



3rd International Conference on

ENERGY & ADVANCED MATERIALS

(ICEAM-2026)

October 8–10, 2026

Department of Physics and Materials Science & Engineering
Jaypee Institute of Information Technology, Noida, India





3rd International Conference on

ENERGY & ADVANCED MATERIALS

ICEAM-2026

ABSTRACT BOOK

October 8–10, 2026

Organized by

Department of Physics and Materials Science & Engineering

Jaypee Institute of Information Technology

A-10, Sector 62, Noida – 201309, Uttar Pradesh, India

iceam.co.in

Message from CEO Digital Learning



Shri. Manu Bhaskar Gaur

Energy is a primary requirement for sustainable growth and development. The growing global need for clean, efficient, and sustainable energy has created significant opportunities for research and innovation in energy technologies and advanced materials. The 3rd International Conference on Energy & Advanced Materials (ICEAM-2026) provides a valuable platform to share ideas, research, and expertise in these important areas.

ICEAM-2026 will bring together scientists, researchers, academicians, and industry professionals to discuss recent scientific and technological advancements in hydrogen energy, batteries, supercapacitors, advanced functional materials, and emerging materials technologies. The interactions among experts will also provide young researchers with opportunities to learn, exchange ideas, and explore new research directions.

I convey my best wishes to the organizers and participants of ICEAM-2026 and wish the conference a grand success.

With compliments and best wishes,

A handwritten signature in black ink, appearing to read 'Manu Gaur', with a stylized flourish at the end.

Manu Bhaskar Gaur
CEO, Digital Learning
Jaypee Institute of Information Technology (IIIT) Online

Message from the Pro-Chancellor



Prof. (Dr.) S.C. Saxena

It gives me immense pleasure to learn that the Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, is hosting the 3rd International Conference on Energy & Advanced Materials (ICEAM-2026) from October 08–10, 2026.

The theme of ICEAM-2026 is highly relevant to the evolving needs and challenges of the present era. The conference will provide a platform for deliberations on recent advances in hydrogen energy, batteries, supercapacitors, and advanced functional materials, with a focus on emerging technologies and their potential applications in sustainable energy and materials development.

ICEAM-2026 is expected to bring together eminent scientists, researchers, academicians, industry professionals, and young researchers from India and abroad. The conference will facilitate the exchange of knowledge, ideas, and experiences among experts from diverse areas of energy and advanced materials. The technical sessions, invited lectures, and scientific discussions will foster meaningful interactions, stimulate new ideas, and provide young researchers with valuable opportunities to engage with leading experts in their respective fields.

I am confident that ICEAM-2026 will contribute significantly to strengthening scientific collaboration, encouraging innovation, and inspiring the next generation of researchers in the areas of energy and advanced materials.

I extend my warm greetings and best wishes to the organizers, delegates, speakers, and participants of ICEAM-2026 and wish the conference great success and a fruitful scientific outcome.

With compliments and best wishes,

A handwritten signature in blue ink, appearing to read 'Saxena', with a horizontal line underneath.

Prof. S. C. Saxena

Pro-Chancellor

Jaypee Institute of Information Technology

Message from the Vice-Chancellor



Prof. Rajive Kumar

I would like to congratulate the PMSE Department for organizing the 3rd International Conference on Energy & Advanced Materials (ICEAM)-2026 during October 08–10, 2026. Nowadays, the whole world is looking for green, clean, and renewable sources of energy, in which advanced materials play a remarkable role. Thus, this conference offers a unique combination of energy and advanced materials, addressing two important and closely interconnected areas of contemporary research.

The vibrant platform created through this conference will go a long way in enabling the participants to learn about new advancements in the field of energy and advanced materials research. Undoubtedly, the conference will attract a large number of national and international participants and provide an excellent opportunity for the exchange of knowledge and ideas. I wish the conference grand success.

With compliments and best wishes,



Prof. Rajive Kumar

Vice-Chancellor

Jaypee Institute of Information Technology

Message from the Conference Chair / Convener

It gives me immense pleasure to welcome you to the 3rd International Conference on Energy & Advanced Materials (ICEAM-2026), being organized by the Department of Physics and Materials Science and Engineering during October 08–10, 2026. ICEAM-2026 brings together two highly interconnected and rapidly evolving areas of contemporary science and technology—energy and advanced materials.

The growing global demand for clean and sustainable energy has created an urgent need for innovative materials and technologies for efficient energy conversion, storage, and utilization. With this vision, ICEAM-2026 provides a platform for researchers, academicians, scientists, industry professionals, and young researchers to present their work, exchange ideas, and discuss recent developments in areas including hydrogen energy systems, batteries, supercapacitors, advanced functional materials, crystalline porous structures, and AI/ML-enabled materials discovery and optimization.

The conference is designed to foster meaningful scientific interactions and encourage new collaborations among participants from India and abroad. The invited lectures, technical sessions, and scientific discussions will provide opportunities to share knowledge, explore emerging research directions, and address the challenges associated with the development of sustainable energy technologies and advanced materials.

I am confident that ICEAM-2026 will provide an enriching and intellectually stimulating experience for all participants and will contribute to strengthening academic and research collaborations in the field.

On behalf of the organizing team, I extend my sincere gratitude to all the distinguished speakers, delegates, researchers, students, and participants for their valuable contribution and support. I warmly welcome you to ICEAM-2026 and wish you a fruitful, engaging, and memorable conference.

With compliments and best wishes,

Conference Chair / Convener



Dr. Ashish Bhatnagar

ICEAM-2026

Department of Physics and Materials Science and Engineering
Jaypee Institute of Information Technology

Preface

It is our pleasure to present the Abstract Book of the 3rd International Conference on Energy & Advanced Materials (ICEAM-2026), organized by the Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology (JIIT), Noida, during October 08–10, 2026.

ICEAM-2026 brings together the closely connected fields of energy and advanced materials, addressing some of the important scientific and technological challenges associated with sustainable energy development. The conference provides a multidisciplinary platform for researchers, academicians, scientists, industry professionals, and young researchers to present their recent work, exchange ideas, and explore emerging research directions.

The scientific programme encompasses a broad range of topics, including hydrogen energy, batteries, supercapacitors, advanced functional materials, two-dimensional materials, crystalline porous structures, and AI/ML-enabled materials discovery and optimization. The Abstract Book brings together contributions from the invited and keynote speakers as well as researchers presenting their work through oral and poster sessions.

We hope that the abstracts compiled in this volume will provide a useful overview of the diverse research activities being pursued in the fields of energy and advanced materials and will stimulate further scientific discussion, collaboration, and innovation.

We sincerely thank all the distinguished speakers, authors, delegates, researchers, students, reviewers, advisory committee members, and organizing team members for their valuable contributions and support. Their collective efforts have been instrumental in making ICEAM-2026 a platform for meaningful scientific interaction and knowledge exchange.

We wish all participants a fruitful, engaging, and memorable conference and hope that the interactions at ICEAM-2026 will lead to new ideas, collaborations, and advances towards a sustainable energy future.

With best wishes,

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Department of Physics and Materials Science and Engineering

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Inaugural, Keynote & Invited Talks

38 Speakers

IT-01 • Inaugural Lecture

08 Oct. 2026, 10:10 to 10:50 AM

Anatomy and Physiology of Soft Materials in Adhesion and Wetting**Prof. Ashutosh Sharma, (Padma Shri)**

IIT Kanpur

Abstract

This talk will focus on instabilities and their control in thin liquid and soft solid films for self-organized micro and nano patterning of polymeric materials, as well as for engineering of reusable adhesives.

**Prof. Ashutosh Sharma****Brief Profile:**

Prof. Ashutosh Sharma is an Institute Chair Professor in the Department of Chemical Engineering at the Indian Institute of Technology Kanpur and a distinguished researcher in nanoscience, nanotechnology, soft matter, and advanced materials. His research interests include soft nanofabrication, functional and nanomaterials, thin films, colloids and interfaces, wetting and adhesion, biomaterials, and micro/nano systems for energy, health, and environmental applications. He has made pioneering contributions to the understanding and engineering of thin films and nanoscale systems. Prof. Sharma served as Secretary, Department of Science and Technology (DST), Government of India, from 2015 to 2021, and served as President of the Indian National Science Academy. He is a recipient of numerous prestigious honours, including the Infosys Prize, Shanti Swarup Bhatnagar Prize, TWAS Science Prize, UNESCO Medal, and the Padma Shri (2025).

IT-02 • Inaugural Lecture

08 Oct. 2026, 10:50 to 11:30 AM

Computational materials science for advanced energy materials**Prof. Rajeev Ahuja**

Indian Institute of Technology Ropar, Rupnagar 140001 Punjab, India

&

Department of Physics & Astronomy, Uppsala University, Uppsala, Sweden

Abstract

Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modelled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

**Prof. Rajeev Ahuja****Brief Profile:**

Prof. Rajeev Ahuja is a Professor of Computational Materials Science at Uppsala University, Sweden, and the Director of the Indian Institute of Technology Ropar since April 2021. He is a leading researcher in computational materials science, with major research interests in batteries, hydrogen storage and production, energy materials, sensors, and high-pressure physics. He has an extensive international research record, with more than 1,200 peer-reviewed scientific publications and a highly cited research profile. Prof. Ahuja has also held academic and research positions at Uppsala University and Harvard University and has supervised numerous doctoral and postdoctoral researchers. His contributions to materials science and energy research have received several international recognitions, including the Benzelius Prize, Wallmark Prize, Beller Lectureship, and honours from the Royal Swedish Academy of Sciences.

IT-03 • Keynote

08 Oct. 2026, 11:45 AM-12:15 PM

Electrochromic studies of atomic/ionic transport kinetics in battery materials**Prof. Guido Schmitz, Univ. Stuttgart, Germany**

Guido Schmitz, Vinit Agarwalla, Monica Mead, Robert Löser
Institute of Materials Science, University of Stuttgart, Germany

Abstract

Diffusion and atomic/ionic transport represent core functional principles of rechargeable batteries. Useful batteries should operate at room temperature. Thus, transport needs to be extremely fast, which hinders application of classical tracer methods established in physical metallurgy. It is quite common to investigate ionic mobilities by electrochemical methods, such as GITT, PITT or even impedance spectroscopy. These methods require delicate assumptions, when interpreting the data in terms of diffusion coefficients. This might be a reason why experimental data on ionic diffusivity not seldom spread on several orders of magnitude.

As an independent alternative, we propose utilizing the electrochromic properties of battery electrodes to enable an in-situ tracing of the ionic transport. By correct calibration / modelling of the optical properties, even detailed evolution of the composition profiles can be determined. The talk demonstrates that way more detailed information can be gathered with the optical method than with established electrochemistry.

In typical thin film geometry, we investigate lateral diffusion profiles on large distances, even several tens of micrometers by optical microscopy. Accurate galvanostatic charging allows producing calibration samples with known composition. The determined functional relation between optical reflectivity and local Li content is used for training machine learning algorithms (support vector regression). Inversely using this regression, the local Li content can be measured during lithiation or delithiation.

In LiMnO_2 , concentration profiles distinguish three phases of different Li content. We observe a very significant difference in diffusivity between these phases. Especially for the Li-poor phase, the diffusivity is very fast, even two orders of magnitude faster than reported in earlier literature. Variation of temperature (20°-80°C) furthermore enables determination of activation energies. It is shown that transport barriers at phase boundaries are so large that for transport lengths less than 10 μm , diffusion coefficients cannot be determined by principle, instead a linear barrier transport coefficient is evaluated that might be misinterpreted as diffusion coefficient in classical PITT.

In reversible processing Si anodes, the Li transport appears in amorphous host. The optical profiles represent a sharp boundary that clearly indicates the presence of two amorphous phases. These phases reveal significantly different ionic mobility (about factor of 50!). This significant asymmetry leads to a way faster lithiation than delithiation process.

IT-04 • Invited

08 Oct. 2026, 12:15-12:45 PM

Uncovering the Potential of Candle Soot Nanocarbon for Energy Storage Applications
Prof.Chandrashekhar Sharma, IIT hyderabad**Abstract**

There has been tremendous focus on carbon nanomaterials, primarily on carbon nanotubes, nanofibers and graphene in the last two decades for a variety of applications including energy storage. Our CARBON Lab however introduced for the first time in 2015 the use of one of the most facile and inexpensive carbon nanomaterial in the form of candle soot nanocarbon as an electrode for Lithium-ion batteries, especially for electric vehicles. Since then, we have explored a number of ways to modify the physicochemical properties of soot derived nanocarbon and extended its application from Metal-ion to Metal-S batteries and supercapacitors. Very recently, we also started exploring a new battery chemistry based on Metal-CO₂ redox reaction in order to find the solutions to overcome the challenges of increased CO₂ emissions on earth. Soot derived nanocarbon is found to play an important role in this case as well. In this talk, I shall present some of our recent findings uncovering the potential of this new form of nanocarbon for energy storage applications.

IT-05 • Invited

08 Oct. 2026, 12:45 to 01:15 PM

Graphene Based Electrode Materials for Efficient Energy Storage as a Supercapacitor

Prof. Dinesh Pratap Singh – University of Santiago, Chile

Physics Department, Faculty of Science, University of Santiago of Chile (USACH), Avenida Victor Jara 3493, Estacion Central, Santiago 9170124, Chile

Corresponding Author Email: singh.dinesh@usach.cl, dineshpsingh@gmail.com

Abstract

The scarcity of fossil fuels such as natural gas, crude oils, coal and simultaneously global energy consumption continue to surge across all energy sectors including daily routine and transportation, have intended researchers to think about more potent energy alternatives. The use of traditional power plants including nuclear energy, increase CO₂ emission hence causes global warming issue and off course significant safety and environmental risks to all living beings. Alternatives of renewable and sustainable energy sources demand highly efficient and ecofriendly system to store energy for uninterrupted continuous 24 hrs. power supplies. Among existing energy storage technologies, Lithium-ion batteries or fuel cells are plagued by scarcity of core materials and environmental issues. In this regard electrochemical double-layer capacitors (EDLCs), or supercapacitors, offer key advantages over commercially available storage systems in terms of fast charging, high power density, rapid power delivery, excellent capacity retention, long cycle life, and eco-friendliness. However, technological and widespread commercial adoption are still far due to limitations of low energy density, narrow operating potential windows, and poor ionic conductivity.

To overcome these challenges, graphene [1] and its composites have emerged as promising candidate for the electrode materials due to their high surface area, superior electronic and ionic conductivity, cost-effective and eco friendliness. This presentation highlights graphene-based electrode materials for efficient energy storage as a supercapacitor. Various rGO based composites (rGO-Au, rGO-CrOOH, rGO-Ag, etc.) [2-4] are synthesized by chemical/ hydrothermal/microwave assisted methods and further utilized as electrode material to evaluate their electrochemical performances by the means of cyclic voltammetry, charge/discharge and electrochemical impedance spectroscopy. The optimized electrode materials are further utilized to design coin cell device and evaluated their performances in two electrode configurations from the prospects of commercial viability. The performances are reported and compared to other related materials and reports by Ragone plot. The details of the synthesis characterizations and device fabrications will be described and discussed in detail at the time of presentation.

Keywords: Graphene; Supercapacitor; rGO-Au; rGO-Ag, Coin cell device

IT-06 • Invited

08 Oct. 2026, 02:15-02:45 PM

Development of sustainable and high energy density Na-ion batteries: Water- stable ‘layered’ transition metal oxide based cathodes and ‘alloying reaction’ based anode**Prof. Amartya Mukhopadhyay- IIT Bombay***Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India*

e-mail ID: amartya_mukhopadhyay@iitb.ac.in

Abstract

For moving up the energy density ladder, both in terms of gravimetric and volumetric energy densities, Na-ion batteries need the development of high capacity, high voltage and electrochemically stable cathode materials, viz., ‘layered’ Na- transition metal (T_M) oxides exhibiting anion-redox, as well as ‘alloying reaction’ based anodes. Furthermore, from the point-of-views of sustainability, ease of handling/storage, cost-cum-energy savings, as well as health/environment-friendly processing, the development of ‘layered’ Na- T_M -oxide cathode materials that are stable upon exposure to humid air and water are also important. The latter can facilitate ‘aqueous’ electrode processing, using water, instead of highly toxic/hazardous NMP, as the medium for preparing the cathode slurry [J. Power Sources 610 (2024) 234716]. Against this backdrop, the talk will discuss about the development of air and water-stable O3-structured, as well as high Na-containing P2-structured, ‘layered’ Na- T_M -oxides by way of either shrinking the ‘inter-slab’ spacing or precise positioning of dopant cation having d^0 electronic configuration (viz., no OSPE) at the tetrahedral site of the Na-layer to suppress spontaneous Na-removal (or Na^+/H^+ exchange) upon exposure to moisture, as well as water [J. Mater. Chem. A 8 (2020) 18064, Chem. Mater. 34 (2022) 10470, Adv. Energy Mater. 13[19] (2023) 2204407, J. Mater. Chem. A 13 (2025) 5807]. This will be followed by a discussion on stable and low hysteretic oxygen redox behaviour, as exhibited by high Na-containing (>0.8 p.f.u.) P2-structured ‘layered’ Na- T_M -oxides, which are built-on high covalency of the T_MO_2 -‘slabs’. On the anode side, considering the disadvantages of hard carbon based anodes due to the low tap density and high 1st cycle irreversible capacity loss, the latter half of the talk will reveal the development of highly stable carbon-free Sn-based anode materials, which exhibit excellent cyclic stability, as well as rate-capability, primarily due to the enhancement of intrinsic strength via metallurgical phenomenon of precipitation strengthening. Challenges associated with the development of ‘full’ Na-ion cells with anion-redox based cathodes and Sn-based anodes will also be discussed, in brief.

Keywords: ‘Layered’ transition metal oxide cathode, Sn-based anode, aqueous electrode processing, electrochemical behavior, ‘full’ Na-ion cell

IT-07 • Invited

08 Oct. 2026, 2:45-3:15 PM

From Advanced Energy Storage Materials to Hydrogen Valley Innovation Clusters: Accelerating India's National Green Hydrogen Mission

Dr. Ranjith Krishna Pai DST, Delhi

Scientist 'F' / Senior Director, Climate, Energy and Sustainable Technology (CEST) Division, Department of Science and Technology (DST), Government of India

Abstract

The global transition towards net-zero emissions demands integrated solutions that combine renewable energy, advanced energy storage, green hydrogen, and circular resource utilization. India's National Green Hydrogen Mission (NGHM) has emerged as a transformative initiative to accelerate industrial decarbonization while strengthening energy security and sustainable economic growth. This keynote presents the Department of Science and Technology's (DST) strategic roadmap for advancing the green hydrogen ecosystem through research, innovation, technology demonstration, and large-scale deployment.

