m/s. The effects on heat transfer and pressure drop were compared to bare tubes. Validated by theoretical and experimental data, the study aimed to enhance heat exchanger performance by optimizing foam thickness and free stream velocity. Results show significant improvements in heat transfer for the metal foam tube bank, as measured by the area goodness factor. The findings highlight the benefits of tube-covering metal foam with low porosity

and low pore density compared to bare tubes, offering insights for the design and optimization of metal foam heat exchangers.

Keywords: Metal foam, Numerical simulations, Fluent, Heat Transfer, Area goodness factor.

ENHANCING BALLISTIC IMPACT PERFORMANCE OF NATURAL FIBER REINFORCED COMPOSITES WITH NATURAL FILLERS

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Abstract: Natural fibre composites offer a superior alternative to existing artificial fibre composites, primarily due to their advantages such as being lightweight, cost-effective, and environmentally friendly, particularly in terms of biodegradability. This study aims to assess the ballistic impact behaviour of Flax/Hemp natural fibre reinforced epoxy composite, incorporating Wooden Charcoal as a filler. Various compositions of flax/hemp/epoxy weight percentages were employed, with ratios varied to evaluate their impact on the ballistic performance of the proposed composites. Wooden charcoal fillers were consistently incorporated at a rate of 5wt%. The ballistic impact testing was carried out according ASTM E3112. The prepared composites samples are subjected to ballistic loading using a gas gun apparatus in the velocity range of 150 m/s to 300 m/s at room temperature. The impact and residual velocity of the projectile was measured by means of a chronograph placed immediately before and after the target. The results indicate that the damage area was determined by the indented point as the centre of the maximum length reached by the defect. Samples D and E, with charcoal as filler, exhibited reduced damage areas along the top ply of 12.35% and 26.48%, respectively, while the bottom ply showed 59.7% and 57.8% damage, respectively, compared to samples without filler. There was a 19.4% and 34.7% increase in energy absorption and ballistic limit velocity for samples D and E, respectively, compared to the other samples. The experimental results have been validated through numerical simulation using Ls-Dyna, demonstrating a close match with the experimental data.

Keywords: *Natural Fiber reinforced composites, Wood Charcoal, Ballistic Impact Test, Energy Absorption, Numerical simulation.*

Harnessing Bonding Heterogeneity: Tailoring Phonon Transport in Ternary Layered Compounds for Enhanced Thermal Management

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Abstract: Efficient thermal energy management employs materials with extreme lattice thermal conductivity (k_L), necessitating the need for the systematic investigation of phonon transport at the microscopic level. In this work, we focus on exploring the lattice dynamics and phonon transport properties in ternary layered compounds through first principles calculations and Boltzmann phonon transport theory. We consider various prototype materials of ternary alkaline-earth halo-fluorides and bismuth oxyhalides, characterized by intrinsic bonding heterogeneity. In bismuth oxyhalides, the presence of lone pair plays a crucial role to further suppress k_L by enhancing anharmonicity, which is absent in alkaline-earth halo-

fluorides. This work critically considers the structure and property correlations for these iso-structural layered materials that probes the interplay of bonding heterogeneity/lone pair activity and atomic mass. Thus, this work demonstrates possible avenues for rational design of phonon transport properties to advance the realization of high-performance materials for thermal management applications.

Keywords: Lattice thermal conductivity, Phonon Transport, thermal management, first principles calculations, Anharmonicity.