The presentation highlights DST's achievements in advanced energy storage materials, hydrogen and fuel cell technologies, Centres of Excellence, and international collaborative programmes that bridge fundamental research with industrial applications. Special emphasis is placed on the development of Hydrogen Valley Innovation Clusters (HVICs), which integrate renewable hydrogen production, storage, transportation, and end-use applications across sectors such as steel, fertilizers, mobility, and chemicals. These regional innovation ecosystems demonstrate how circular energy systems can accelerate technology commercialization while fostering collaboration among academia, industry, startups, and government.

The keynote also discusses India's progress under the National Green Hydrogen Mission, including policy interventions, pilot projects, indigenous technology development, skill enhancement, and global partnerships that support the transition toward a low-carbon economy. Finally, future opportunities for scaling Hydrogen Valleys, circular hydrogen value chains, and sustainable energy systems are outlined, highlighting India's growing role in the global clean energy transition.

Keywords: Green Hydrogen, National Green Hydrogen Mission, Hydrogen Valley Innovation Clusters, Energy Storage, Circular Economy, Industrial Decarbonization, Sustainable Energy, Net Zero, Clean Energy Technologies.

IT-08 • Invited

08 Oct. 2026, 04:00-04:30 PM

A walk through the realm of atomically thin materials: From Graphene to beyond
Prof. Anchal Srivastava – BHU, India*Department of Physics, Institute of Science, Banaras Hindu University, Varanasi, India*

Email: anchalbhu@gmail.com

Abstract

Two-dimensional (2D) materials have revolutionized materials science, beginning with the discovery of graphene—an atomically thin carbon sheet with extraordinary carrier mobility, mechanical strength, and thermal conductivity. However, the absence of an intrinsic band gap in graphene limits its application in semiconductor electronics. To overcome this challenge, research has advanced toward the development of 2D materials beyond graphene, such as transition metal dichalcogenides (TMDs) including MoS₂, WS₂, and WSe₂, which exhibit direct band gaps at the monolayer limit and show strong excitonic behavior in the visible range.

This presentation explores the evolution of 2D materials from graphene to other layered systems, highlighting advances in synthesis techniques like vacuum-assisted CVD and APCVD for large-area, uniform films. Our group has demonstrated scalable growth of high-quality graphene and TMD monolayers, verified by Raman, AFM, and photoluminescence studies. Additionally, hybrid systems such as h-BNC (boron nitride–graphene composites) and “Glaphene” (graphene–silica hybrids) represent the next frontier, enabling tunable band gaps and multifunctional device architectures. The study of these materials opens avenues for flexible electronics, photodetectors, sensors, and next-generation optoelectronic devices.

IT-09 • Invited

08 Oct. 2026, 4:30-5:00 PM

Hydrogen Storage Materials: A structural perspective on thermodynamics and kinetics

Prof. M.A. Shaz-BHU, India

Department of Physics, Institute of Science, Banaras Hindu University, Varanasi

Abstract

Hydrogen carries roughly three times the energy of petrol per kilogram, however, per litre it is among the poorest fuels. This makes storage the weak link in a hydrogen economy rather than production or end use. This talk discusses storage as a structural problem which is governed by three questions: where hydrogen sits, how fast it diffuses, and whether it comes back out. Interstitial site geometry sets the capacity ceiling. For example, in high-entropy alloys, lattice distortion opens octahedral sites which are not utilized in simple body-centred metals, raising that ceiling. On the other hand, atomic size mismatch even predicts the transformation pathway. Which links a purely geometric parameter to hydrogen kinetics. Diffusion distance and activation barriers set the rate, while catalysts or nano-structuring also changes it without altering the bond enthalpy. The shape of a PCT curve reports the spread of hydrogen absorption site energies, which connects thermodynamics to local structure. Against this background, the talk presents carbon aerogel work from Banaras Hindu University. Resorcinol-formaldehyde aerogels physically activated using CO₂ rise in surface area from 580 to 800 m²/g and absorb 5.28 wt.% hydrogen at 77 K and 22 atmospheres. Further, in-situ copper and nickel incorporation with chemical activation using KOH enhances uptake to 5.94 wt.%, yet a 2.7-fold gain in surface area delivers only a 20 percent gain in capacity, showing that pore-size distribution governs storage more strongly than total area. No material class yet satisfies capacity, kinetics and ambient thermodynamics together.

IT-10 • Invited

09 Oct. 2026, 09:00-09:30 AM

2D Materials for THz Application
Prof. Gagan Kumar – IIT Ropar, India*Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab 140001**Email: gk@iitrpr.ac.in***Abstract**

The field of terahertz photonics has grown rapidly due to its immense potential for developing next-generation devices and components [1]. The advent of artificially engineered materials, known as metamaterials, has opened new avenues for research and development in terahertz photonic components. This talk will discuss terahertz metasurfaces and their potential for building terahertz devices for applications in 6G and beyond.

This talk will delve into the intricacies involved in designing metamaterials, their fabrication in cleanroom ambience, and various related phenomena at terahertz frequencies, such as bound states in the continuum, toroidal excitations, flexible broadband metasurfaces, machine learning assisted meta-designs and electromagnetically induced transparency [2,3]. These phenomena can have significance in the development of photonic components at terahertz frequencies. Some of our recent research work on the excitation of high Q-metasurface using the approach of toroidal excitations and bound states in the continuum will also be discussed that can enable ultrasensitive biomolecular sensing with enhanced sensitivity.

IT-11 • Invited

09 Oct. 2026, 09:30-10:00 AM

Sodium ion Conducting Gel Polymer Interlayer for Suppressing Polysulfide Shuttle and Enhancing Performance of Room Temperature Sodium-Sulfur Batteries**Prof. Rajendra K. Singh, BHU Varanasi, India**

Rajendra Kumar Singh* and Samriddhi

Department of Physics, Banaras Hindu University, Varanasi

*email:rajendrasingh.bhu@gmail.com

Abstract

Room-temperature sodium sulfur (Na-S) batteries are attractive for cost effective energy storage, but their practical development is limited by polysulfide dissolution and shuttle, sluggish sulfur redox kinetics, and rapid capacity degradation. In this work, a flexible, free-standing sodium ion conducting gel polymer interlayer (IC-IM) based on PVDF-HFP, NaTFSI, and BMIMTFSI ionic liquid was developed. The influence of ionic liquid/salt solution content on the structural, thermal, ionic-transport, and electrochemical properties of the membrane was systematically investigated. Incorporation of the ionic liquid/salt phase promotes disruption of the crystalline structure of PVDF-HFP and increases its polar character, thereby generating favorable pathways for sodium ion transport. Among the investigated compositions, IC-IM70 (70% IL containing membrane) exhibited favorable ionic conductivity, low activation energy, high overall ionic transference, and appreciable Na^+ transport capability. The membrane also showed good electrochemical stability, supporting its application as an interfacial layer in room temperature Na-S batteries.

The interlayer substantially improved the rate performance and cycling stability of the cell by promoting sodium ion transport while limiting polysulfide migration toward the sodium anode. The enhanced electrochemical behavior is attributed to the combined effects of the ion-conducting polymer network and the negatively polarized PVDF-HFP/TFSI-rich interface, which facilitates Na^+ transport while contributing to electrostatic rejection and interfacial trapping of polysulfide species. The results demonstrate that a sodium ion conducting gel-polymer interlayer can provide an effective interfacial strategy for mitigating polysulfide shuttle and improving the reversibility and cycling stability of room-temperature Na-S batteries.

IT-12 • Invited

09 Oct. 2026, 10:00-10:30 AM

Magnesium-Sodium Hybrid Battery with Flexible Dual-Ion Gel Polymer Electrolyte**Prof. S.A. Hashmi, University of Delhi**

Pratibha Kumari and S.A. Hashmi*

Department of Physics and Astrophysics, University of Delhi, Delhi – 110007, India

E-mail: sahashmi@physics.du.ac.in

Abstract

Lithium-ion batteries (LIBs), a promising storage technology, are widely used in various technological applications including electric vehicles (EVs) or hybrid electric vehicles (HEVs). Although LIBs offer high energy and power densities and long cycle life, they face a great competition in the market, as a result, their potential alternatives are under active investigations. Magnesium batteries, particularly, are one of the promising alternatives, which have capability to fulfil most of the requirements. However, Mg-ion batteries (MIBs) are still far away from commercialization due to the requirements of proper cathodes and suitable electrolytes. Recently, magnesium-lithium or magnesium-sodium hybrid batteries having electrolytes containing dual-cations Mg^{2+} and Li^+ or Na^+ , known as “Mg-Li hybrid batteries (MLHBs) and Mg-Na hybrid batteries (MNHBs),” are found as promising replacement of LIB-technology. Various issues of MIB-technology are tackled by this novel concept. The MLHBs/MNHBs comprise Mg-metal or Mg-nanocomposites as anode and Li or Na-ion insertion-type compounds as cathode, separated by liquid or polymer-based electrolytes containing dual-cation (Mg/Li or Mg/Na) salts.

In this report, a promising Mg-Na dual-ion hybrid gel polymer electrolyte (hGPE) comprising $\text{Mg}(\text{ClO}_4)_2$ and NaClO_4 , dissolved in diglyme, immobilized in poly(vinylidene fluoride-co-hexafluoropropylene) is presented. Free-standing and flexible hGPE-films, optimized via various physical and electrochemical techniques, are found suitable for MNHBs. High conductivity ($\sigma_{\text{RT}} \sim 3.6 \text{ mS cm}^{-1}$), wide electrochemical stability window ($\sim 3.8 \text{ V}$) and high Mg-ion transport number ($t_{\text{Mg}^{2+}} = 0.75\text{--}0.81$) are attractive features of the hGPE-films. The electrolyte-film shows excellent interfacial stability with MWCNTs-dispersed Mg-anode, as evident from long-term electrochemical impedance spectroscopy (EIS) and stripping/plating. Performance of the hGPE-film-incorporated MNHB-cell with MWCNTs-dispersed Mg-powder and $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ as anode and cathode, respectively, have been evaluated via CV and galvanostatic charge-discharge tests. The MWCNTs-dispersion in anode/cathode materials shows the excellent improvement in device performance in terms of specific capacity ($\sim 78 \text{ mAh g}^{-1}$ after 50 GCD cycles with $\sim 53\%$ capacity retention at 1 C-rate), cyclic stability (up to 140 cycles) and Coulombic efficiency ($\sim 99\%$).

IT-13 • Invited

09 Oct. 2026, 10:30 to 11:00 AM

Design, development and testing of metal hydride based devices for hydrogen storage, purification and compression applications**Prof. P. Muthukumar – IIT Tirupati, India***Professor, Department of Mechanical Engineering, Indian Institute of Technology Tirupati*

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Abstract

Considering the global energy scenario and the significant increase in atmospheric CO₂ concentrations, there is a need to shift toward a hydrogen-based economy to meet future energy demands without harming the environment. The Metal Hydride–Hydrogen System (MHHS) emerges as a suitable alternative for addressing growing energy demands by offering clean and sustainable energy solutions for both stationary and mobile energy storage applications. The exothermic and endothermic nature of hydrogen absorption and desorption in MHHS makes it suitable for various heating and cooling applications. The composition of the metal hydride (MH) alloy can be readily tailored to achieve the required absorption and desorption conditions for specific applications. Key engineering applications of MHHS include hydrogen storage, purification, compression, refrigeration, heat pumps, heat transformers, and thermal energy storage. Despite several advantages, including reversible hydrogen storage, long cycle life, high energy density, and a wide operating temperature range, MHHS requires specific design considerations because of the poor thermal conductivity of MH alloys. Reactor design plays a crucial role in the efficient operation of MHHS, as the absorption and desorption kinetics depend significantly on the heat and mass transfer characteristics of the reactor. Therefore, appropriate reactor design is crucial and often incorporates heat-transfer enhancement techniques, such as embedded cooling tubes and external cooling jackets.

Prof. Muthukumar's research team at IIT Tirupati has successfully designed and developed several metal hydride-based hydrogen storage systems with capacities ranging from 1 to 50 Nm³, employing novel reactor configurations such as spiral-finned-tube reactors, tube-bundle reactors, embedded cooling-tube reactors, and disc-fin reactors for onboard and stationary applications. A novel methodology has been proposed for the design of these large-scale reactors and has been demonstrated to be effective. Additionally, several pre-industrial-scale metal hydride-based hydrogen purification systems, with capacities ranging from 10 to 24 Nm³, were fabricated and successfully demonstrated at a National Thermal Power Corporation (NTPC) power station. These systems can purify hydrogen from 20% purity to 99.999% purity using thermal inputs corresponding to temperatures ranging from 25 to 95 °C. Furthermore, MHHS can produce a significant cooling effect during hydrogen discharge because of the endothermic nature of the reaction. Recently, the group developed a large-scale metal hydride-based hydrogen compressor capable of compressing hydrogen from 1 bar to 400 bar using low-grade thermal input at temperatures ranging from 25 to 90 °C. Following parametric studies at the laboratory scale, the system was installed at NTPC. The group also developed a compression-driven, metal hydride-based cooling system for automobile air-conditioning applications, achieving a coefficient of performance (COP) ranging from 2.5 to 3.2. Several working prototypes of metal hydride reactors for thermal upgrading and space-heating applications were also developed and tested.

Keywords: Metal Hydride; Solid state hydrogen storage; Hydrogen Thermal Compression; Hydrogen purification; Hydrogen based heating and cooling systems

IT-14 • Invited

09 Oct. 2026, 11:40-12:10 PM

High-Entropy Alloys for Hydrogen Energy: From Production to Solid-State Storage

Prof. T.P. Yadava- University of Delhi

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Abstract

Hydrogen is widely recognized as one of the most promising clean energy carriers for a sustainable energy future. However, its widespread deployment depends critically on the development of safe, efficient, and high-capacity hydrogen storage materials. Among the available storage strategies, solid-state hydrogen storage using metal hydrides offers significant advantages in terms of volumetric density and operational safety. Despite decades of research, conventional metal hydrides have not yet achieved the combination of storage capacity, reversibility, and rapid kinetics required for practical applications. High-entropy alloys (HEAs), composed of five or more principal elements in near-equiatomic or substantial concentrations, have recently emerged as a new class of hydrogen storage materials owing to their unique structural and thermodynamic characteristics. The severe lattice distortion, high configurational entropy, and tunable crystal structures of HEAs create favorable interstitial sites for hydrogen occupation, enabling enhanced hydrogen uptake. Unlike conventional transition-metal hydrides, which typically exhibit a hydrogen-to-metal (H/M) ratio below 2, certain HEAs have demonstrated H/M ratios approaching 2.5, resulting in significantly improved hydrogen storage capacities. This presentation provides an overview of the recent advances in HEA-based hydrogen storage materials, with particular emphasis on the relationship between crystal structure and hydrogen storage performance. Our investigations reveal that body-centered cubic (BCC) HEAs exhibit superior hydrogen storage capacities compared with intermetallic phases due to their larger interstitial volume and higher lattice strain. In contrast, intermetallic HEAs, particularly those containing the C14 Laves phase, demonstrate remarkably faster hydrogen absorption and desorption kinetics at room temperature. A representative Ti–Zr–V–Ni–Cr/Fe HEA exhibits a reversible hydrogen storage capacity of approximately 1.7 wt% with rapid absorption/desorption kinetics at 303 K without requiring high-temperature activation. The alloy readily absorbs and releases hydrogen under a hydrogen pressure of 3.9 MPa at room temperature, highlighting its excellent practical potential. The findings demonstrate that crystal structure plays a decisive role in balancing hydrogen storage capacity and reaction kinetics in HEAs. The insights presented in this work provide valuable guidelines for the rational design of next-generation high-performance hydrogen storage alloys for future hydrogen energy systems. The defect-engineered high-entropy alloy unlocks enhanced hydrogen evolution performance and notable catalytic activity of for hydrogen sorption in MgH_2 will also discussed and presented.

Keywords: High-Entropy Alloys (HEAs), Hydrogen Storage, Metal Hydrides, Body-Centered Cubic (BCC) Alloys, Hydrogen Absorption-Desorption Kinetics, Laves Phase Alloys, Structure-Property Relationship

IT-15 • Invited

09 Oct. 2026, 12:05- 12:30 PM

**From Defects to Intelligence: Engineering Semiconductors for Sustainable Sensing
Dr. Vinayak Kamble – IISER Trivandrum, India****Abstract**

Semiconducting materials offer a powerful platform for developing sustainable sensing technologies, where defects, interfaces, and charge transport govern device functionality. This talk explores our efforts to engineer semiconductor materials and heterostructures for sensitive, selective, and energy-efficient sensing. We demonstrate how defect and interface engineering can tailor electronic transport and surface interactions in metal oxides, two-dimensional materials, and hybrid structures, enabling room-temperature chemical sensing and multifunctional devices. By integrating sensor arrays with machine learning, we move from conventional detection toward intelligent identification and quantification

IT-16 • Invited

09 Oct. 2026, 12:10- 12:35 PM

AI-Enabled Digital Twin for Energy Management, HVAC and Storage Solutions for Healthcare Buildings**Dr. Sudhakar Kumarasamy, University of Malaysia Pahang****Abstract**

The increasing energy demand of healthcare buildings, particularly in tropical climates, presents significant challenges in achieving energy efficiency, operational reliability and climate resilience while maintaining acceptable indoor air quality and uninterrupted healthcare services. Integrating artificial intelligence (AI), digital twin technologies, renewable energy systems and energy storage solutions offers considerable potential for intelligent energy management and sustainable building operation. However, the integration of real-time building data, predictive analytics, HVAC optimisation and energy storage management within a validated digital twin framework remains an emerging research area. This study proposes an AI-enabled digital twin framework for intelligent energy management in healthcare buildings, integrating field-verified Level of Development 500 (LOD500) Building Information Modelling (BIM), Internet of Things (IoT) monitoring, predictive equipment-health analytics, HVAC energy optimisation and prospective renewable energy and storage integration. The framework was developed and deployed at Klinik Kesihatan Sri Jaya, Maran district, Pahang, Malaysia, linking 28 air-conditioning and mechanical ventilation (ACMV) and mechanical and electrical (M&E) assets through 36 IoT monitoring channels. A prospective mixed-method evaluation combining real-time field monitoring, weather- and operation-normalised energy-performance analysis, and a paired human-decision experiment was conducted to assess operational performance. The analytics framework detected 18 operational anomalies, of which 83.33% were validated. Integration of digital decision support reduced median facility-management decision time from 12.0 to 4.2 minutes and improved the first-correct-action rate from 54.7% to 89.1%. Following human-authorised operational interventions, ACMV energy consumption decreased by 15.0% (95% confidence interval: 12.9%–17.1% reduction), while occupied-hour compliance with the assessed indoor environmental parameters remained at 97.9% for temperature, 96.6% for relative humidity and 99.2% for carbon dioxide (CO₂). Building on these validated results, the proposed framework establishes a pathway for integrating AI-based energy forecasting, HVAC control, solar photovoltaic generation and battery or thermal energy storage to improve load management, reduce peak electricity demand and enhance energy flexibility. The study provides a human-supervised digital twin architecture for advancing intelligent, low-carbon and climate-resilient healthcare infrastructure, with potential applications in distributed renewable energy integration and next-generation smart energy management systems.