Recent Developments in Thermoelectric Properties of Bi_2Te_3-based Hybrid Nanocomposites

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Abstract: Energy generation and storage have become significant challenges for humanity today. Thermoelectricity is one of the renewable sources of energy which are utilized in low-powered but critical applications, ranging from remote IoT devices to radioisotope thermoelectric generators (RTG) used in spacecraft to power their communication devices. The efficiency of thermoelectric materials is evaluated by dimensionless constant thermoelectric figure-of-merit ZT of materials, based on Seebeck coefficient (S), electric conductivity (s) and thermal conductivity (s) at temperature T as $zT = S^2\sigma\,\kappa\,T$

Alloys based on bismuth telluride thermoelectric material is state of art materials at room temperature. Recently, hybrid nanocomposites of organic-inorganic materials, *viz.* inorganic compounds (such as Bi_2Te_3, PbTe, and SnSe), 2D materials (like graphene, transition metal dichalcogenides, black phosphorus, and MXene), organic materials (such as conducting polymers like polyacetylene, polyaniline, polypyrrole, and PEDOT), ceramics (such as CoO and CdO) are being studied for their thermoelectric properties. These hybrid nanocomposite thermoelectric materials show promise for harvesting energy in wearable devices, as they offer mechanical flexibility due to irregular surfaces, utilize simple solution-based deposition techniques, and deliver enhanced output power density. In this presentation results obtained from both experimental and computational studies of hybrid nanocomposites of pristine and doped of bismuth tellurides samples will be discussed.

Keywords: *Thermoelectric, Bismuth Tellurides, hybrid nanocomposites*

Enhanced Optoelectronic Devices Engineered with Lead (Pb) or Lead-Free Halide Perovskites Tailored for Environmental Stability

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Abstract: Since the unveiling of state-of-the-art hybrid halide perovskites, their application in optoelectronics has gathered substantial attention. Integrating materials with diverse functionalities stands out as a versatile approach to realizing advanced optoelectronic devices. This study underlines the synthesis of both Pb and Pb-free perovskite-based optoelectronic devices, employing a straightforward device architecture with a larger active area, demonstrating efficient performance under the self-powered/photovoltaic mode. In particular, this work highlights the fabrication of low-temperature

processed inorganic-rich perovskites based on cesium, emerging as an appealing alternative to hybrid organic-inorganic perovskites. Explorations involving dilute additive engineering and various anti-solvent engineering techniques have been conducted to tailor and stabilize single and double cation Pb-based films at lower processing temperatures. Consequently, well-oriented structures with a more compact crystal lattice volume are achieved. Additionally, noteworthy enhancements in phase stability and robustness against external erosions have been observed, even under a relative humidity of 65±2% in ambient air conditions. The solar cell devices exhibit remarkable power conversion efficiencies ranging from 12.6% to 23.2%.

Keywords: *Optoelectronics, Photovoltaic, Inorganic-rich, Hybrid, Halide Perovskite*

Magnetic Field Dependent Magnetoresistive Variations in Trilayer ($La_{2/3}Sr_{1/3}MnO_3$/γ Fe_2O_3/$La_{2/3}Sr_{1/3}MnO_3$) Hetero-structure

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Abstract: We report the magnetic field dependent magnetoresistance (MR) properties of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO)/γ-Fe_2O_3/LSMO trilayer heterostructure and single layer LSMO film grown on SiO_2/Si (100) substrates by Pulsed Laser Deposition technique. The metal-insulator-metal configuration is a magnetic tunnel junction topology[1,2], which is a parallel network of two metallic layers (LSMO) and one insulating layer (γ-Fe_2O_3) in current-in-plane (CIP) geometry. The MR-H [MR = (ρ (H)-ρ (0))/ρ (0)] behavior of the films is studied under two regimes namely, Low Field Magnetoresistance (LFMR) and High Field Magnetoresistance (HFMR)[3,4] at 5 K and 300 K in the field range of 0-7 T. Several equations were developed to simulate the experimental MR-H data. We obtained significantly better MR-H results for the trilayer in current-perpendicular-to-plane (CPP) configuration, where the two metallic layers and an insulating layer are in series. In CPP configuration, MR is 21% @ 5 K and 1 T, while it reached to 44% at 5 K and 7 T. At a field of 9 T, trilayer film in CPP mode exhibits MR of 48% @ 5 K and 23% @ 300 K. Further, the anti-parallel and parallel magnetization states of the MIM device are well manifested in CIP and CPP geometries.

Keywords: Current-in-plane, Current-perpendicular-to-plane, Low field magnetoresistance, High field magnetoresistance, Magnetic Tunnel Junction.

Enhanced synaptic characteristics under applied magnetic field in V2O5/NiMnIn based switching device for neuromorphic computing

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Abstract: The present study reports a memory structure Al/V2O5/NiMnIn on a flexible stainless-steel (SS) substrate for neuromorphic applications. The fabricated device exhibits gradual SET and RESET switching characteristics with an OFF/ON resistance ratio of ~100, good consistency of 4500, and excellent data retention capability up to 3000 s. The resistance versus temperature measurement (R-T) in the LRS and HRS of the device signifies that oxygen vacancies form the conduction filament. We further analyze the synaptic functioning by applying identical consecutive voltage pulses, and the device's conductance change has been observed. These characteristics show a good representation of the biological memory synapse in

terms of the artificial memory device. Long-term potentiation (LTP) and long-term depression (LTD) show nonlinear and asymmetery behavior, which is substantial for neuromorphic applications. A considerable shift in LTP and LTD was detected by applying external temperature and magnetic field. This is explained via temperature and magnetic field strain in the functional NiMnIn bottom electrode of the fabricated device. The mechanical flexibility of the memory structure was tested by exploring the switching characteristics with various bending angles and bending cycles. Therefore, the present study offers new avenues for flexible devices with high data storage capability for futuristic neuromorphic applications.

Keywords: *Neuromorphic, RRAM devices, thin film, 2D materials, functional materials*.

Navigating the Potential of Nanomaterial in Thermal Systems Evaluating Performance, Stability and Overcoming Limitations with Innovative Solutions: A Comprehensive Review

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Abstract: This comprehensive review explores the intersection of thermal systems and nanomaterial, focusing on their impact on overall performance, stability, and the associated limitations and potential solutions. Nanomaterial, with their unique properties at the Nano scale 0-100 nm have emerged as a promising avenue for enhancing heat transfer characteristics and energy efficiency in many thermal applications systems, such as air conditioning and refrigeration, heat exchangers, solar thermal systems, chillers etc. However, this combination comes with a wide range of challenges, including issues such as stability, material corrosion as well as environmental impact. This review works enlightened about categorizing nanomaterial's used in variant thermal systems, each category is examined in terms of its synthesis mode, properties. The enhancement of heat transfer and energy efficiency is discussed in detail, showcasing the potential benefits that nanomaterial's offer in thermal systems. This review critically examines the constraints inherent in employing nanomaterial across thermal systems, encompassing issues like agglomeration, toxicity, and elevated pressure drop. It explores pragmatic remedies, including the utilization of surfactants, tailored nanoparticle design, and meticulous base material selection. This review paper furnishes a thorough synopsis of nanomaterial integration into Refrigeration, IC engines systems, accentuating their potential to augment overall performance and energy efficiency. As research progresses, the prospect of nanomaterial revolutionizing thermal systems towards a more sustainable, compact and energy-conscious future remains a compelling and continually evolving area of investigation.

Keywords: *Nano materials, Thermeophysical Properties, Stability, Challenges*.

A Dual emitting carbon dot-based ratiometric fluorescent probe for polarity sensor

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Abstract: Carbon dots are luminescent nanoparticles composed of a carbon core and surface structure

having functional groups such as amine, carboxyl, and hydroxyl groups, etc. Their properties, such as high emission quantum yield, non-toxicity, and biocompatibility, make them suitable candidates for bioimaging, sensing, and optoelectronic applications. The emission properties of carbon dots primarily depend on the surface states. This allows tunability of emission wavelengths, efficiency, and selectivity by optimizing the precursors and dopants used during synthesis as well as the surrounding environment where the carbon dots are dispersed. The synthesis of dual-emitting carbon dots with a longer emission wavelength by using a facile strategy is of great importance for the fabrication of ratiometric fluorescent nanoprobes. The dual emitting carbon dots, synthesized by the solvothermal method, exhibit emission in blue and red wavelength regions, showing a systematic dependence on the polarity of the solvent. Moreover, dual-emitting carbon dots demonstrate aqueous solubility and excellent fluorescence stability. Their polarity-dependent emission displays high sensitivity and inherent reliability, making them suitable for ratiometric in vitro polarity sensors.