IT-17 • Invited

09 Oct. 2026, 12:30- 12:55 PM

2D Halide-based Hybrid Perovskite Nanomaterials for Efficient Solar and Heat Energy Harvesting

Prof. Dheeraj K. Singh – University of Delhi, India

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Abstract

Fossil fuels are the primary energy sources, which generate greenhouse gases that lead to environmental pollution, global warming and climate change. However, solar energy is cost effective and crucial to fulfil the energy demands. In recent years, the halide-based hybrid perovskite materials revealed remarkable progress in the field of solar energy conversion. These materials show tunable structural characteristics, excellent physical properties and performance, however, the perovskite solar cells possess stability issues due to moisture, light exposure and heat. Therefore, during my presentation, the role of two-dimensional (2D) perovskite nanomaterials will be explored to overcome the recent challenges and efforts will be shown for excellent photostability, and thermal and moisture resistance, which makes them superior to the 3D perovskites. For this purpose, density functional theory calculations (DFT) will be used for the 2D Ruddlesden–Popper (2DRP) phase of halide perovskite $(\text{BA})_2(\text{MA})\text{Pb}_2\text{I}_7$, and the 2D derivative of the MAPbI_3 . Further, the role of excellent Rashba splitting of band edges will be discussed for better efficiency of solar energy. In order to avoid the toxicity, substitution of Pb by Sn in 5-ammonium valeric acid-based 2D perovskites for highly efficient Pb-free perovskite solar cells will be also explored.

IT-18 • Invited

09 Oct. 2026, 03:05-03:35 PM

Machine Learning–Assisted Advancement of Environmental Remediation Using Metal–Organic Frameworks**Prof. Manika Khanuja – JMI Delhi, India***Centre for Nanoscience and Nanotechnology, Jamia Millia Islamia, New Delhi-110025, India*

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Abstract

Machine learning (ML) is an emerging powerful tool for extracting meaningful relationships from complex experimental datasets and accelerating the development of intelligent materials for environmental applications. Metal–organic frameworks (MOFs), have tunable porosity, high surface area, structural diversity, and the ability to integrate with functional nanomaterials, providing a versatile platform for developing advanced environmental remediation systems. However, optimizing the reaction parameters and deploying them in real-time sensing and catalytic activity remains limited by slow experimentation cycles. Integrating ML frameworks can accelerate application pipelines for MOFs by facilitating the development of insights and discoveries from a large amount of data in a short time, and the use of supervised learning and feature-importance analysis to uncover the dominant reaction drivers. By employing data-driven ML models, one may predict and optimize material performance through various parameters, thereby reducing the number of required experiments significantly. Here, we explore ML-assisted MOF-engineered nanomaterials for two interconnected applications: colorimetric sensing and photocatalytic treatment of water pollutants. For colorimetric sensing, experimentally observed color changes were transformed into quantitative RGB- and HSV-based features and correlated with analyte concentration using different regression algorithms. For photocatalytic degradation of water pollutants, material engineering was used to improve light utilization, interfacial charge transfer, and reactive-species generation. Ensemble and nonlinear ML models enabled prediction beyond conventional interpretation, while explainable ML approaches were employed to identify the features governing model predictions. This combined experimental-computational approach could contribute to the development of rapid water-quality monitoring and sustainable wastewater-treatment technologies.

Keywords: MOF, ZIF, Machine learning, Nanomaterials, Explainable AI

IT-19 • Invited

09 Oct. 2026, 03:15-03:35 PM

Realizing Dendrite Free Sodium Metal Anodes using Hybrid Artificial Solid Electrolyte Interphase (SEI) Layer for Energy Storage Application**Prof. Ranjit Thangavel, IIT Tirupati***Department of Chemical Engineering, IIT Tirupati***Abstract**

Attempts to develop high-performance energy storage system with high energy – high power – high cycle life combination has been the focus of increasing attention in recent years. Owing to the natural abundance of sodium resources and the similar working mechanism with lithium-ion batteries (LIBs), sodium-ion batteries (SIBs) are an appealing and low-cost candidate for large-scale applications. However, the capacity limitations in anode and cathode have severely limited the energy output of the SIBs. Increasing the energy density of the SIBs equivalent to LIBs is a key to achieve its commercialization in EVs and grid storage. Sodium metal (Na) anodes are considered the most promising anode for high-energy-density sodium-ion batteries, sulfur/solid state batteries because of their high capacity (~1166 mAh g⁻¹) and low electrochemical potential (-2.71 vs SHE). Na metal has several limitations such as stability, reversibility, and safety due to their thermodynamic instability with organic electrolytes that lead to severe dendrite formation. The current talk will cover the engineering contributions in achieving a dendrite free and stable Na metal anode using artificial solid electrolyte interphase (SEI) layer for next-generation sodium-based energy storage systems. The multifunctional approach adapted to realize a dendrite free, long life and safer Na anode will also be presented.

IT-20 • Invited

09 Oct. 2026, 03:35-04:05 PM

Morphology-Dependent Electrocatalytic Performance of Co₃O₄ Nanostructures for Alkaline Water Splitting**Prof. Prabhakar Singh***Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University) Varanasi-221005, India*

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Abstract

Transition-metal-based electrocatalysts are promising electrocatalysts for anion exchange membrane water electrolyzer because of their low cost and earth abundance, however sluggish reaction kinetics and limited utilization of catalytically active surface site can restrict their catalytic efficiency. Improving the catalytic performance of such materials requires effective control over their surface structure and morphology. In this context, morphology engineering offers a promising strategy for tuning surface characteristics, active-site accessibility, and electrode-electrolyte interactions without altering the fundamental chemical composition of the catalyst. Here, in this work three distinct Co₃O₄ nanostructures, namely nanocubes, nanorods, and nanosheets, were synthesized through a hydrothermal route followed by thermal treatment to systematically investigate the influence of morphology on their structural, optical, and electrocatalytic properties. X-ray diffraction confirmed the formation of cubic spinel Co₃O₄, while electron microscopy revealed well-defined morphology-dependent architectures. Raman and UV-visible spectroscopic analyses further demonstrated variations in the local structural environment and optical response associated with the different morphologies. The electrocatalytic performance of the synthesized Co₃O₄ nanostructures was evaluated toward the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline medium. At a current density of 10 mA cm⁻², Co₃O₄ nanosheets exhibited the lowest HER overpotential of 174 mV, followed by nanocubes (206 mV) and nanorods (242 mV). Similarly, the nanosheets demonstrated the best OER performance, requiring an overpotential of 230 mV, compared with 269 mV for nanorods and 302 mV for nanocubes. The superior performance of the nanosheets may be attributed to their two-dimensional framework, which can provide greater exposure of catalytically accessible surface regions and facilitate efficient electrolyte-electrode interactions and charge transfer. Overall, this study demonstrates that morphology engineering is an effective approach for tuning the electrocatalytic properties of Co₃O₄ and provides insights into the rational design of earth-abundant bifunctional electrocatalysts for alkaline water electrolysis.

IT-21 • Invited

09 Oct. 2026, 03:35-03:55 PM

Bias-Driven Transition from Capacitive Coupling to Nonvolatile Resistive Switching in PVA–Graphene Oxide Thin-Film Devices

Prof. Neeraj Panwar, CCS University

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Abstract

Polyvinyl alcohol-graphene oxide (PVA-GO) composite thin-film devices with an Ag/PVA-GO/FTO structure were fabricated to investigate the transition from capacitive coupling to nonvolatile resistive switching. A bias-driven evolution from capacitively coupled behaviour to purely resistive switching was observed with increasing applied voltage and graphene oxide concentration. The Ag/PVA-GO (0.2 wt.%) /FTO device exhibited forming-free bipolar resistive switching with a set voltage of ~ 1.72 V, a reset voltage of ~ 1.83 V, and a switching ratio of $\sim 10^3$. At a read voltage of 0.1 V, the device demonstrated two well-defined resistance states with stable endurance over 2500 switching cycles and retention for 4020 s without noticeable degradation. The charge-flux linkage exhibited the characteristic double-valued hysteresis of memristive behavior, while the time-domain charge and flux responses showed asymmetric and symmetric profiles, respectively. Finally, the electrical conduction and resistive switching mechanisms were interpreted using appropriate transport models, providing insight into the bias-controlled switching transition in PVA-GO thin-film devices.

Keywords: PVA-GO composite; Resistive switching; Memristor; High- and low-resistance states

IT-22 • Invited

09 Oct. 2026, 4:05-04:30 PM

Ways to improve charge storage and tackle dendrite issue at anode in Zinc Ion Battery**Dr. Neetu Jha***Department of Physics, Institute of Chemical Technology, Mumbai, Nathalal Parekh Marg, Matunga, Mumbai- 400019, India***Abstract**

Aqueous zinc ion batteries (AZIB) possess high potential for the next generation grid energy storage applications. These batteries are inherently safer and cheaper, making them more economically viable. The metallic zinc anode has a pivotal role in extending the cyclability of the AZIB. The plating and stripping of zinc at the anode electrolyte interface (AEI) is preferential to the uneven protruded sites of zinc, which increases the probability of dendrite formation, thereby reducing the overall cycle life. To overcome this drawback, various techniques are employed, which varies from adding additives to the electrolyte to the formation of an interphase layer at the anode surface. Here, my research group is focusing on the formation of a thin film at the interface of the anode and electrolyte. This technique is popular among material scientists to reduce the dendrite formation and enhance the life cycle of the batteries. My discussion will focus more on the property of the materials, which is forming layer and the science behind the mechanism of manipulating the diffusion of ions during intercalation and deintercalation, which ultimately leads to the life-cycle enhancement in batteries.

IT-23 • Invited

09 Oct. 2026, 03:55-04:15 PM

Advanced Porous Carbon Aerogels for Energy Storage and Efficient Dye Removal from Water**Dr. Sweta Singh, Mahatma Gandhi Central University, Motihari, Bihar***Department of Physics, Mahatma Gandhi Central University, Motihari, Bihar 845401*

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Abstract

The growing demand for sustainable energy storage technologies and effective water treatment strategies has stimulated considerable interest in multifunctional porous carbon materials. The rational design of hierarchical porous carbon materials from renewable biomass is of significant interest for sustainable energy storage and environmental remediation. In the present work, carbon aerogels (CAs) and activated carbon aerogels (ACAs) synthesized using *Mangifera indica* peel ash (MIPA) as a biomass-derived catalyst will be discussed. KOH activation was employed to tailor the porous architecture, resulting in interconnected micro–mesoporous carbon networks with specific surface areas of $1309 \text{ m}^2 \text{ g}^{-1}$ and $1961.7 \text{ m}^2 \text{ g}^{-1}$ for ACA@0.05MIPA and ACA@0.005MIPA, respectively. The multifunctional performance of these ACAs for aqueous-phase dye adsorption and supercapacitor applications will be highlighted. ACA@0.05MIPA exhibited adsorption capacities of 198.41 mg g^{-1} , 180.83 mg g^{-1} , and 221.23 mg g^{-1} for methylene blue, methyl orange, and methyl red, respectively, demonstrating efficient removal of organic pollutants. The enhanced adsorption is associated with the high accessible surface area, hierarchical pore structure, and abundant surface-active sites. Furthermore, the interconnected three-dimensional carbon framework facilitated efficient ion diffusion and charge transport, yielding specific capacitances of 270.39 and 443.15 F g^{-1} for ACA@0.05MIPA and ACA@0.005MIPA, respectively, at 1 A g^{-1} in 3 M KOH . Overall, the talk will highlight the potential of biomass-derived activated carbon aerogels as multifunctional porous platforms for electrochemical energy storage and wastewater remediation, while demonstrating a sustainable route for converting agricultural residues into value-added advanced carbon materials.

Keywords: carbon aerogels, Biomass-derived catalyst, Supercapacitors, Dye adsorption, Wastewater treatment

IT-24 • Invited

09 Oct. 2026, 4:30-5:00 PM

Emerging Materials for Interfacial Electrochemistry: Fundamental Insights to Sustainable Technologies**Dr. Ramendra Sundar Dey – INST Mohali, India***Institute of Nano Science and Technology, Sector-81, Mohali, Punjab-140306, India*

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Abstract

The transition towards a sustainable and electrified society demands energy-efficient chemical processes and reliable energy-storage technologies. Electrochemical approaches provide a promising platform for integrating renewable electricity with both chemical synthesis and energy storage. In this context, our research explores materials and interfacial electrochemistry for sustainable ammonia synthesis through the nitrogen reduction reaction (NRR). Unlike the energy- and carbon-intensive Haber–Bosch process, electrochemical NRR offers the prospect of ammonia production under ambient conditions using renewable electricity. Our studies demonstrate how rational control over the electronic structure and interfacial environment of catalytic materials can regulate N_2 adsorption and activation while modulating the competing hydrogen evolution reaction. By establishing structure–function relationships and combining electrochemical measurements with in situ/operando investigations, we seek to unravel the elementary processes governing ammonia formation and develop efficient materials for practical electrochemical ammonia synthesis.

A deeper understanding of electrochemical interfaces is equally important for advancing rechargeable energy-storage systems. We therefore employ ultramicroelectrode (UME)-based electrochemical methodologies to probe localized interfacial processes in Zn-ion batteries. The high sensitivity of UME measurements provides valuable insights into electrode kinetics, Zn nucleation and growth, and electrode–electrolyte interactions that are difficult to resolve using conventional electrodes. These studies enable us to understand and control Zn deposition/stripping behavior, thereby improving the reversibility, stability, and cycling performance of Zn-based energy-storage systems. Collectively, these studies highlight how materials engineering coupled with advanced interfacial electrochemistry and UME-based investigations can bridge fundamental mechanistic understanding with the development of sustainable ammonia synthesis and next-generation Zn-ion energy-storage technologies.

IT-25 • Invited

10 Oct. 2026, 09:00-09:25 AM

Future Materials for Thermoelectric and Field Emitter Materials**Prof. Jai Singh, University of Delhi***Department of Physics, University of Delhi, Delhi, 110007*

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Abstract

The human sustainability and development are strongly reliant on energy use. Advanced functional materials are attracting considerable attention for next-generation energy conversion and electronic applications. Thermoelectric materials enable the direct conversion of waste heat into electrical energy, whereas field-emission materials offer potential applications in electron sources, flat-panel displays, electron sources, and vacuum microelectronic devices. This research focuses on the development of multifunctional nanocomposites based on Bi_2Se_3 , Sb_2Te_3 , carbon nanotubes (CNTs), and ZnO for thermoelectric applications, alongside MoS_2 and ZnO nanostructures for field emission. For thermoelectric applications, Bi_2Se_3 - and Sb_2Te_3 -based composites incorporating CNTs and ZnO nanostructures will be investigated to understand the influence of interfacial engineering, nanostructuring, and hybrid conductive pathways on electrical conductivity, Seebeck coefficient, and thermal conductivity. The objective is to enhance the thermoelectric figure of merit (ZT) by optimizing electronic transport while suppressing lattice thermal conductivity. For field-emission applications, MoS_2 and ZnO nanostructures will be explored to exploit their favorable electronic properties, high aspect-ratio morphologies, and interfacial effects for improving electron emission. The field-emission performance will be evaluated through current density, turn-on field, threshold field, field-enhancement factor, and emission stability. Structural, morphological, compositional, and electronic characterizations will be performed to establish structure–property–performance relationships. The proposed research aims to develop efficient, stable, and potentially cost-effective nanocomposite materials for waste-heat recovery and advanced electron-emission technologies, contributing to sustainable energy utilization and next-generation electronic devices.

IT-26 • Keynote

10 Oct. 2026, 09:25-09:55 AM

Investigations on Hydrogen From Sources Of Natural Origin In Russia**Prof. Dimitry Dunikov, Russian Academy of Sciences**

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Abstract

Climate change is one of the major challenges of the 21st century. Russia's Climate Doctrine envisions achieving carbon neutrality by 2060, and Russia is implementing programs to cut greenhouse gas emissions, to introduce innovative technologies, to improve energy efficiency, and to promote energy conservation. Hydrogen is considered as a clean and efficient secondary energy carrier for energy transition. In 2024 global hydrogen production has reached almost 100 Mt, though, less than 1% of hydrogen is produced by low-carbon paths [1], and efforts are needed to increase the role of low-carbon hydrogen. The Russian "Road Map for the development of the high-tech direction "Development of Hydrogen Energy" for the period until 2030" includes 34 critical technological areas in the field of technologies for the production, storage, transportation and energy use of hydrogen [2]. These directions should assist modernization of Russia's heavy industries, such as the metallurgy, petrochemicals, fertilizers, and energy sectors, and ensure the competitiveness of Russian exports in Asia, the Middle East, Africa and Latin America.

Currently low-carbon hydrogen is produced mostly by water electrolysis. Some alternative natural sources of hydrogen, such as hydrogen of biological origin (biohydrogen) and geological origin (natural hydrogen), have great potential, but stay mostly unused. These sources have a low carbon footprint and their reserves are potentially huge, and their advantage over solar and wind energy lies in their constant generation over time. Biohydrogen is actively investigated since the 2010s, though the wide commercial use is still uncertain. From the 1950-1960s, it had become clear that molecular hydrogen (natural H_2) is present in almost all mineral occurrences but its use in energy production has not been considered until recently.