Keywords: *dual emitting carbon dots, ratiometric fluorescent nanoprobe, polarity sensor, Bioimaging*

Unveiling the Non-enzymatic Electrochemical Glucose Sensing Properties of NiO Polyhedra synthesized through a Simple Thermal Decomposition Approach

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Abstract: Maintaining a stable glucose level is vital for overall health, as both high and low blood sugar levels can lead to various complications. Different glucose monitoring methods exist, but electrochemical glucose sensing is the most popular and promising detection technique. Herein, nickel oxide polyhedra was synthesized via direct thermal decomposition of $Ni(NO_3)_2.6H_2O$. The glucose-sensing properties of NiO-modified Glassy carbon were evaluated in 0.1 M NaOH. The NiO/GCE exhibited an excellent sensitivity of 1109 $\mu AmM^{-1}cm^{-2}$ and 737.7 $\mu AmM^{-1}cm^{-2}$ in the glucose range 5 µM to 1 mM and 1 mM to 6 mM, respectively, with a limit of detection 1.1 µM. Additionally, it showed good selectivity towards glucose compared to other interferents and a reproducible and stable performance. In addition, the influence of varying potentials and concentrations on glucose oxidation was investigated through Electrochemical Impedance Spectroscopy (EIS). The EIS consisted of two semicircles in the lower and higher frequency domains, and the diameters of the semicircles changed with the potential and concentration of glucose. Negative resistance was observed at some polarizing potentials. To the best of our knowledge, there are no published reports on utilizing NiO synthesized through a direct decomposition approach for glucose sensing coupled with a thorough impedance investigation.

Keywords: *Nickel oxide, Glucose sensing, Non-enzymatic, Thermal decomposition, Electrochemical impedance Spectroscopy*

Heterojunction of Natural Clay Minerals and Carbon Nanotubes as Robust Moisture Electric Generator

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Abstract: Among various sustainable energy harvesting devices, moisture electric generators (MEG) possess distinct advantages like portability, minimum human intervention, absence of moving parts, unnecessity of fuels, and potential for off-grid power generation. However, maturing this emerging technology requires the exploration of a diverse range of materials and device configurations. Here, we report the fabrication of heterojunction-based robust MEGs by using reconstructed layers of natural vermiculite clay (VM) and HNO_3-treated oxidized multi-walled carbon nanotubes (o-CNT). The heterojunction of negatively charged VM and o-CNT membranes (o-CNT-VM) prepared through a facile water-assisted fusion process yielded voltages of ~ 790 mV for more than 2000 seconds (at 75% RH). Assembling multiple o-CNT-VM devices in series connection output potentials up to 98 V were achieved. The mechanistic studies revealed the junction potential between VM and o-CNT to be the major contributor to the observed potential, with minor contributions arising from evaporation-driven streaming of ions through the 2D nanofluidic channels. The o-CNT-VM devices can function in extreme conditions such as temperatures ranging from 0 to 80 °C. The practical applicability of the flexible o-CNT-VM-based MEG devices is demonstrated by lighting LED, and powering calculators by assembling o-CNT-VM devices in simultaneous series and parallel connection.

Keywords: *Heterojunction; Vermiculite; Carbon nanotubes; Moisture electric generator; Junction potential; Streaming potential.*

High sensitivity and speed from heterostructure of few-layer MoS_2 and reduced graphene oxide-based photodetector

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Abstract: In recent years, there has been significant interest in two-dimensional transition metal dichalcogenides (2D-TMDC) because of their exceptional properties such as high mobility, high absorbance, and excellent performance in generating excitons (electron and hole pairs). Particularly, 2D molybdenum disulfide (MoS2) has been widely employed in optoelectronic and photovoltaic applications. Pristine MoS2-based devices are not suitable for these applications due to their poor photo-to-dark current ratio and low speed. So, they need some improvements, i.e., by adding layers or decorating with materials of the opposite types of majority carriers. In this study, we enhanced the properties of pristine MoS_2 by decorating reduced graphene oxide (rGO), resulting in improved dark current, photo-to-dark current ratio, and response time. Upon comparing the performance of a device based on pristine MoS_2 and a device based on rGO decorated MoS_2, it was observed that the rGO/MoS_2-based device exhibited an enhanced responsivity of 3.36 A/W, along with a photo-to-dark current ratio value of around 154. The heterojunction device demonstrated a detectivity of 4.75×10^{12} Jones, coupled with an exceptionally low response time of 0.184 ms. The device's stability is also exceptional, maintaining consistent repeatability tests even after a period of six months [1].

Keywords: *2D materials, MoS_2, rGO, Photodetector, Heterojunction*.

Design, Synthesis and Characterization of Tetrabenzofluorene Derivatives with Tailored Properties for Fluorescent Sensing Application

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Abstract: Extended π-conjugated molecules have garnered significant attention for their potential application as fluorescent sensors in diverse industry applications, environmental monitoring and bioimaging. Molecules exhibiting desirable properties including high sensitivity and selectivity, high quantum yield and having emission in easily detectable region are of importance. Butterfly-shaped tetrabenzofluorene (TBF) molecule poses as a highly appealing system due to its core structure consisting of fused benzene and fluorene rings. This enhances the desirable characteristics of TBF and its derivates giving a class of compounds with versatile properties. In this work, we have synthesized four novel TBF derivatives with preferred functional groups by Suzuki coupling reaction and subsequently purified. These molecules were characterized by 1D and 2D NMR spectroscopy, mass spectrometry and FTIR. The photophysical properties were investigated using UV-VIS and fluorescence spectroscopy. The results of these studies provide valuable insight into the structural and photophysical properties of the synthesized TBF derivatives, highlighting their potential use as fluorescent sensor.

Keywords: *Tetrabenzofluorene, π-conjugated molecules, fluorescent sensors, Suzuki coupling reaction*

Graphene based Transparent conducting electrode for OLEDs

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Abstract: Indium Tin Oxide (ITO) is the most widely used transparent conducting electrode (TCE) for Organic Light Emitting Diode (OLEDs) application due to its high electrical conductivity and highoptical transmittance. However, the scarcity of indium is the major concern for its use as it leads to increase in the production cost of the device. Moreover, due to its brittle nature, it is unsuitablefor flexible and foldable display technology. Apart from these drawbacks, deposition of ITO involves unpleasant high temperature processing methods. Graphene being highly flexible, transparent, and conducting, could be used as the potential candidate for replacing ITOs. However,for graphene there are some challenges like high sheet resistance, low work function, zero-band gap, and scalability. Recent research is focused on various methods to overcome these drawbacks.In this work, we did the traditional wet transfer etching method for transferring graphene on to theglass substrate. Other part of the work is to reduce the sheet resistance and increase transmittanceof the transferred graphene via doping with HNO3. Further, we have performed a comparative study of the ITO and Graphene as TCE for the OLED device application.