The main barrier to the use of these natural sources of hydrogen is that their feedstocks are low-pressure (less than 1 MPa) gas mixtures based on methane (natural gas), carbon dioxide or even helium with a low concentration of hydrogen (up to 10 mol.% or less). The extraction of such hydrogen by traditional methods is currently difficult and economically unjustified, thus there are currently no effective and affordable ways for practical use of hydrogen from mixtures of natural origin. Commercial technologies (adsorption, membrane and cryogenic) for hydrogen purification have been developed to extract hydrogen from mixtures with an increased hydrogen content (more than 70%) and operate at pressures above 1 MPa. It is possible to solve the problem of hydrogen separation from low quality mixtures using substances that selectively absorb hydrogen even at low pressures, for example, metal hydrides. Purification, compression and storage of hydrogen by reversible metal hydrides is the safest and most compact option [3].

Successful extraction of hydrogen by metal hydride was demonstrated both for H_2/CO_2 and H_2/CH_4 mixtures representing biohydrogen and natural hydrogen, as well as for the concentrated natural gas probe (ca. 4% mol. H_2). The probe was delivered by the "Gazprom Hydrogen LLC" and produced by the membrane separation using the raw gas from the Kovyktinskoye gas and condensate field (0.07% mol. H_2) [4]. However, commercialization potential of natural hydrogen is uncertain today, and one of the main challenges is low H_2 concentration in geological sources, thus cost of purification and compression is unpredictable on the current stage of development. A promising direction in reducing cost of natural hydrogen exploitation is a possible co-production with helium, because two gases often co-exist. Using $LaNi_5$ type metal hydrides we were able to successfully separate 50% H_2 / 50% He mixture

Practical implementation of the technologies for hydrogen production and extraction from natural sources could be done within the framework of the Russian Roadmap for "The development of high-tech direction Hydrogen energy up to 2030", in which PJSC Gazprom is the leading company in natural hydrogen.

Keywords: natural hydrogen; biohydrogen; metal hydrides; hydrogen purification; hydrogen storage; helium

IT-27 • Invited

10 Oct. 2026, 09:55-10:25 AM

Sustainable Green Nano Materials for Waste Water Remediations**Prof. Ajay Mishra -- University of the Western Cape (UWC), South Africa***Department of Chemistry, University of the Western Cape, Robert Sobukwe Road, Bellville 7535, South Africa***Abstract**

Environmental pollution raised bigger concerns on the discharge of waste water. 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 waste water. The current invited talk will be focused on the recent development, advancement and applications of green sustainable nano materials for wastewater remediation.

IT-28 • Invited

10 Oct. 2026, 10:50-11:20 AM

Manifesting multifunctions in PrFeO₃**Prof. R. Nagarajan, University of Delhi***Materials Chemistry Group, Department of Chemistry, University of Delhi, Delhi-110007***Abstract**

Research on functional oxide ceramics has tremendous translational potential for technological applications. Despite sharing a similar formula, BiFeO₃ and REFeO₃ (RE = rare earth) perovskites differ widely in structure and properties.^[1-3] The cooperative octahedral tilting about the [011] and [100] axes of the cubic unit cell in REFeO₃ (RE = rare earth) distorts the structure, playing an influential role towards the magnetism. The Fe³⁺–Fe³⁺ interactions dominate over a wide temperature range (typically high temperatures), giving rise to an antiferromagnetic transition (T_{N1} (the Neel temperature)). Antisymmetric and anisotropic superexchange interactions of RE³⁺–Fe³⁺ ions determine the TSR (spin reorientation transition temperature). In low-temperature regions, RE³⁺–RE³⁺ interactions determine the antiferromagnetic transitions at T_{N2} .^[4,5] These complex exchange interactions of the magnetic ions in orthoferrites have given rise to various magnetic properties, along with the existence of competing ferromagnetic (FM) and antiferromagnetic (AFM) orderings in RE- and Fe-sublattices, giving researchers an additional handle to tune it to exhibit exchange bias (EB), spin-reorientation (SR), and magnetoelectric (ME) effects. The chemical substitution at the rare-earth site, Fe site, or both sites is a well-established and straightforward procedure for tuning the magnetic properties of REFeO₃. In this talk, we will present the results of magnetic dilution at the RE and Fe sites in imparting multiple functions, using PrFeO₃ as a model system.^[6-8]

IT-29 • Invited

10 Oct. 2026, 11:55- 12:20 PM

Strongly Correlated Electron Materials for Energy Applications**Dr. Dinesh Kumar Shukla – Scientist-F, UGC DAE Indore Centre***UGC-DAE Consortium for Scientific Research, Indore 452001, India***Abstract**

This talk focuses on vanadium dioxide (VO_2), a benchmark strongly correlated material in which electron-electron interactions drive a sharp, first-order insulator-to-metal transition (IMT) near room temperature, accompanied by a structural phase transition and profound optical property modulations. We will present distinct paradigms for harnessing these phase transition characteristics in energy technologies. First, we discuss how tailoring the IMT temperature and the accompanying optical response enables the development of smart window materials for energy conservation. Additionally, we showcase some of the first experimental evidence of multiple exciton generation (MEG) in a strongly correlated system, a phenomenon with significant implications for the future efficiency of solar cells.

IT-30 • Invited

10 Oct. 2026, 12:20- 12:50 PM

Waste to Wealth: Computational Design of Waste-Derived Graphene for Sustainable Energy Storage**Prof. A. Srivastava, IIITM, Gwalior***Advanced Material Research Group, Department of Engineering Science, ABV-Indian Institute of Information Technology and Management, Gwalior, Madhya Pradesh, 474015, India*

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Abstract

The rapid generation of tyre, plastic, and other carbon-rich waste presents a major environmental challenge while offering an untapped source of functional carbon materials for energy storage. Our research explores a “Waste-to-Wealth” computational framework that transforms carbonaceous waste into graphene-based electrodes for next-generation energy storage. Using spin-polarized DFT, we demonstrate that intrinsic defects and chemical heterogeneity in waste-derived carbon can be engineered to tune electronic structure and charge-storage behavior. Building on our earlier studies, we established a defect–dopant trade-off in graphene, where nitrogen functionalization enhances both stability and quantum capacitance. Transition-metal decoration further improved capacitance, reaching $220 \mu\text{F cm}^{-2}$ for Fe, driven by localized 3d states near the Fermi level. Extending this design logic to real waste-derived precursor chemistries, we construct realistic reduced-graphene-oxide models from waste tyres, incorporating co-existing N/S dopants, oxygen functionalities, and Fe/Zn adsorbates. These models exhibit substantially enhanced electronic states near the Fermi level relative to pristine graphene, with Fe-functionalized configurations delivering a peak quantum capacitance of $\sim 180 \mu\text{F cm}^{-2}$ — falling within the high-performance window established by our prior transition-metal-decorated systems, and notably exceeding the capacitance reported for experimentally synthesized Zn-doped tyre-waste rGO ($59.63 \mu\text{F cm}^{-2}$ at -0.38 V , itself $5.5\times$ pristine graphene, with a specific capacitance of 316 F g^{-1} and energy density of 36.94 Wh kg^{-1}). This positions computational screening as a predictive front end capable of identifying superior defect–dopant combinations ahead of expensive synthesis and testing. Extending this framework to plastic-derived and other waste-derived carbons, we establish structure–property relationships that link specific defect/dopant motifs to quantum-capacitance enhancement, offering a rational, atomistic-modelling-guided pathway for converting low-value waste into high-value electrode materials.

Keywords: Waste Valorization, DFT, Graphene, Quantum Capacitance, Supercapacitors, Circular Carbon Economy, Defect Engineering

IT-31 • Invited

10 Oct. 2026, 12:55- 1:20 PM

2D Materials for Zinc and Iron Based Batteries**Prof. Ashish Mishra, IITBHU**

*Nano Photonics & Energy Materials Laboratory (NPEML), School of Materials Science and Technology,
Indian Institute of Technology (Banaras Hindu University), Varanasi*

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Abstract

Currently, Li-ion battery technology is a dominant force working in the market and Na-ion batteries are being explored as alternative. However, safety issues and relatively high cost of lithium and sodium have led to the investigation of next generation clean energy storage devices such as Zn-, Al- and Fe-batteries [1]. Carbon materials are known to be good cathode materials for metal-ion hybrid capacitors/batteries like Zn-ion and Fe-ion ones due to their large surface area and good electrical conductivity [2, 3]. Transition metal dichalcogenides (TMDs) are known to be good electrocatalysts for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), suitable for metal-air batteries like Zn-air batteries due to their unique electronic properties, abundant active sites, and high surface area [4, 5].

Here, we discuss the role of Carbon and TMDs nanostructures and their nanocomposites with different metal oxides in Zn- and Fe-ion hybrid capacitors/batteries and Zn-air batteries. We have demonstrated the electrochemical activity of these materials and further examined the design and performance of these devices. The results underscore the potential of the work in advancing the sustainable energy storage technology.

Keywords: Carbon, Transition metal dichalcogenides, Fe-ion batteries, Zn-air batteries.

IT-32 • Keynote

10 Oct. 2026, 02:20- 02:50 PM

Compound Semiconductor Technology: Enabling India's Future in RF, Power and Photonics**Dr. D.S. Rawal, Associate Director, DRDO****Abstract**

Compound semiconductors such as GaAs, GaN, and InP are driving transformative advances in high-frequency electronics, power devices, photonics, and emerging quantum technologies. Their superior electrical and optical properties make them indispensable for applications in 5G/6G communications, radar systems, satellite technologies, renewable energy, and quantum networks.

This talk will highlight India's progress in the indigenous development of compound semiconductor technologies, including GaAs and GaN-based RF devices, photonic components, and advanced semiconductor platforms. Recent developments in RF electronics, power devices, photonics, and strategic initiatives under the National Quantum Mission will be discussed, along with future opportunities for building a self-reliant semiconductor ecosystem in India.

IT-33 • Invited

10 Oct. 2026, 02:20- 02:50 PM

Pumped Hydro, Hydrogen And Batteries For Hybrid Microgrids: A Techno-Economic Assessment

Dr. Saiful Anwar Che Ghani, University of Malaysia Pahang

Saiful Anwar Che Ghani^{1,2}, Ahmad Tarmizi Haron¹, Azim Arshad², Anuar Pawan³, Abdul Murad Zainal Abidin³

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Abstract

Digital twins are now common in building operation, energy management and predictive maintenance, yet most stop at monitoring or prediction. Few show that the information a twin produces actually reaches an operator, changes what that operator does, and is then checked against how the physical system responds. The gap matters most in healthcare facilities in hot-humid climates, where cutting air-conditioning and mechanical ventilation (ACMV) energy cannot be allowed to erode indoor air quality (IAQ), equipment reliability or continuity of care. We report a human-in-the-loop operational digital twin that ties together a field-verified LOD500 Building Information Model (BIM), live Internet of Things (IoT) monitoring of energy, indoor environmental quality and ACMV operating states, equipment-health analytics, and an Augmented Reality (AR) interface for decision support. The system was deployed at a small operational healthcare facility in Klinik Kesihatan Sri Jaya, Maran district, Pahang, Malaysia, and evaluated with a prospective mixed-method design that combined field monitoring, weather-normalised building-performance analysis and a paired human-decision experiment. The deployed twin linked 28 ACMV/M&E assets across 36 IoT channels; the analytics layer flagged 18 anomalies (83.33 % validated); and median facility-management decision time moved from 12.0 minutes (IQR: 9.0–15.5) to 4.2 minutes (IQR: 3.0–6.0), while the first-correct-action (FCA) rate rose from 54.7% to 89.1 %. After human-authorised interventions, weather- and operation-normalised ACMV energy changed by -15.0 % (95 % CI: -12.9 % to -17.1 %), and occupied-hour compliance with the assessed IAQ parameters was 97.9 % for temperature, 96.6 % for relative humidity, and 99.2 % for CO₂. The study extends the building digital twin from a visualisation-and-prediction tool into a closed sense–infer–explain–act–verify loop, and frames the healthcare facility as a distributed, human-supervised node that could later be federated across critical public infrastructure to support climate-resilient urban governance.

Keywords: Digital twin; Human-in-the-loop decision support; Building information modelling; Augmented reality; Climate-resilient healthcare infrastructure

IT-34 • Invited

10 Oct. 2026, 02:50-03:20 PM

Hierarchal 3D Plasmonic Structures: Fabrication and Their Applications**Prof. J. P. Singh, IIT Delhi**

J.P. Singh, Lakshay Bhardwaj, Sneha Senapati and Sarjana Yadav

*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016***Abstract**

We will present complex 3D plasmonic nanostructures formed by glancing angle deposition (GLAD) method. The fabricated plasmonic structures have shown their applications as surface enhanced Raman spectroscopy (SERS) substrates for the detection of bio pathogen. The method was found to be highly sensitive, selective, rapid and field deployable. Some experimental findings of ultralow detection of clinical samples for HIV, Dengue, malaria and COVID-19 will be shown as examples. We will also our present results on enantioselective discrimination by using chiral SERS platform.

IT-35 • Invited

10 Oct. 2026, 02:50-03:20 PM

Biomass-Assisted Defect Engineering of Metal Oxide Nanomaterials for Sustainable Environmental Applications**Dr. Gaurav, FRI, Dehradun****Abstract**

The transition from conventional nanomaterial synthesis to resource-efficient and environmentally responsible processing requires more than replacing synthetic reagents with biological extracts. It calls for a mechanistic understanding of how biomass-derived molecules influence nucleation, crystal growth, surface chemistry and defect formation, and how these changes govern material performance. This invited talk examines biomass-assisted synthesis and defect engineering of ZnO, CuO and TiO₂ as a platform for developing multifunctional materials for environmental applications. Particular attention is given to the roles of phytochemicals and biomass-derived functional groups as complexing, reducing, stabilizing and morphology-directing agents, together with the effects of extract composition, pH, precursor chemistry, thermal treatment and synthesis route on crystallinity, oxygen vacancies, surface states and band-gap behaviour.

The discussion links structural and surface characteristics to photocatalytic, antimicrobial and remediation mechanisms, including adsorption, charge-carrier separation, reactive oxygen species generation and contaminant transformation. It also considers opportunities offered by ZnO-, CuO- and TiO₂-based heterostructures for improving visible-light response and suppressing charge recombination. Drawing on experimental experience with diverse waste plant biomass, the talk highlights reproducibility, mechanistic validation and scale-up as central challenges. A fit-for-purpose characterization strategy integrating XRD, vibrational spectroscopy, electron microscopy, BET analysis, UV–visible diffuse reflectance, photoluminescence and XPS is proposed to distinguish credible structure–property relationships from descriptive claims. Finally, the presentation places performance within a broader sustainability framework encompassing biomass valorization, material recovery, life-cycle impacts, ecotoxicity, safe and sustainable-by-design principles and regulatory relevance. This integrated perspective can help move green-synthesized metal oxide nanomaterials from laboratory demonstrations toward reproducible and environmentally responsible technologies.

Keywords: Biomass valorization; defect engineering; metal oxide nanomaterials; ZnO; CuO; TiO₂; photocatalysis; environmental remediation

IT-36 • Invited

10 Oct. 2026, 03:20-3:50 PM

Dual-Waste Porous Carbon Composites for High-Performance Sustainable Supercapacitor Electrodes

Prof. V.C. Srivastava, IIT Roorkee

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Abstract

Advancing circular-economy strategies for energy storage, this work develops supercapacitor electrode materials by jointly valorizing complementary agricultural and industrial waste streams. Peanut-shell-derived activated carbon and red mud hematite nanoflakes were used to create an electric double-layer and pseudocapacitive charge storage composite in the first investigation. In a three-electrode cell, the optimized 10 wt.% hematite composite had 284.3 F/g at 2 A/g, while a symmetric coin-cell device achieved 7.6 Wh/kg at 720 W/kg with 106% capacitance retention, representing, to our knowledge, the first supercapacitor electrode obtained entirely from two waste streams. The second study co-activated graphite from spent lithium-ion batteries with peanut-shell biochar to produce a composite that delivered 197 F/g at 0.4 A/g and retained 94% of its capacitance over 5000 cycles, outperforming pristine activated carbon and a commercial graphite reference. This composite showed that recovered battery graphite can also replace conductive carbon black additives in electrode materials. Hierarchical porosity, tailored surface chemistry, and controlled interfacial dispersion between the carbon matrix and secondary phases dictate electrochemical performance in both systems. These dual-waste-derived materials are competitive with or better than state-of-the-art composites synthesized from commercial precursors, establishing a scalable, circular-economy pathway for low-cost, high-performance supercapacitor electrode development.

IT-37 • Invited

10 Oct. 2026, 3:50-04:15 PM

Wide-Bandgap Semiconductor Materials: Silicon Carbide for Advanced Electronic and Power Applications**Prof. O.P Thakur, DRDO Delhi***Solid State Physics Laboratory, Timarpur, Delhi-110054***Abstract**

Wide-bandgap (WBG) semiconductor materials have emerged as key enablers for next-generation power electronics, high-frequency electronics, optoelectronics, and harsh-environment applications. Compared with conventional silicon, materials such as silicon carbide (SiC), gallium nitride (GaN), gallium oxide (Ga_2O_3), and diamond offer larger bandgaps, higher critical electric fields, higher thermal conductivity, and the capability to operate at elevated temperatures and frequencies. These properties enable semiconductor devices with higher breakdown voltage, lower switching losses, higher power density, and improved energy efficiency.

Among the WBG materials, silicon carbide, particularly 4H-SiC, has attained significant technological maturity and is increasingly being adopted for high-voltage and high-power applications. Its wide bandgap (~ 3.26 eV), high critical electric field, high thermal conductivity, and high saturation velocity make it particularly attractive for power MOSFETs, Schottky barrier diodes, high-temperature electronics, electric vehicles, renewable-energy systems, smart grids, and high-power industrial applications. The development of high-quality bulk SiC single crystals, low-defect wafers, epitaxial layers, and device fabrication technologies is therefore critical for realizing the full potential of SiC.

The presentation will discuss the fundamental properties of WBG semiconductors and particular emphasis will be placed on 4H-SiC bulk crystal growth, wafer fabrication, defect control, material characterization. Challenges associated with SiC crystal growth, including micropipes, threading dislocations, basal-plane defects, polytype stability, doping control, and wafer processing, will be highlighted. Recent advances in indigenous SiC technology and the pathway from bulk crystal growth to wafer processing will also be discussed. The role of SiC in high-efficiency power conversion and emerging strategic applications will be outlined.

Role of Quantum Materials and Devices for Quantum Technology applications**Prof. Rajendra Singh, IIT Delhi***Department of Physics, IIT Delhi, New Delhi - 110016***Abstract**

Quantum materials and devices form the bedrock of the next technological revolution, offering unprecedented capabilities for quantum computing, sensing, and secure communications. This abstract explores the synthesis and implementation of Novel Quantum Materials (NQMs), including topological insulators, two-dimensional van der Waals heterostructures, and engineered semiconductors. By exploiting intrinsic quantum phenomena such as entanglement, superposition, and topological protection, these advanced materials overcome the coherence and scalability limitations of traditional silicon electronics. In this talk, I will inform about various thematic Hubs under National Quantum Mission (NQM) and then elaborate on the Quantum Materials and Devices (QMD) Hub established at IIT Delhi. I will discuss about various activities being pursued under the QMD Hub and also the kind of technologies that are being developed under this theme.

AI for Materials Science and Engineering: Leveraging GNNs, LLMs, XAI, and Nanocombinatorics

DR. ANKIT AGRAWAL

Department of ECE, Northwestern University, USA

Abstract

The increasing availability of data from the first three paradigms of science (experiments, theory, and simulations), along with advances in artificial intelligence and machine learning (AI/ML) techniques has offered unprecedented opportunities for data-driven science and discovery, which is the fourth paradigm of science. Within the arena of AI/ML, deep learning (DL) has emerged as a game-changing technique over the last decade with its ability to effectively work on raw big data, bypassing the (otherwise crucial) manual feature engineering step traditionally required for building accurate ML models, thus enabling numerous real-world applications. In this talk, I will present some of the ongoing AI/ML/DL research in our group with illustrative real-world applications in materials science and engineering, by leveraging graph neural networks (GNNs), large language models (LLMs), explainable AI (XAI), and generative AI (GenAI). We will also see how AI can be used to accelerate nanocombinatorics workflows to facilitate rapid structure characterization of megalibraries with millions of nanoparticles on a chip.



Oral Presentations

38 Papers

O0007 • Pawan Kumar Soni

ICEAM2026-ORAL-0007 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT1

Improvement of hydrogen storage properties of reactive hydride via catalytic interface.**Pawan Kumar Soni***IILM University, Knowledge Park II, Plot no. 18, Greater Noida, Uttar Pradesh, India*

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Abstract

The high intrinsic energy barriers and multi-step transformation pathways are a major challenge for the improvement of the hydrogen storage performances of the RHC systems. We report that the hydrogen storage characteristics of $2\text{LiH} + \text{MgB}_2$ system are significantly improved by the introduction of Co@C and Ni@C catalysts through the action of the interface. Kinetic measurements reveal significantly accelerated hydrogenation and dehydrogenation processes, accompanied by reduced apparent activation energies. Multi-scale structural characterization shows that the catalysts induce a refined hydride matrix and generate stable nanoscale interfaces that are preserved during cycling. The catalyst-hydride interfaces increase active site density, facilitate mass transport, and induce electronic interactions that weaken B-H bonds and lower the energy barrier for hydrogen release. Further DFT calculations also demonstrate that the interface interaction of LiBH_4 with transition metal sites causes charge transfer and BH_4^- distortion which reduces the dehydrogenation energy barrier and weakens the B-H bond. As can be seen from these results, these improvements in hydrogen storage do not reflect bulk catalysis, but rather interface driven processes. The interfaces between the catalyst and the hydride promote the density of active sites, mass transport, and electronic interactions that weaken B-H bonds, and reduce the energy barriers for hydrogen release. This work provides a mechanistic framework for catalyst design through interfacial engineering, offering a general strategy for optimizing reactive hydride composites for energy storage applications.

Keywords: Hydrogen Storage, Catalytic Interface, Density Functional Theory, Reactive Hydride

O0022 • Dr. Yogita Jain

ICEAM2026-ORAL-0022 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT1

TEMPERATURE-DRIVEN ENHANCEMENT OF BIOHYDROGEN PRODUCTION FROM *BENINCASA HISPIDA* WASTE: TOWARD CIRCULAR BIOECONOMY APPLICATIONSYogita Jain^{1*} and Radhika Singh²¹*B.Voc Water Sanitation and Waste Management, Department of Civil Engineering, Faculty of Engineering, Dayalbagh Educational Institute, Agra 282001*²*Department of Chemistry, Faculty of Science, Dayalbagh Educational Institute, Agra 282001*

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Abstract

In the present scenario of energy and fuel crisis, demand for the sustainable renewable energy production have been emphasized around the globe. Biohydrogen production from waste is considered as a dual process focusing on the waste management and energy recovery but the yield of biohydrogen depends on the concentration of organic matter in the substrate and can be affected by the operational parameters like temperature, pH, bacterial consortium etc. This study explores the potential of the *Benincasa hispida* (Petha) waste as a substrate discarded in the large amount from the industries in Agra, for the biohydrogen production. To enhance the yield of biohydrogen, mixed culture source was pretreated at different temperatures ranges from 60°C to 120°C which was also compared with the untreated culture source. The highest biohydrogen production was found in the reactor which was pretreated at 100°C i.e. 69.4 mmol L⁻¹ day⁻¹ which was about ten times more in the untreated reactor (6.8mmol L⁻¹ day⁻¹). HAC/HBu was also found to be maximum (1.37) in the same reactor with the maximum COD degradation of 71.5%. The study is also supported by the statistical models like one way ANOVA, t-test and principal component analysis. This study showed the feasibility of the temperature pretreatment of mixed consortia for biohydrogen production following the circular economy pathway.

Keywords: Fermentation; Petha; Sustainable Energy; Waste valorization; Pretreatment.

O0030 • Krishnamraju Putta

ICEAM2026-ORAL-0030 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT1

Synergistic Enhancement of a Pyramidal Solar Still with Reflector, PCM and Active Glass Cooling: 3E AnalysisKrishnam Raju Putta¹, Nagendra Prasad Pandey², Prafull Hishikar³¹ *Department of Mechanical Engineering, Parul University, Vadodara, Gujarat, India*^{2,3} *Department of Automobile Engineering, Parul University, Vadodara, Gujarat, India*

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Abstract

This study experimentally investigates the performance enhancement of a pyramidal solar still through the synergistic integration of a fixed solar reflector, phase change material (PCM), and active fan-based glass-cover cooling. Two experimental configurations, namely the integrated pyramidal solar still (IPSS) incorporating the proposed enhancements and a conventional pyramidal solar still (CPSS), were experimentally evaluated under similar operating and climatic conditions. The objective was to assess the effectiveness of the integrated configuration in enhancing freshwater production and energy performance while examining its thermodynamic and economic characteristics. The performance was evaluated using energy, exergy, and economic (3E) analyses, with particular emphasis on the effect of active cooling and its associated electrical energy consumption. The IPSS achieved a freshwater yield of 8.4 L/m²/day, compared with 3.7 L/m²/day for the CPSS, representing a substantial improvement in productivity. The corresponding energy efficiencies were 65% and 32%, respectively. The exergy efficiencies of the CPSS and IPSS were 3.40% and 8.60%, respectively, while the costs of freshwater (CPL) were estimated at \$0.09/L for IPSS and \$0.016/L for CPSS. Although the integrated system resulted in higher freshwater production and energy efficiency, the additional components and active cooling increased the freshwater production cost. Overall, the results demonstrate that the combined use of solar energy intensification, latent heat storage, and active condensation enhancement can substantially improve the freshwater productivity of pyramidal solar stills, while highlighting the need to balance thermodynamic gains with economic performance.

Keywords: Pyramidal solar still; Solar reflector; Phase change material; Active glass cooling; Energy analysis.

O0031 • Prof. Sandeep Chhoker

ICEAM2026-ORAL-0031 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT1

TERNARY 2D-MoO₃/g-C₃N₄/CNDs Z-SCHEME HETEROJUNCTION FOR SOLAR-DRIVEN PHOTOCATALYTIC WATER SPLITTINGAmbika Pathak¹, Satish Kumar Verma², Sandeep Chhoker¹¹*Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, Gautam Buddha Nagar, Uttar Pradesh, India*²*Laboratory for Energy Storage Devices, Department of Physics, SSBSR, Sharda University, Uttar Pradesh, India*

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Abstract

Solar-driven photocatalytic water splitting offers a promising route for sustainable hydrogen production, provided that efficient light harvesting, spatial charge separation and sufficiently strong redox potentials are simultaneously achieved. In this work, a carbon-nanodot (CND)-modified 2D-MoO₃/g-C₃N₄ Z-scheme photocatalyst is investigated as a multifunctional platform for solar-assisted water splitting. The heterostructure integrates layered 2D-MoO₃ and visible-light-responsive g-C₃N₄ with green-precursor-derived carbon nanodots to facilitate interfacial charge transport and broaden solar-light utilization. Structural, morphological and compositional characteristics are established through X-ray diffraction, FTIR, FESEM and EDX analyses, while UV-visible spectroscopy, photoluminescence and Raman spectroscopy are employed to elucidate the optical and electronic characteristics of the heterostructure. The constituent materials exhibit band gaps of 3.48, 2.81 and 2.76 eV for 2D-MoO₃, g-C₃N₄ and CNDs, respectively, with the integrated composite exhibiting enhanced light absorption extending into the visible region. Pronounced photoluminescence quenching following heterostructure formation indicates suppressed electron-hole recombination and improved carrier separation. The Z-scheme architecture is proposed to retain the highly reducing electrons of g-C₃N₄ and strongly oxidizing holes of 2D-MoO₃, thereby providing spatially separated charge carriers with appropriate redox potentials for proton reduction and water oxidation. The CND component further contributes to interfacial charge-transfer pathways and modified surface electronic interactions. This rationally engineered 2D/2D carbon-functionalized Z-scheme therefore provides a promising photocatalytic architecture for solar-to-hydrogen conversion and sustainable hydrogen generation.

Keywords: Z-scheme photocatalyst; 2D-MoO₃; g-C₃N₄; carbon nanodots; photocatalytic water splitting

BATTERY–SUPERCAPACITOR HYBRID ENERGY STORAGE FOR ISLANDED PV OPERATION AND SINGLE-PHASE SHUNT ACTIVE POWER FILTERING USING REINFORCEMENT LEARNING-BASED MPPT

Nikhil Agrawal¹, Neha Yadav², Anurag Das¹, Anshul Agarwal⁴

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Abstract

Rapid load switching, irradiance fluctuation and transients are very detrimental to the performance of PV-powered standalone systems and power quality compensators operating in grid connected mode. The batteries used as the only storage medium in such systems will suffer from faster degradation from frequent exposure to high magnitude transient currents. In this work, the integration of the supercapacitor with the battery is explored to reduce the battery stress and boost the overall system performance in two applications: (1) islanded PV operation and (2) a PV-fed single-phase shunt active power filter (SAPF), and an intelligent maximum power point tracking (MPPT) strategy for PV power extraction is investigated. The proposed hybrid energy storage system consists of two storage devices: a supercapacitor to provide fast transient power during load switching and fluctuations, and a battery to provide sustained steady state power. The coordinated power management strategy distributes power between the two storage elements depending on transient severity, and voltage regulation at the DC-link. On the PV-side control, a reinforcement learning (RL)-based MPPT algorithm are implemented, where different irradiance and partial shading conditions are used. The entire system consisting of the PV array, hybrid storage, MPPT controllers, islanded load and single-phase distribution system (SAPF) is designed and simulated in MATLAB/Simulink.

Simulation results demonstrate that the battery–supercapacitor hybrid storage module is able to deliver a considerable decrease of the peak and current stress of the battery when subjected to load transients, without compromising the stability of the DC-link voltage. The RL-based MPPT, in comparison to the conventional algorithm, shows better convergence and tracking to the global MPPT for dynamic and partially shaded conditions. The hybrid-storage system enables the system to achieve the improved harmonic compensation and reactive power support at the point of common coupling as per IEEE-519 limits in SAPF application. The proposed battery–supercapacitor hybrid architecture, along with the RL MPPT, successfully mitigates battery degradation, enhances transient response and power quality during islanded PV operation and in PV connected SAPF applications. The outcomes show its appropriateness for dependable and efficient stand-alone PV-based power systems, and its great potential for extending to real-time hardware implementation.

Keywords: Battery Energy Storage; Supercapacitor; Islanded PV Mode; Shunt Active Power Filter; MPPT; Reinforcement learning; Power Quality.

O0048 • Kritika Bansal

ICEAM2026-ORAL-0048 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT1

Physics-Informed MARL and Digital Twins for Carbon-Indexed Hybrid Second-Life Battery TradingSurya Karan Singh¹, Salil Kumar², Amit Kumar Singh³ and Kritika Bansal^{4*}^{1,2,3} *National Institute of Technology Delhi, Department of Electrical Engineering, New Delhi, India, 110036*⁴ *School of Electronics Engineering, VIT-AP University, Amaravati, Andhra Pradesh, India, 522241*

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Abstract

The largest near-term storage reservoir is the battery bank of retired EVs, the largest homogeneous new asset, and the tools for dealing with homogeneous new assets, lithium-plating blind degradation models and price signals which incentivise emissions-increasing arbitrage, are used to manage this asset. This paper aims to examine the possibility of linking per-pack digital twins – with a physics-based approach – with the trading of carbon using competitive trading aggregators. The neural operator model trained with single-particle-with-electrolyte-and-thermal-residuals with thermodynamics constraints of lithium inventory conservation and capacity monotonicity as differentiable constraints, achieves 3,100× faster terminal voltage reproduction (RMSE: 8.7 mV compared with pseudo-2D reference model), terminal voltage state of health (0.94% MAE compared with pseudo-2D reference model) and lithium-plating onset (AUROC: 0.97 compared with pseudo-2D reference model, AUROC: 0.71, and 26% loss of detection for data-driven ablation). The proximal policy optimisation (PPO) with multiple agents has a barrier-certified safe set where actions are projected and a twin-derived policy price of capacity degradation is learned. Under a carbon price of 100 USD tCO₂e⁻¹, more than 1.4 GWh of mixed-vintage capacity over 12 months with a 5-min resolution show a higher NPV (+21.7%), a lower carbon-intensity of delivered energy (-14.9%), a longer time to 60% State of Health (+19%) and no plating excursions (on 3.4% of the unconstrained steps). The 88% recovery of all-new revenue at 46% embodied emissions is achieved by hybridising with 15% new lithium iron phosphate (LFP).

Keywords: Second-life electric-vehicle batteries; Physics-informed digital twins; Carbon-aware energy trading; Multi-agent reinforcement learning; Lithium-plating-aware degradation

O0001 • Naseem Ahmad

ICEAM2026-ORAL-0001 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT4

Fe-Induced Structural and Electrical Transport Modulation in MnWO_4 Naseem Ahmad^{*,1}, and Kimoon Lee^{#,1,2}¹*Department of Physics, Kunsan National University, Gunsan, South Korea 54150*²*Institute of Basic Science, Kunsan National University, Gunsan, South Korea 54150*

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Abstract

Transition-metal doping is a well-established and effective strategy for tuning the physical characteristics of oxide-based systems. Before these materials can be effectively deployed in practical applications, achieving controlled modification and a thorough fundamental understanding of their behavior is essential. This study focuses on the ternary manganese tungstate oxide (MnWO_4) system, exploring how iron (Fe) doping tunes its physical properties. Rietveld refinement of powder X-ray diffraction (PXRD) data, along with Raman spectroscopy, confirmed that both pristine and Fe-doped MnWO_4 samples maintain a pure monoclinic wolframite phase. A closer look at the PXRD and Raman results reveals a highly selective substitution process, where Fe ions exclusively replace Mn ions rather than W sites. Furthermore, a 20% Fe concentration drastically boosts electrical conductivity by five orders of magnitude (10^5) and amplifies overall polarization. Also, the introduction of Fe not only enhances space-charge polarization but also maintains an optimized dissipation factor. These improved dielectric and electronic characteristics demonstrate that Fe-doped MnWO_4 systems hold strong potential for next-generation electronic device applications.

Keywords: Fe-doped MnWO_4 , Wolframite-monoclinic phase, Rietveld refinement, Space-charge polarization, Enhanced conductivity.

*Abstract adapted from our published work in *Journal of Molecular Structure* (2026),

DOI: 10.1016/j.molstruc.2026.145681.

O0021 • Shakshi Choudhary

ICEAM2026-ORAL-0021 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT4

Comparative Kinetic and Diffusion Analysis of NO₂ Gas Adsorption on Single-Walled Carbon Nanotubes and Functionalized Single-Walled Carbon Nanotubes

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Abstract

Understanding the adsorption kinetics and diffusion mechanisms of toxic gases on carbon nanotube-based sensors is essential for improving their sensing performance and designing high-sensitivity gas detection systems. In the present study, a comprehensive computational kinetic analysis is carried out to compare the adsorption behaviour of nitrogen dioxide (NO₂) on pristine single-walled carbon nanotubes (SWNTs) and tin oxide (SnO₂)-functionalized SWNTs. The adsorption process is analysed using multiple nonlinear and diffusion models, including the pseudo-first-order, pseudo-second-order, Avrami, Elovich, Linear Driving Force (LDF), Weber–Morris intraparticle diffusion, and Boyd models. Model parameters are estimated through nonlinear regression to minimize fitting errors, and the goodness of fit is evaluated using appropriate statistical criteria. Comparative analysis of the extracted kinetic parameters, diffusion coefficients, and rate constants is performed to elucidate the adsorption mechanism and identify the dominant rate-controlling step for each sensing material. The study aims to determine the influence of SnO₂ functionalization on adsorption kinetics and diffusion behaviour relative to pristine SWNTs. Functionalization alters the adsorption pathway, modify the rate-controlling mechanism, and enhance gas–surface interactions, resulting in improved NO₂ sensing performance. The findings provide mechanistic insights into gas adsorption on carbon nanotube-based nanocomposites and establish a systematic framework for evaluating adsorption kinetics and diffusion processes in nanostructured gas sensors.