Keywords: *Organic Light Emitting Diode (OLED), Transparent conducting electrode (TCE), Graphene, Indium Tin Oxide (ITO).*

Stimuli-Responsive Nanofluidic Device for Controlled Delivery of Ions

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Abstract: The elegance and accuracy of biological ion channels inspire the fabrication of artificial devices with similar properties. Here, we report the fabrication of iontronic devices capable of delivering ions at the nanomolar (nmol) level of accuracy. The triangular nanofluidic device prepared with reconstructed vanadium pentoxide (VO) membranes of thickness 45 ±5.5µm can continuously deliver K^+, Na^+, and Ca^{2+} ions at the rate of 0.44 ±0.24, 0.35±0.06, and 0.03 nmol/min, respectively. The ionic flow rate can be further tuned by modulating membrane thickness and salt concentration at the source reservoir. The triangular VO device can also deliver ions in miniscule doses (~132 ± 9.7 nanomole) by electrothermally heating (33°C) with a nichrome wire (NW) or applying lights of specific intensities. The simplicity of the fabrication process of reconstructed layered material-based nanofluidic devices allows the designing of various complicated iontronic devices like the three terminal-Ni-VO (3T-Ni-VO) devices. Such devices can find applications in various fields such as Energy conversion and storage, drug delivery, neurological signaling.

Keywords: *Nanofluidics, Iontronics, Controlled delivery, Ion selectivity, Energy Conversion*

Thermoelectric and photovoltaic properties of 12-$BaBi_2S_4$

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Abstract: We present the structure and properties of 12-$BaBi_2S_4$, which crystallizes in the hexagonal crystal system with the space group $P6_3/m$ as revealed by a single crystal X-ray diffraction study. The refined lattice parameters of the structure are $a = b = 25.2687(10)$ Å, $c = 4.1859(2)$ Å ($Z = 12$) at RT. The 12-$BaBi_2S_4$ structure is made up of fifteen unique crystallographic independent sites: 3 × Ba, 4 × Bi, and 8 × S atoms. A polycrystalline 12-$BaBi_2S_4$ sample was found as a semiconductor with a direct optical bandgap of 1.3(1) eV, as confirmed by a UV-visible absorption study. We have also carried out thermal conductivity measurements, which reveal ultralow values varying from 0.47 $Wm^{-1}K^{-1}$ at 323 K to 0.43 $Wm^{-1}K^{-1}$ at 773 K. The polycrystalline sample shows a high value of Seebeck coefficients varying from $S = -300$ µV/K to −210 µV/K (323 K to 773 K). We have utilized the 12-$BaBi_2S_4$ sample for photovoltaic (PV) applications by fabricating a liquid junction solar cell, TiO_2/CdS/12-$BaBi_2S_4$/S_n^{2-}/S^{2-}/MWCNTs@Ni. The solar cell showed an improvement in efficiency of ~12% compared to the control cell, which was based on sole CdS as the photosensitizer.

Keywords: *X-ray diffraction, Thermal Conductivity, Seebeck coefficients, Photovoltaic, Solar cell.*

Enhancement in SO_2 Sensing Performance by Functionalizing Thiazole Polymer with Benzoselenadiazole Ring

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Abstract: Gas sensors with sensitivity, fast response, selectivity and room temperature operation (RT) but current materials like metal oxides or inorganic polymers often fail to meet these criteria. Herein, we have successfully synthesized two conjugated polymers (CPs), one was decorated with only thiazole rings denoted as BBT and other contains benzolselenadiazole and thiazole rings denoted as BBTBSe. Furthermore, both were fabricated on interdigitated electrodes and employed to detect sulphur dioxide (SO_2) at RT. The BBTBSe sensor exhibited ~4 times improved response (R_g/R_a = ~199) to 100 ppm of SO_2 with fast response/recovery time of 60/70 s, as compared to BBT (R_g/R_a = ~45). Moreover, BBTBSe sensors

exhibited linear increase in the response with concentration with limit of detection and limit of quantification values of 0.23 and 0.76 ppb, respectively. Furthermore, BTBBSe sensor shows excellent selectivity against other interfering toxic gases, complete reversibility and pro-longed durability at RT. The possible sensing mechanism involves SO_2 molecules interaction with nitrogen atoms within benzolselenadiazole and thiazole rings on the surface of BBTBSe. Such remarkable results provide a feasible approach for highly sensitive and selective detection of SO_2 gas by BBTBSe sensor and suggest its application in industries and environmental monitoring.