Keywords: Carbon nanotube, tin oxide functionalized, Pseudo first order, pseudo second order, Avrami, Elovich, LDF, Weber Morris models

SYNTHESIS OF 2D MOSSE JANUS STRUCTURE BY HYDROTHERMAL METHODKushal Mazumder¹¹*Department of Physics, School of Sciences, IILM University, Greater Noida, Uttar Pradesh, India*

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Abstract

Two-dimensional (2D) TMD based Janus structure such as MoSSe has garnered significant attention due to its unique electronic properties like intrinsic dipole moment, band gap tunability and enhanced carrier mobility, optical properties such as strong photoluminescence and light-matter interaction, and improved catalytic properties. Due to inversion symmetry breaking, MoSSe Janus structures exhibit strong second harmonic generation, making them useful for frequency conversion, optical signal processing, and other photonic applications. Out of different polytypes of MoSSe, such as 1T, 2H, and 3R, which refer to various stacking sequences and symmetries of the MoSSe layers, the 1T phase is often considered better than the 2H and 3R phases due to its higher electrical conductivity and catalytic activity, making it more suitable for applications in electronics and catalysis. There are different synthesis techniques for 1T MoSSe, such as chemical vapor deposition (CVD), mechanical exfoliation, hydrothermal method and each offer unique advantages. However, hydrothermal method is considered the best due to its ability to produce high-quality, uniform crystals with controlled morphology and stoichiometry. Due to the limited literature on hydrothermal synthesis of 1T phase MoSSe, the present study aims to explore this method and fill the knowledge gap by reporting the hydrothermal synthesis of high-quality 1T phase MoSSe Janus structures. The phase formation of the prepared structures has been verified by different characterization techniques such as XRD, FESEM, Raman and PL spectroscopy.

XRD analysis confirms the crystal structure and phase purity of the synthesized MoSSe, with distinct diffraction peaks and the (002) peak specifically indicating the 1T phase. FESEM imaging shows continuous and uniform flower like morphology with the size of few hundred nanometers. Raman spectroscopy shows characteristic peaks for J_2 , E_{1g} , and J_3 phonon modes of the 1T-phase indicating successful synthesis. PL spectroscopy further reveals no distinct emission peaks which indicates the formation of metallic 1T phase MoSSe. The synthesized Janus structure can be useful for catalytic applications including hydrogen evolution reactions, CO_2 reduction, and water splitting.

Keywords: 2D Materials; MoSSe Janus Structure; Symmetry breaking; Hydrothermal Synthesis; 1T Phase.

O0019 • Raghav Sharma

ICEAM2026-ORAL-0019 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT4

Nonlinear Quantum Materials for energy harvesting, Harmonic Generation and Frequency-MixingRaghav Sharma¹¹ *Department of Electrical Engineering, IIT Ropar, Rupnagar, Punjab, India*Corresponding Author Email: raghav.sharma@iitrpr.ac.in**Abstract**

Recently, second and higher-order nonlinear electrical responses have emerged as important phenomena in quantum materials. These responses can originate from intrinsic mechanisms related to crystal symmetry and Berry curvature dipole [1,2], as well as extrinsic scattering mechanisms such as skew scattering and side-jump processes. For example, nonlinear Hall responses can arise in non-centrosymmetric materials through Berry curvature dipole related mechanisms [1,2], while nonlinear longitudinal and Hall responses have also been observed in materials such as Bi₂Te₃ [3]. Second-order nonlinear responses, including nonlinear magnetoresistance [4] and the nonlinear Hall effect [5], generate both a second-harmonic voltage at (2 ω) and a dc component through rectification when driven by an alternating current. These effects provide a route toward zero-bias, room-temperature wireless RF rectification, frequency doubling, and potentially higher-order harmonic generation without requiring an external magnetic field, with promising applications including energy harvesting, wireless communication, and THz detection. Beyond harmonic generation and rectification, nonlinear responses enable frequency mixing when multiple input frequencies are applied, producing intermodulation frequencies that encode information, which can potentially be used as nonlinear computational states or features, allowing quantum materials to serve as physical nonlinear kernels for neuromorphic computing and frequency-domain information processing. This presentation will discuss the fundamental origins of nonlinear electrical responses in quantum materials and their manifestations as dc signals, harmonics, and frequency-mixing products, followed by how these intrinsic and extrinsic nonlinearities can be harnessed for emerging applications in RF electronics, THz technologies, and neuromorphic computing.

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O0023 • Tanmoy Majumder

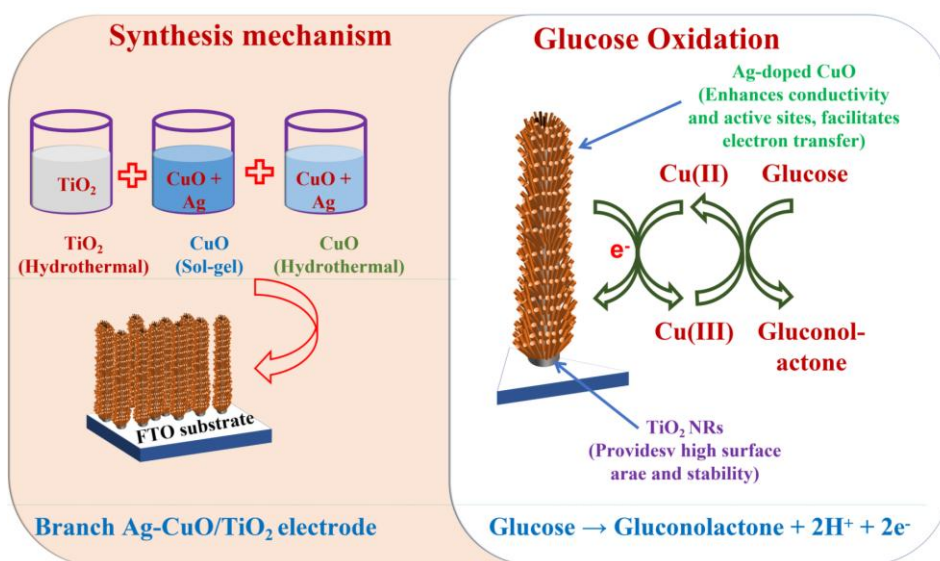
ICEAM2026-ORAL-0023 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT4

Ag-ENGINEERED CuO/TiO₂ BRANCHED HETEROSTRUCTURE FOR HIGH-PERFORMANCE NON-ENZYMATIC AND NON-INVASIVE ELECTROCHEMICAL GLUCOSE SENSINGKaberi Saha¹, Kamalesh Debnath¹, Tanmoy Majumder^{2*},¹Department of Electronics and Communication Engineering, National Institute of Technology Agartala, Agartala, Tripura, India-799046²Centre for Nanoelectronics and VLSI Design, Vellore Institute of Technology Chennai, Chennai, Tamil Nadu, 600127

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Abstract

Diabetes mellitus is a major global health concern that requires regular and reliable monitoring of blood glucose levels for effective disease management. However, the conventional glucose monitoring methods are usually invasive and painful, and the enzyme based sensors may have limited stability and sensitivity under different environmental conditions. Thus, it is highly desirable to develop non-enzymatic and non-invasive glucose monitoring technologies for convenient and reliable glucose assessment. In this study, an electrochemical glucose biosensor based on an Ag-doped CuO/TiO₂ branched heterostructure was fabricated by combining the high catalytic activity of CuO, the good charge-transport properties of TiO₂ and the increased electrical conductivity and electrocatalytic properties resulting from Ag doping. The branched heterostructure offers a large number of electrochemically active sites and enables efficient interfacial charge transfer, which in turn promotes the electrochemical oxidation of glucose in an alkaline environment. The optimized Ag-doped CuO/TiO₂ electrode shows a quick and strong amperometric response to glucose, together with high sensitivity and a broad linear detection range, demonstrates its capability toward detecting glucose in both low and relatively high concentrations. The improved sensing performance is due to the synergistic effect of Ag, CuO and TiO₂, since this leads to better electron transport, greater surface accessibility and enhanced catalytic activity for the oxidation of glucose. Moreover, the sensor shows excellent selectivity with respect to common interfering substances, as well as good repeatability, reproducibility and operational stability, which confirms the reliability of the sensing performance. In order to show its practical applicability, the sensor was successfully employed for glucose detection in commercially available soft drinks, such as Diet Coke and Mountain Dew along with glucose-spiked raw human saliva, giving satisfactory responses and recovery values. These results show the promise of the Ag-doped CuO/TiO₂ branched heterostructure as a potential electrode material for sensitive, selective, and practical non-enzymatic glucose monitoring and offer a valuable approach to electrochemical sensing in real samples.

Keywords: heterostructure, CuO, TiO₂, glucose, Ag-doping, LOD, sensitivity, selectivity

Sensitivity Analysis of an InGaAs Junctionless Gate-All-Around Nanowire MOSFET with High-k Underlap Spacer for Multi-VOC Gas Detection

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Abstract

This work presents a numerical investigation of an InGaAs Junctionless gate-all-around (JL-GAA) nanowire MOSFET with an underlap S/D high-k spacer for volatile organic compound (VOC) gas sensing applications. The proposed device exploits the strong electrostatic control of the gate-all-around architecture and the high surface-to-volume ratio of the nanowire channel to enhance drain-current modulation upon gas adsorption. The sensing performance is evaluated in terms of the variation in ON-state current (I_{ON}) for five target VOCs, namely methanol, isopropanol, chloroform, hexane, and dichloromethane (DCM). The gas response is measured using the normalized ON-current sensitivity, defined from the relative change in I_{ON} between the reference and gas-exposed conditions. At $V_{DS}=0.2$ V and $V_{GS}=1.0$ V, chloroform and DCM exhibit a sensitivity of approximately 0.4, whereas hexane shows a substantially lower sensitivity of approximately 0.04, signifying the competence of the proposed device to categorize between different VOC GAS molecules. A comprehensive parametric analysis is further performed by varying the operating temperature, high-k spacer dielectric constant, underlap length, channel doping concentration, channel length, and nanowire radius. These parameters are investigated to determine their influence on carrier transport, electrostatic control, and gas-induced I_{ON} modulation. The comparative gas response and device-parameter optimization demonstrate the potential of the proposed InGaAs JL-GAA nanowire MOSFET as a compact and sensitive platform for VOC detection and environmental monitoring applications.

Keywords: InGaAs; Junctionless GAA MOSFET; Nanowire FET; High-k Spacer; Underlap Engineering; ON-Current Sensitivity.

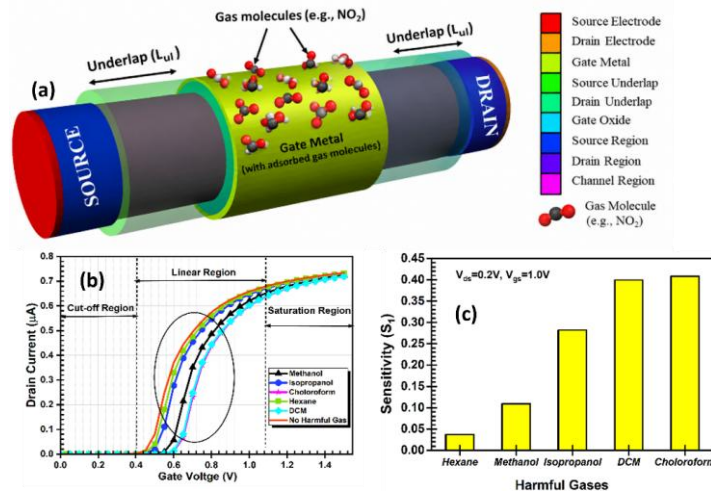


Fig. 1: (a) Schematic of InGaAs JL-GAA nanowire MOSFET, (b) Drain characteristics, and (c) Sensitivity for various gas molecules.

O0042 • Dr. Soniya Juneja

ICEAM2026-ORAL-0042 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT5

SIZE- AND MEDIUM-DEPENDENT OPTICAL RESPONSE OF CdSe@ZrN CORE-SHELL NANOPARTICLES FOR PHOTONIC APPLICATIONS**Soniya Juneja¹, Manmohan Singh Shishodia², Vipin Kumar¹, Kapil Kumar Sharma¹**¹Department of Applied Sciences and Humanities, KIET Deemed to be University, Ghaziabad, India²Department of Applied Physics, Gautam Buddha University, Greater Noida, India**Corresponding authors: Manmohan Singh Shishodia, Soniya Juneja***Abstract**

CdSe@ZrN core-shell nanoparticles are of interest for photonic applications because their optical behaviour can be controlled through both particle geometry and the surrounding environment. The CdSe core provides a wavelength-dependent semiconductor response, while the ZrN shell contributes to the plasmonic behaviour of the structure. In this work, the absorption, scattering, and extinction efficiencies of CdSe@ZrN nanoparticles are studied in the visible and near-infrared regions. The effects of particle size, core-to-shell radius ratio, and refractive index of the embedding medium are examined. Changes in the core-to-shell ratio modify the resonance position and the strength of the optical response. Similarly, variation in the surrounding medium produces a noticeable change in the resonance behaviour of the nanoparticle. These parameters therefore provide different ways to tune the interaction of light with the core-shell structure. The study may support the design of wavelength-selective optical components and other nanoscale photonic devices.

Keywords: CdSe@ZrN; core-shell nanoparticle; zirconium nitride; aspect ratio; embedding medium; optical efficiency; plasmon resonance; photonic applications

Electronic Structure, Optical Response and Photovoltaic Performance of BaZrS₃: An Integrated DFT–SCAPS-1D Approach

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Abstract

Chalcogenide perovskites such as barium zirconium sulfide (BaZrS₃) have emerged as promising, non-toxic absorber materials for next-generation thin-film photovoltaics. In this study, a combined density functional theory (DFT) and SCAPS-1D device simulation framework was employed to evaluate the fundamental physical properties and solar cell performance of BaZrS₃. The ground-state crystal structure was optimized using variable-cell relaxation, followed by self-consistent field (SCF) calculations. Electronic property analysis via total and projected density of states (DOS/PDOS) elucidated the contribution of specific atomic orbitals to the valence band maximum and conduction band minimum. Furthermore, the frequency-dependent dielectric function and optical absorption spectrum were computed to assess light-harvesting capability. Utilizing the DFT-derived electronic and optical properties as baseline inputs, a BaZrS₃-based thin-film heterojunction solar cell was designed and simulated in SCAPS-1D. Key photovoltaic parameters, including open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE), were evaluated under standard AM1.5G illumination. Systematic optimization of critical device parameters provides practical design guidelines to optimize device performance, confirming the strong potential of BaZrS₃ for efficient thin-film solar cells.

Keywords: Chalcogenide perovskite, BaZrS₃, DFT, SCAPS-1D

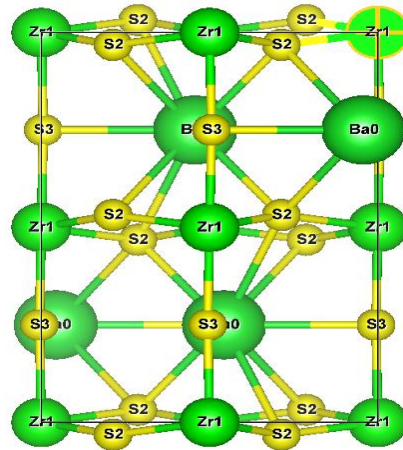


Fig-1 Unit cell structure of BaZrS₃

UNRAVELING CAPACITANCE–STRUCTURE RELATIONSHIPS IN BIOMASS-DERIVED CARBON ELECTRODES THROUGH MACHINE LEARNING

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Keywords: Supercapacitor, Machine learning, Energy Storage, Random Forest, Feature Importance

Objective

The objective of this work is to develop a machine learning (ML)-based framework for predicting the specific capacitance of biomass-derived activated carbon electrodes and to elucidate the influence of key physicochemical and operating parameters on supercapacitor performance.

Methodology

Abstract

A literature-derived dataset containing 785 experimental data points was compiled using key descriptors, including specific surface area, pore size, pore volume, potential window, Raman ID/IG ratio, and current density, with specific capacitance as the target parameter. Six ML models—XGBoost, Gradient Boosting, Random Forest, Kernel Ridge Regression, K-Nearest Neighbours, and CatBoost—were evaluated using R^2 , MAE, and RMSE. SHAP analysis was further employed to interpret model predictions and quantify the contribution of individual descriptors.

Major Results

The comparative analysis revealed a clear difference in predictive capability among the investigated ML models. XGBoost demonstrated the most accurate and robust prediction of specific capacitance, achieving an R^2 of 0.91, MAE of 26.71 Fg^{-1} , and RMSE of 48.47 Fg^{-1} . The high R^2 indicates that the model successfully captures the complex and nonlinear relationships governing the electrochemical response of biomass-derived activated carbon electrodes. The relatively low MAE further demonstrates its ability to predict specific capacitance with good accuracy across diverse experimental conditions. SHAP analysis provided additional insight into the model behaviour by identifying the relative contribution of material characteristics and operating parameters to capacitance prediction. The results highlight the importance of surface characteristics and pore-related properties in governing the electrochemical performance of activated carbon electrodes.

Conclusions

The findings demonstrate that ML, particularly XGBoost, can effectively predict the specific capacitance of biomass-derived activated carbon electrodes and provide meaningful insights into the underlying material–performance relationships. The proposed approach offers a data-driven alternative to extensive trial-and-error experimentation, enabling rapid screening of biomass-derived carbon materials while reducing experimental time, cost, and effort. This framework can support the rational design and optimization of sustainable, high-performance supercapacitor electrodes for advanced energy-storage applications.

O0054 • DR. DHIRENDRA KUMAR SHARMA

ICEAM2026-ORAL-0054 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT5

Probing Exciton and Defect Physics in Lead-Free $\text{Cs}_2\text{AgBiBr}_6$ Double Perovskite Nanocrystals

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Abstract

Lead-free double perovskites are emerging as one of the most promising routes to non-toxic, stable alternatives to lead halide perovskites. Simple homovalent substitutes such as Sn^{2+} or Ge^{2+} readily oxidise and degrade, while trivalent-only substitutions (e.g., Bi^{3+}) distort the desirable cubic perovskite framework into a less favorable hexagonal structure. Double perovskites overcome both limitations through heterovalent substitution, replacing two Pb^{2+} ions with a monovalent-trivalent pair ($\text{Ag}^+/\text{Bi}^{3+}$), which preserves the cubic framework while using oxidation-resistant, low-toxicity ions. This makes them uniquely attractive for scalable, air-stable optoelectronics, but their indirect bandgap remains a key barrier to high-performance devices. Here, we synthesise $\text{Cs}_2\text{AgBiBr}_6$ nanocrystals at room temperature and unpack their structural and optical behaviour through a combined TEM/STEM, static absorption, photoluminescence (PL), and transient absorption spectroscopy (TAS) study. TEM and STEM imaging confirm well-formed ~ 12.5 nm nanocubes, alongside trace $\text{Cs}_3\text{Bi}_2\text{Br}_9$ and silver byproducts that trace back to a partial degradation pathway. Strikingly, PL measurements reveal a dual-emission signature with broad peaks at 2.5 eV and 1.8 eV, challenging the single-peak emission. We propose two competing explanations: a coexistence of direct and indirect bandgap recombination pathways, or an indirect transition intertwined with defect-mediated trap emission. TAS further captures this complexity, showing excitonic ground-state bleaching at 2.9 eV that decays as carriers recombine, set against a broad photo-induced absorption background from carriers migrating to higher-energy states. Together, these findings sharpen the emerging picture of exciton and defect physics in silver-bismuth double perovskites and point to concrete design levers, defect passivation and band engineering, to unlock their potential in next-generation, lead-free optoelectronic devices.

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O0051 • Shubham Kumar Singh

ICEAM2026-ORAL-0051 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT5

Energy-Aware Digital Twins for Coupled Strain Defect Dynamics and Adaptive Recovery in Perovskite PhotovoltaicsSurya Karan Singh¹, Shubham Kumar Singh^{2*}, Sameer Bhambri³, Amit Kumar Singh⁴^{1,2*,3} *National Institute of Technology Delhi, Department of Electrical Engineering, New Delhi, India, 110036*

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Abstract

Mechanical fatigue, ionic defects, and irreversible degradation at the interface are the main factors limiting the long-term stability of perovskite PVs. In this, a digital twin of a strain–defect–passivation system is developed that combines spatial damage evolution, vacancy transport, reversible polymer kinetics, Kalman state estimation, and safety-constrained predictive recovery, together with a 5-parameter photovoltaic model. Under cyclic strain and synthetic irradiance, 41 spatial nodes and 0.25 h of integration are analyzed for 5 recovery strategies over 96 h. When the devices are treated without any treatment, the efficiency drops from 20.74% to 17.37%, while static passivation, open-loop thermal treatment, threshold control, and predictive control result in efficiencies of 19.26%, 21.23%, 20.09%, and 20.11%, respectively, for an identical simulated power-conversion efficiency of 20.74%. Corresponding net energy yields reach 0.4946, 0.5287, 0.5340, 0.5306, and 0.5296 Wh cm^{−2} after accounting for thermal actuation. Predictive recovery involves only one intervention at 329.75K, which is kept below the set safety limit of 335.15K. Notably, periodic treatment yields higher simulated net energy than predictive control, highlighting trade-offs among control complexity, actuator consumption, and recovery effectiveness. The performance metrics are derived from uncalibrated simulations, while the fabrication of the materials, autonomous healing, and operational durability are yet to be proven through controlled experiments and device-level validation.

Keywords: Perovskite photovoltaics; Digital twin; Strain–defect coupling; Autonomous defect passivation; Self-healing materials; Predictive recovery control; Photovoltaic degradation

O0002 • Dr. Prakash Yadav

ICEAM2026-ORAL-0002 | Oral Presentation | Day 2, 09 Oct 2026, 08:00-09:00 AM, LT5

Interfacial Properties of PTFE–ZnO Nanosheet for Triboelectric Nanogenerator: A Density Functional Theory Investigation

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Abstract

Triboelectric nanogenerators (TENGs) have attracted significant attention as sustainable energy harvesting devices for powering self-powered electronics. In this study, Density Functional Theory (DFT) calculations were performed to investigate the interfacial properties of PTFE adsorbed on a ZnO nanosheet for triboelectric energy generation. Six stable adsorption configurations were optimized, and their electronic structures, adsorption energies, Mulliken charge transfer, dielectric constants, surface-bound charge densities, and output voltages were systematically analyzed. The calculated adsorption energies confirm strong interfacial interaction between PTFE and ZnO, while noticeable charge transfer demonstrates efficient electron redistribution across the interface. PTFE adsorption increases the band gap of the pristine ZnO nanosheet from 1.70 eV to 1.82–1.92 eV, indicating modified electronic characteristics favorable for triboelectric performance. Furthermore, the calculated surface-bound charge density and output voltage reveal that the z-direction exhibits the highest electrical response, highlighting the importance of vertical polarization during sliding operation. These findings provide atomic-level insights into the PTFE–ZnO triboelectric interface and establish this heterostructure as a promising candidate for high-performance triboelectric nanogenerators and future self-powered energy harvesting applications.

Keywords: Density Functional Theory; Triboelectric Nanogenerator; PTFE; ZnO Nanosheet; Charge Transfer; Energy Harvesting

O0013 • Manoj Tripathi

ICEAM2026-ORAL-0013 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

Thermochemical Valorization of Sugarcane Bagasse through Fast Pyrolysis: Bio-Oil Production and Recovery of Phenolic Compounds

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Abstract

Biomass derived bio-oil has emerged as an amazingly effective and sustainable energy alternative. In this study, bio-oil is produced from the fast pyrolysis of sugarcane bagasse at three different temperatures i.e. 500 °C, 600 °C & 700°C. Bio-oil yield was obtained as 20.4 wt.%, 26.3 wt.% & 33.6wt.% respectively for these temperatures. Viscosity, pH, density, acid number and heating value of SB-500, SB-600 & SB-700 were examined. The chemical composition of the produced bio-oil was determined by gas chromatography-mass spectrometer (GC-MS), which confirmed the presence of a significant amount of phenols in it. To estimate the phenolic compounds, Gallic acid calibration standards were used. Total phenolic component in SB-500, SB-600 & SB-700 were in the range of 44.8%, 51.5% & 58.4% respectively. Effect of temperature and the stirrer speed on the extraction of phenolic compounds was also studied in the present study. The temperature range for the study was 30°C to 50°C while the stirrer speed range was 200 rpm to 300 rpm. The optimum temperature and the stirrer speed was 40°C and 250 rpm for all the three samples. The optimum phenolic extract was 45.3%, 49.8% & 56.8% for SB-500, SB-600 & SB-700 respectively.

Keywords: Bio-oil; Fast Pyrolysis; Phenolic extraction; Sugarcane Bagasse

O0035 • Dr. J. Joseph

ICEAM2026-ORAL-0035 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

AI-Enabled Sensor-Integrated Seaweed-Based Functional Coatings for Atmospheric CO₂ Capture, Smart Monitoring, and Sustainable Energy-Efficient Buildings

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Abstract

The rising level of atmospheric carbon dioxide (CO₂) leads to a need for eco-friendly material. Seaweed-based functional coating has been developed in this research, which is made of renewable raw materials, including naturally available biopolymers derived from seaweeds (alginate, carrageenan, and chitosan), cellulose acetate, coconut fibre biochar, conch shell powder, beeswax, and Vinca rosea pigment along with other materials like limestone and linseed oil. The developed coating has been characterized using methods such as SEM, FTIR, XRD, BET, TGA. All these techniques confirm the porous microstructure, the presence of various functional groups on the surface of the coating, and its good thermal stability. The CO₂ adsorption ability has been tested using an atmospheric capture chamber designed and applied for this research. The chamber includes the environmental sensors connected with the IoT platform for continuous monitoring. The functional coating that was developed, which is made from seaweed, has the ability to adsorb CO₂ in the amount of $15.20 \pm 0.42 \text{ mg g}^{-1}$, which is better than wall paints that are produced commercially, under the same conditions. The efficiency of the adsorption process followed the pseudo-second order relationship ($R^2 = 0.992$), while the analysis of Langmuir isotherm proved the existence of favorable monolayer adsorption. The results of statistical analyses (ANOVA, $p < 0.05$) indicated that the variables of humidity and airflow have an important impact on the efficiency of the system. In addition, the artificial intelligence technology made it possible to make continuous adjustments of the operating parameters of the system. Long-term experiments proved that the coating is able to retain 76% of CO₂ results over the period of time, which shows that the coating is durable and practically applicable.

Keywords: Seaweed-based paint; CO₂ capture; Smart coatings; Artificial intelligence; Carbon sequestration; Sustainable materials.

O0045 • Abhinav Adarsh

ICEAM2026-ORAL-0045 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

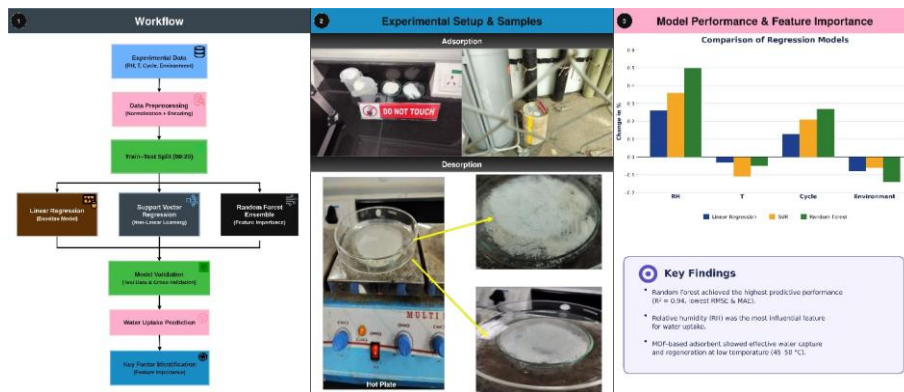
MACHINE LEARNING-ASSISTED EVALUATION OF MOF-303 AND MOF-801 FOR ATMOSPHERIC WATER HARVESTING IN REAL-WORLD CONDITIONS

Pawan Kumar Chauhan¹, Abhinav Adarsh², Raju Patel^{3*}^{1,2}Department of Advanced Computer Science and Engineering, Vignan's Foundation for Science, Technology and Research (Deemed to be University), Vaddlamudi, 522213, Guntur, India³School of Electronics Engineering, Vellore Institute of Technology, Chennai, India-600127*Corresponding author email-raju.patel@vit.ac.in

Abstract

Atmospheric water harvesting using metal–organic frameworks (MOFs) is a promising approach for sustainable water generation, however, most studies remain limited to controlled laboratory conditions. This work presents a hybrid experimental–AI framework to evaluate MOF-303 and MOF-801 under realistic indoor and outdoor environments across day and overnight cycles. Experimental results show that MOF-303 consistently outperforms MOF-801, exhibiting higher water uptake and faster adsorption kinetics, with most adsorption occurring within 60–90 minutes. Both materials demonstrate efficient regeneration at low temperatures (45–50 °C). To complement experimental analysis, machine learning models, Linear Regression ($R^2 = 0.78$), Support Vector Regression ($R^2 = 0.86$), and Random Forest ($R^2 = 0.94$) were applied to predict adsorption behaviour. Random Forest achieved the best performance, accurately capturing non-linear relationships between relative humidity, temperature, and environmental conditions. Feature importance analysis identified relative humidity as the dominant factor influencing water uptake, consistent with experimental observations. Thus, the integration of real-environment experimentation with AI modelling provides enhanced predictive capability and deeper insight into adsorption dynamics. Overall, the superior performance of MOF-303 and the proposed hybrid framework offer a scalable and application-oriented pathway for optimizing next-generation atmospheric water harvesting systems.

Keywords: Atmospheric Water Harvesting; Metal–Organic Frameworks (MOFs); Machine Learning; Adsorption Performance Prediction



O0050 • Shubhangi Saxena

ICEAM2026-ORAL-0050 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

WASTE-TO-RESOURCE PATHWAYS: A REVIEW OF PRODUCT INNOVATIONS FROM CROP RESIDUESShubhangi Saxena¹, Tiju T. Thomas²¹ *University School of Design & Innovation, Guru Gobind Singh Indraprastha University, New Delhi, Delhi, India*² *University School of Design & Innovation, Guru Gobind Singh Indraprastha University, New Delhi, Delhi, India*

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Abstract

Stubble Burning is one of the most difficult problems faced by Northern parts of India especially- parts of Delhi NCR, Haryana, Punjab and some parts of Uttar Pradesh. The pressure on a farmer's head for making the fields ready for the next crops leads to burning of waste stubble. The reason waste stubble is reused and utilized in a productive way is to be used as an eco-friendly alternative to many non-renewable solutions and products that are harming the environment. Technological advancements nowadays have added to the preparation of eco-friendly answers and product innovations executed by many start-ups, new companies working on the execution of market-ready products while taking care of their procurement and easy handling. Ample amount of product range is available in current market scenarios ranging from tableware, packaging material, acoustic material, paper bags, stationery packing, particleboards and many more. Stubble has taken over universally, the trail that leads to remarkable wonders from waste.

Keywords: *Crop Residue Utilization, Stubble Burning Mitigation, Waste-to-Resource Conversion, Sustainable Product Innovation, Circular Economy, Biodegradable Materials*

O0055 • Manisha Bajpai

ICEAM2026-ORAL-0055 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

STRUCTURAL, OPTICAL, VIBRATIONAL AND MORPHOLOGICAL CHARACTERIZATION OF PLANT MEDIATED GREEN SYNTHESIS OF ZnO NANOPARTICLES using *Moringa oleifera* EXTRACT

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Abstract

In the present study, Zinc oxide nanoparticles were synthesised through a green and eco-friendly approach using *Moringa oleifera* extract. The synthesised ZnO nanoparticles were comprehensively characterized by using UV-vis spectroscopy, Raman spectroscopy, X-ray diffraction (XRD), Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDX). UV –Vis spectroscopy was employed to investigate the optical absorption of synthesised nanoparticles whereas PL spectroscopy was used to determine emission behaviour and optical properties of nanoparticles. Raman spectroscopy was performed to investigate the vibrational characteristics and structural features of ZnO nanoparticles. XRD analysis was carried out to determine the crystalline structure , phase composition and crystallinity of the synthesised particles. SEM analysis also provided information regarding the surface morphology, particle distribution, and agglomeration behaviour. The elemental composition of synthesised nanoparticles was confirmed through EDX analysis. The combined characterises results provide comprehensive insights into the optical , vibrational , structural , morphological and elemental properties of green synthesized ZnO nanoparticles . The study demonstrates the successful synthesis of ZnO nanoparticles through an environmentally sustainable route and highlights the suitability of the synthesized material for further exploration in advanced functional and optoelectronic applications.

Keywords: Zinc Oxide nanoparticles; Green synthesis; XRD; SEM–EDX; *Moringa oleifera*; Photoluminescence

O0008 • AJAY KUMAR

ICEAM2026-ORAL-0008 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT1

SAME MOLECULE, OPPOSITE OUTCOME: SOLVENT-MEDIATED INTERFACIAL ENGINEERING IN INVERTED PEROVSKITE SOLAR CELLSAjay Kumar¹, Dr. Mukta Sharma ², Dr. C L Tsai¹¹ Dept. Of Electronics Engg, Chang Gung University, Taiwan² Dept. Of Prospective Tech Of electrical Engg. And Computer Science, National Chin-Yi University of Technology, Taiwan

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Abstract

Molecular passivation at the perovskite/fullerene interface is widely used in inverted (p–i–n) perovskite solar cells, but the role of processing solvent is often overlooked. Here, we investigate solvent-mediated interfacial modification using N-(2-Aminoethyl)-3-Aminopropyltrimethoxysilane (AEAPTMS), introduced between the perovskite absorber and PCBM electron-transport layer. The molecule was processed from toluene, ethanol, or 2-propanol, with and without a post-deposition rinse. A strong dependence on processing conditions was observed. Ethanol followed by rinsing produced the best overall performance, delivering an average efficiency of 17.9% compared with 14.2% for the reference, and a champion efficiency of 19.5%. The improvement was mainly driven by an approximately 190 mV increase in open-circuit voltage, while the fill factor remained comparable to the reference. In contrast, removing the rinse preserved the voltage enhancement but caused a pronounced reduction in fill factor, indicating less favourable charge extraction. Toluene treatment showed little benefit. These results suggest that the solvent and rinse protocol influence how AEAPTMS modifies the perovskite/PCBM interface. We propose that ethanol promotes effective interfacial interaction, while rinsing helps remove excess material and avoids extraction losses. The findings highlight processing conditions as an important design parameter for molecular passivation in inverted perovskite solar cells.

Keywords: AEAPTMS, heterojunction, device simulation, broadband detection, detectivity

O0018 • Varsha

ICEAM2026-ORAL-0018 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

INVESTIGATING THE ROLE OF DEFECT AND ION-MIGRATION DYNAMICS ON CURRENT–VOLTAGE HYSTERESIS IN PEROVSKITE SOLAR CELLS: A COMSOL MULTIPHYSICS-BASED STUDYVarsha¹, Kapil Kumar¹, Vinod Prasad²¹ *Department of Physics, Kalindi College, University of Delhi, Delhi-110008, India*² *Department of Physics, Swami Shraddhanand College, University of Delhi, Delhi-110036, India*

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Abstract

Perovskite solar cells (PSCs) have emerged as one of the most promising third-generation photovoltaic technologies, with power conversion efficiencies now exceeding 25%. However, their commercial viability remains hindered by current density–voltage (J–V) hysteresis, an anomalous behaviour in which the backward and forward voltage-scan characteristics differ significantly, making accurate efficiency determination difficult. This hysteresis has been largely attributed to ion migration within the perovskite absorber layer, interfacial charge trapping, and defect-mediated recombination at the transport-layer interfaces, though the physical origin — particularly of the less-understood inverted hysteresis — remains unresolved. Building on our prior work on impurity and defect effects on the optical and electronic properties of low-dimensional semiconductor nanostructures, we propose to extend this framework to perovskite-based solar cells by numerically investigating how defect density, ionic species mobility, and interfacial trap states govern the hysteretic response of the device. Using the Semiconductor Module of COMSOL Multiphysics, we will self-consistently solve the coupled Poisson and carrier-continuity equations along with ion-migration transport equations for an FTO/TiO₂/MAPbI₃/Spiro-OMeTAD/Au device architecture. The dependence of the hysteresis index on scan rate, carrier mobility, pre-bias voltage, and ion flux across the electron- and hole-transport layers will be systematically studied and correlated with the underlying recombination and band-alignment mechanisms at the perovskite interfaces. The proposed study aims to identify defect-engineering and interface-passivation strategies that can suppress both normal and inverted hysteresis, thereby contributing toward the design of hysteresis-free, high-efficiency, and stable perovskite solar cells.