Keywords: *Conjugated polymers, thiazole, benzoselenadiazole, sulphur dioxide, complete reversibility and highly sensitive.*

Non-volatile resistive switching based on halide perovskite materials for memory applications

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Abstract: Perovskite materials present compelling attributes for memristor applications owing to their rapid ion migration, adjustable band gaps, mechanical flexibility, and cost-effective fabrication. Notably, the high ion mobility and presence of point defects in perovskites augment memristor functionality, facilitating low threshold values and swift switching speeds, thus positioning them favorably for advanced electronic utilization. This investigation introduces solution-processable CsFAPbI3 perovskite-based memristor devices, integrating thorough structural, morphological, and electrical assessments to elucidate their memory characteristics. A comprehensive array of characterization techniques scrutinizes the impact of a few nanometres thin NiOx interfacial layer on memory attributes. The device manifests notably diminished set and reset voltages alongside a heightened on-off ratio when juxtaposed with alternative materials. Furthermore, the demonstrated device exhibits sustained performance across multiple scans and preserves consistent set voltages over protracted periods. This memristor's observed stability and reliability endorse its versatility for an array of applications encompassing information retention and memory-driven computing paradigms.

Keywords: *Memristor, Resistive switching, solution-processable, set voltage, neuromorphic computing.*

Flexible 2D MXene Based High Performance Piezoelectric Nanogenerators

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Abstract: Ti_3C_2, one of the two-dimensional layered structure material from MXene family which made up of titanium and carbon atoms has recently gained intensive interest due to its outstanding mechanical strength, optical property, ability to conduct electricity and their potential applications in area of catalysis, supercapacitors, molecular separation, and electromagnetic shielding effect. However, piezoelectric property of the MXene is rarely reported. In this work, single crystalline pure phase of Ti3C2 was synthesized using Ti_3AlC_2 MAX phase via chemical etching and solution route. Crystalline nature structure

and nanosheet like morphology of the as grown Ti3C2 phase were investigated by XRD and HR-TEM techniques. Nanoscale piezoelectricity in the 2D Ti3C2 was investigated by piezoelectric force microscopy and results was discussed. The PFM analysis revealed very high piezoelectric charge coefficient of 180 pm/V. The piezoelectric flexible nanogenerator based on as grown MXene was also fabricated and output performance was measured under vertical compressive strain. MXene-based piezoelectric materials hold the potential for enhancing energy harvesting and advancing versatile energy conversion technologies.

Keywords: *Ti_3C_2 (MXene), PDMD, piezoelectric nanogenerator, characterization, energy harvesting.*

Reduced Graphene Oxide/Silicon Heterojunction Solar Cells: Technical Strategies for Future High Efficiency Devices

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Graphene and its derivatives have garnered significant attention in Si heterojunction solar cells due to their exceptional electronic properties and compatibility with Si substrates [1,2]. Herein, we present a novel reduced graphene oxide (rGO)/Si heterojunction solar cell (HSC) aimed at systematic optimization of device parameters, significant advancements in power conversion efficiency (PCE), stability, and scalability of Si solar cells. The HSC was fabricated by depositing a thin layer of graphene oxide (GO) onto a Si substrate followed by its thermal reduction at 450 ℃ for 1h in the N2/H2 gaseous atmosphere to obtain rGO/Si junction. Silver (Ag) grid pattern was then deposited by thermal evaporation as front electrode and In:Ga alloy as full area rear electrode (schematic layout of device is presented in Fig. 1 (a)). The improved electrical conductivity of >20 S/cm after reduction with respect to the insulating GO layer and reduced ID/IG ratio (1.41 for GO; 0.95 for rGO) in the Raman spectroscopy revealed a significant removal of the oxygen functional groups, therefore efficient reduction of the GO. Detailed morphological and optical study before and after reduction revealed a uniform coverage of rGO over micro pyramid textured n-Si substrate along with matched optical reflectance with the textured Si (<11%). Quite impressive improvement of ~1% (absolute) in the PCE of the rGO/Si HSC as compared to that of the GO/n- Si (without reduction) based HSC was obtained. The reduced GO facilitated efficient charge separation and collection, leading to improved Jsc (7.80 to 9.77 mA/cm^2) (see Fig. 1 (b)). Also, high integrated Jsc of 21.04 mA/cm^2 from the quantum efficiency, tunable optical and electrical properties indicate the potential capability of the optimized rGO layer for high efficiency low- thermal budget heterojunction based solar cells.

Keywords: *Reduced graphene oxide, Silicon, Heterojunction solar cells, Electrical conductivity, Photovoltaic performance.*

Artificial Intelligence techniques in buildings for energy-savings: A review

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Abstract: Worldwide, buildings are considered a significant energy consumer and provide a comfortable indoor environment and conveniences to occupants. The rate of development of urban architecture in the World needs to adopt advance smart techniques in the dwellings which are eco-friendly and maintain the

indoor temperature close to thermal comfort condition. The artificial intelligence and a sustainability approach to the dwellings provide a better environment for human beings in the future prospective. The adoption of digital innovative and sustainable technologies is needed to improve the energy performance rating of the buildings. For current scenario, IoT, robotics AI, edge computing, and drones are the emergent technologies renowned as critical performers in accomplishing energy-efficient digitalized technology that will utilize in the urban area in buildings. The present studies include these technologies with advance passive techniques to enhance the energy efficiency measures in the building infrastructures.

Keywords: *Artificial intelligence, buildings, energy-saving, IoT, Sustainability, Thermal comfort*

Optimizatization of temperature by Hydrothermal synthesis of Nickel sulfide for Application as energy storage device

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Abstract: Nanomaterials have emerged as an exciting new class of materials that are in high demand for a range of different practical applications. Metal sulfides have recently gained considerable attention due to their distinctive optical, electrochemical, and structural attributes. The electrochemical efficacy of sulfide-based electrode materials is contingent upon factors such as structure, size, porosity, and morphology. Nickel sulfide holds particular significance within the metal sulfide category, owing to its diverse phases like such are, α-NiS, NiS_2, Ni_3S_2, Ni_7S_6, etc. among which its phases, β-NiS (rhombohedral) and α-NiS (hexagonal) emerge as the most stable and sulfur-rich forms of nickel sulfide. Here β-NiS is synthesized hydrothermally at different temperatures in the range 140 to 200 ^oC using ammonia as a reducing agent. The synthesized material underwent comprehensive characterization through techniques such as X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), UV-Vis Spectroscopy and Fourier Transform Infrared (FTIR) Spectroscopy. The synthesized nanoparticles are then evaluated for their electrochemical performance as electrode materials demonstrating a good capacitance making it an appropriate candidate for supercapacitor application.

Keywords: *Nanoflakes, electrolyte, electrode, Nickel sulfide*

Development of Electrochemical Energy Storage Device Thorough Fused Filament Fabrication

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Abstract: This paper explores a novel approach in the field of electrochemical energy storage devices (EESD) while investigating the mechanical (tensile, compression, impact, and flexural strength), electrical (electrical conduction), and thermal (thermal transition and thermogravimetric behaviour) properties of the developed PLA and its sixteen composite materials through fused filament fabrication. The polymer-matrix composites are developed with PLA (as thermoplastic matrix) and different combinations of additives, including carbon fibres, graphene nanoplatelets, multi-walled carbon nanotubes, lithium titanate oxide, and lithium manganese oxide. Through experimentation and analysis, this research studies how additives influence material behaviour for enhanced design and application in the field of EESD.

Keywords: *polymer-matrix composites; electrical properties; mechanical properties; thermal properties; fused filament fabrication.*