Keywords: Perovskite solar cells; J–V hysteresis; ion migration; drift–diffusion simulation; COMSOL Multiphysics

O0020 • Priya Siwach

ICEAM2026-ORAL-0020 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

POLYANILINE HYDROGEL DECORATED ON Ni-Mn-Zn LAYERED DOUBLE HYDROXIDE AND ORANGE PEEL-DERIVED POROUS CARBON FOR NEXT- GENERATION ENERGY STORAGE APPLICATIONS

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Abstract

Polyaniline (PANI) is a widely studied conductive polymer owing to its impressive electrical conductivity, reversible redox behaviour, and easy synthesis. As a hydrogel, PANI contains a porous three-dimensional network that provides continuous electron pathways and increased electrolyte accessibility. In the present work, a ternary nanocomposite (PLC) comprising NiMnZn layered double hydroxide (NMZ LDH), PANI hydrogel and orange peel-derived porous carbon (OPC) have been rationally designed and synthesized to construct a multidimensional electrode architecture. The NMZ LDH was synthesized via a hydrothermal route to provide abundant multivalent redox-active sites, followed by incorporation of OPC as a conductive porous scaffold. Then, the PANI hydrogel was grown atop the NMZ/OPC network, forming an interconnected conducting network. The PLC3 electrode exhibits commendable specific capacitance (C_s) of 2638.5 F/g at 1 A/g. The 100% capacitance retention over 13000 cycles attests to the electrode's excellent structural stability. The practicality of the material has been tested with the fabrication of an asymmetric device PLC3//OPC. The device delivers a specific capacitance of 166.2 F/g at 1 A/g, along with specific energy and specific power valued 75.8 Wh/kg and 2131.6 W/kg, respectively. The device demonstrates remarkable capacitance retention of 90% and 100% coulombic efficiency after 12000 continuous cycles. The combined contribution of all materials in the ternary composite leads to superior electrochemical performance, providing an effective strategy for sustainable, economical, and high-performance supercapacitors.

Keywords: Polyaniline; Layered double hydroxides, Biomass, Supercapacitors; Asymmetric device

O0029 • Prof. Narendra Kumar Singh

ICEAM2026-ORAL-0029 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

ROLE OF A-SITE SUBSTITUTION IN THIOSPINEL PHASE OF $\text{CoCo}_2\text{S}_4/\text{rGO}$ WITH NI, CU AND ZN FOR EFFICIENT ELECTROCHEMICAL ENERGY STORAGE AND WATER SPLITTING APPLICATIONS

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Abstract

Understanding how lattice-level electronic modulation governs charge transfer and electrochemical performance is critical for the rational design of advanced electrocatalyst; however, the role of A-site substitution in thiospinel sulphides and its influence on orbital interactions and graphene coupling remains insufficiently explored. In this context, the A-site of $\text{CoCo}_2\text{S}_4/\text{rGO}$ with late 3d transition metals (Nickel (Ni), Copper (Cu) and Zinc (Zn)) via modified Hydrothermal synthetic route. Comprehensive physicochemical analysis, including Rietveld refinement, validated the strong interaction between reduced graphene oxide and transition metal sulphides, elucidating the crystal structure, phase purity, morphology, surface area and pore size determination, and electronic properties of materials. Furthermore, Ni substitution alters the sp^2/sp^3 carbon ratio through charge redistribution, suppressing the D-band and enabling enhanced electron transport.

Among the synthesized nanocomposites, $\text{NiCo}_2\text{S}_4/\text{rGO}$ (GNIS) achieved an impressive specific capacitance of 1919.6 F g^{-1} at 1 Ag^{-1} . It reached a maximum energy density of 66.6 Wh kg^{-1} at 1 Ag^{-1} and power density of 2119.8 W kg^{-1} at 8 Ag^{-1} , respectively. Furthermore, the GNIS electrocatalyst requiring only 243.2 mV and 274 mV overpotentials to achieve a current density of 100 mA cm^{-2} for OER and HER, respectively, along with favourable Tafel slopes of 46.9 and 57 mV/dec, respectively. These results, supported by a low charge-transfer resistance (0.85Ω) and high electrochemical surface area, position GNIS as a high-performance material for integrated energy storage and conversion.

Keywords: Transition metal sulphides, rGO, Rietveld refinement, Specific capacitance, Energy storage.

O0036 • Pariksha Malik

ICEAM2026-ORAL-0036 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

TEMPERATURE-DEPENDENT IONIC TRANSPORT IN GRAPHITE ELECTRODES: AN EIS AND TLM STUDYPariksha Malik¹, Abbas Ali Hor², Sylvain Franger^{3*}¹ICMMO-ERIEE, Université Paris-Saclay, France²ICMMO-ERIEE, Université Paris-Saclay, France³ICMMO-ERIEE, Université Paris-Saclay, France

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¹Present address: Department of Applied Physics, Delhi Technological University, India.**Abstract**

Lithium-ion battery performance is strongly governed by ionic transport through porous electrode architectures, particularly under high-rate operation where electrolyte transport limitations can contribute significantly to cell polarization [1,2]. Electrode tortuosity is a key microstructural parameter describing the complexity of electrolyte transport pathways within porous electrodes and is closely related to their effective ionic conductivity and transport resistance [1,5]. Electrochemical impedance spectroscopy (EIS) combined with symmetric-cell measurements provides a non-invasive approach for evaluating ionic transport in porous electrodes, while transmission line model (TLM) analysis enables the determination of ionic resistance and estimation of electrode tortuosity [1,3,4]. In this work, temperature-dependent EIS measurements were performed on graphite symmetric cells using LP30 electrolyte (1 M LiPF₆ in EC/DEC, 1:1 vol.) to investigate the influence of electrode structure and temperature on ionic transport. Graphite electrode formulations with different mass loadings, thicknesses, and porosities were investigated over a temperature range from 20 to –10 °C. The impedance spectra were analyzed using TLM fitting to determine ionic transport resistance and evaluate the corresponding tortuosity. A systematic increase in impedance was observed with decreasing temperature, reflecting the reduction in electrolyte ionic conductivity and increasingly hindered Li⁺ transport at lower temperatures. The comparative analysis further showed that the electrode with the more favorable porous structure exhibited lower ionic resistance and lower tortuosity despite having a slightly higher mass loading. These results highlight the importance of electrode pore structure and tortuosity in governing ionic transport and demonstrate that optimization of electrode microstructure, rather than mass loading alone, is essential for minimizing transport limitations in graphite electrodes. The study further demonstrates the applicability of temperature-dependent EIS combined with TLM analysis for evaluating ionic transport characteristics of porous battery electrodes [3–5].

Keywords: Lithium-ion batteries; Graphite symmetric cell; Electrode tortuosity; Electrochemical impedance spectroscopy; Transmission line model; Ionic transport; LP30 electrolyte

O0044 • Dr. Raju patel

ICEAM2026-ORAL-0044 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

Binder -Free CuO Nanostructures grown on Nickel Foam for Non-Enzymatic Glucose Sensing and Electrochemical Energy Storage

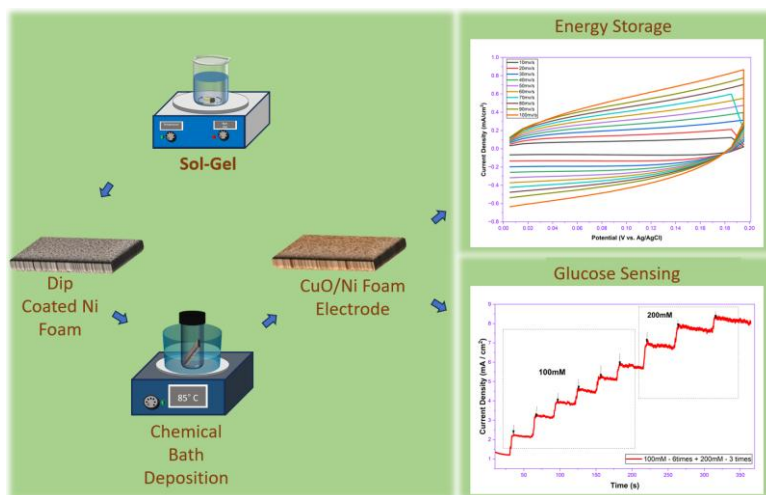
S Jayaprakash¹, Vinuta Shetty², Chandramauleshwar Roy³, Raju Patel^{4*}^{1,2}School of Applied Science, Vellore Institute of Technology Chennai, Chennai, India-600127^{3,4}School of Electronics Engineering, Vellore Institute of Technology Chennai, Chennai, India-600127

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Abstract

CuO nanostructures were directly grown on nickel foam without the binder by two step chemical bath deposition and the electrode is investigated for electrochemical glucose sensing and energy storage application. The porous conductive nickel foam which acts as an excellent current collector supports the growth of CuO nanostructures. This electrochemically active CuO/Ni foam electrode facilitates efficient electron transfer pathways in alkaline electrolytes with enhanced redox activity and charge transfer resistance. The electrodes surface morphology and compositional properties are characterised by SEM and XRD respectively. The electrochemical glucose sensing studies were carried out in alkaline medium revealed excellent response towards glucose. Cyclic voltammetry and chronoamperometry are performed at different concentration of glucose solution and sensitivity and LOD is determined to be $5.33 \text{ mA mM}^{-1} \text{cm}^{-2}$ and $1.51 \mu\text{M}$ respectively. The Selectivity, reproducibility and repeatability is also studied. The electrode demonstrated a significant pseudocapacitive behaviour with high charge storage capabilities which are studied by performing CV, GCD and EIS in the alkaline medium. This study highlights a simple binder free strategy to develop a CuO/Ni foam electrode that supports combined energy storage and non-enzymatic glucose sensing functionalities within a single electrochemical platform.

Keywords: Copper oxide nickel foam electrode, Glucose sensing, Energy storage



00009 • Khushboo Gupta

ICEAM2026-ORAL-0009 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

Cs₂AgBiBr₆ Double Perovskite: A Multifunctional Material for Energy Conversion and StorageKhushboo Gupta^{1*}¹Department of Physics, School of Sciences, IILM University, Greater Noida 201308, Uttar Pradesh, India**Abstract**

Lead-free double perovskites have emerged as promising materials for sustainable energy technologies owing to their favorable structural, electronic, optical, and electrochemical properties. In this study, Cs₂AgBiBr₆ was investigated as a multifunctional material for energy conversion and storage applications. X-ray diffraction with Rietveld refinement and density functional theory calculations confirmed its cubic **Fm $\bar{3}$ m** structure and semiconducting nature. Theoretical and experimental investigations revealed suitable band-gap characteristics, with a calculated band gap of **1.32 eV** and experimentally determined direct and indirect band gaps of **1.84 and 1.71 eV**, respectively, indicating its potential for light-driven energy conversion. In addition, Cs₂AgBiBr₆ exhibited pronounced pseudocapacitive behavior, achieving a specific capacitance of approximately **327 F g⁻¹ at 1 A g⁻¹**. The material delivered an energy density of **29.05 Wh kg⁻¹** at a power density of **800 W kg⁻¹**, demonstrating its potential for electrochemical energy storage. The low series and charge-transfer resistances further indicate favorable charge-transfer kinetics and efficient electrochemical performance. The combination of suitable electronic properties and high charge-storage capability highlights Cs₂AgBiBr₆ as a promising lead-free double perovskite for multifunctional energy conversion and storage systems. The findings also suggest that further optimization through defect engineering, compositional modification, and heterostructure formation could enhance its performance and facilitate the development of stable and efficient next-generation energy devices.

O0047 • Dr. Kapil Kumar

ICEAM2026-ORAL-0047 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

Enhancing Near-Infrared Photo-Response in Sb_2Se_3 Thin Films through Laser-Induced Periodic Surface Structures: Ultrafast Spectroscopy Insights into Carrier Dynamics

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Abstract

The present research delves into creating periodic surface structures on thermally grown Sb_2Se_3 thin film using femtosecond pulse laser technology for various optoelectronic applications. Raman spectroscopy validates the formation of these periodic structures on the Sb_2Se_3 film. The periodic structures formed are HSFL with a calculated periodicity of 400 nm. The structured film demonstrates a significant increase in photocurrent owing to this periodic pattern on the film. We utilise Ultrafast Transient Reflectance Spectroscopy to gain insight into the transient mechanisms linked to the excitation and subsequent relaxation of charge carriers within the structured Sb_2Se_3 film. We conducted an in-depth analysis of charge carrier dynamics using the analysis software Surface Explorer and the Glotaran. The in-depth analysis and insights into surface defects and carrier dynamics play a crucial role in comprehending the potential applications in photovoltaics and optoelectronic devices. Our investigation is centred on exploring carrier concentration, charge transfer properties, and the dynamics of ultrafast carriers. Additionally, confirming the periodicity and orientation of these patterns, scanning electron microscopy and SPIP (Scanning Probe Image Processor) analysis validate our findings. We underscore the advantages of micro/nanofabrication on thin films for optoelectronic devices. However, achieving subwavelength structuring, especially within the optical wavelength range, remains a considerable challenge despite advancements facilitated by femtosecond laser structuring techniques.

Keywords: Thin film; Spectroscopy; Microscopy; Optoelectronic; photocurrent.

P0074 • UZMA AFREEN

ICEAM2026-POSTER-0074 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

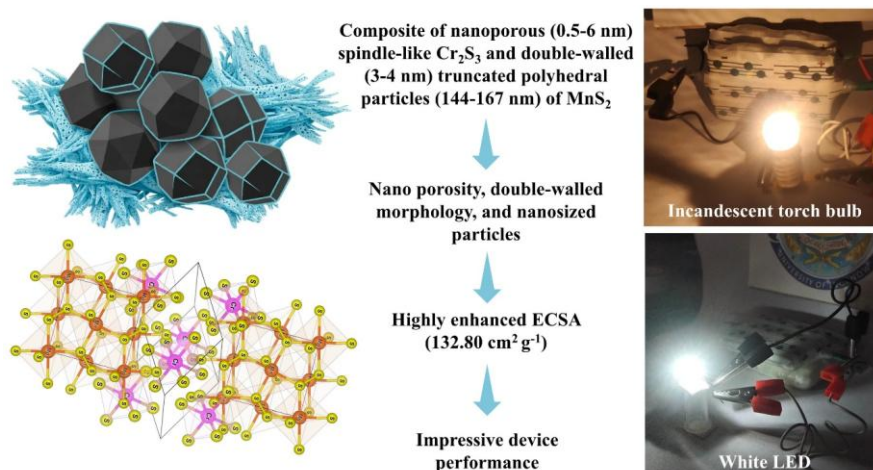
Cr₂S₃@MnS₂ NANOCOMPOSITE: ENHANCED SUPERCAPATTERY PERFORMANCE DRIVEN BY NANO-ARCHITECTURAL MORPHOLOGY**Uzma Afreen, Ushna Afreen, Narendra Kumar Singh***

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Abstract

Modern electronics and electric transportation demand energy storage devices that can simultaneously deliver high energy density and rapid power delivery. The persistent trade-off between the energy density of batteries and the superior power density of supercapacitors has driven intensive research into hybrid energy storage paradigms. Bridging this performance gap stands as a cornerstone goal of modern electrochemical engineering for developing high-performing energy storage technologies. The current study involves the synthesis of Cr₂S₃, MnS₂, and their nanocomposites (Cr₂S₃@MnS₂) in varying weight ratios. Rigorous physicochemical characterization has been performed to validate successful synthesis of the materials. Electrochemical evaluation has been performed in both half-cell and full-cell configurations using 1M KOH electrolyte. The Cr₂S₃@MnS₂ (1:2) nanocomposite, having nanoporous Cr₂S₃ and double-walled truncated polyhedral MnS₂ particles, delivered the best performance amongst the synthesized nanocomposites by delivering the highest specific capacitance (14060.4 F g⁻¹), energy density (372.6 W h kg⁻¹), and power density (2620.8 W kg⁻¹) at a high current demand of 12 A g⁻¹. A supercapattery, fabricated using Cr₂S₃@MnS₂ (1:2) as the cathode material, delivered impressive energy storage. Two supercapatteries in parallel combination successfully powered an incandescent torch bulb and in series combination powered a white LED, providing a solid proof of its practical viability.

Keywords: Cr₂S₃; MnS₂; supercapattery; energy storage; high energy density**GRAPHICAL ABSTRACT**

P0077 • Awanish Gupta

ICEAM2026-POSTER-0077 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

STUDIES ON ION-CONDUCTING POLYMER ELECTROLYTES AND NA/LI BATTERIES

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Abstract

The present thesis focuses on the preparation and characterization of polymer electrolytes (PEs) for sodium-ion batteries (SIBs) and flexible paper-based batteries for lithium-ion battery (LIB) applications. The PEs were successfully prepared, and obtained PEs were free-standing, flexible, and mechanically stable. The prepared PEs exhibited enhanced ionic conductivity and increased amorphous character with increasing salt concentration. The blend of poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and poly(methyl methacrylate) (PMMA) containing NaClO_4 salt and EC: DEC plasticizer demonstrated improved electrochemical performance. To further enhance the electrochemical performance, the 2D material VS_2 was incorporated as an active filler into the gel polymer matrix, resulting in the formation of composite gel polymer electrolytes (CGPEs). The incorporation of VS_2 improved salt dissociation and facilitated ion transport through surface interactions with ClO_4^- anions, thereby enhancing the sodium-ion transference number. The optimized GPE/CGPE exhibited an ionic conductivity of the order of $10^{-3} \text{ S cm}^{-1}$, as and the temperature-dependent conductivity studies. The predominantly ionic conducting nature of the electrolytes was confirmed by DC polarization measurements. Furthermore, the sodium-ion transference number, determined using the combined AC/DC polarization technique. The prepared electrolytes also exhibited a wide electrochemical stability window of approximately 3.5–5.0 V. The fabricated SIB delivered a specific discharge capacity of $\sim 195 \text{ mAh g}^{-1}$ at a current density of 50 mA g^{-1} , with stable cycling performance for up to 100 cycles. In addition, a flexible paper-based battery was successfully developed, demonstrating low weight, mechanical flexibility, and potential applicability in wearable electronic devices. The results presented in this thesis demonstrate that the strategic preparation of GPEs and CGEPs can significantly improve the electrochemical performance, safety, and flexibility of next-generation SIBs/LIBs.

Keywords: Composite gel polymer electrolytes; Sodium-ion batteries; Lithium-ion batteries; Paper-based batteries; energy storage devices.

P0056 • Manoj Goswami

ICEAM2026-POSTER-0056 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

BIOMASS-DERIVED ACTIVATED CARBON/SULPHUR CATHODE AND HYBRID ELECTROLYTE ENGINEERING FOR AQUEOUS ZINC-SULPHUR BATTERIES

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Abstract

Aqueous zinc-sulphur batteries (AZSBs) are promising electrochemical energy storage devices owing to their high theoretical capacity (1675 mAh g^{-1}), cost-effective, zinc abundance, safety, and compatibility with aqueous electrolytes¹. However, the practical application of AZSBs is hindered by the poor electrical conductivity ($1 \times 10^{-15} \text{ S m}^{-1}$), sluggish redox kinetics, side reactions, and hydrophobic nature of sulphur². In this work, biomass-derived activated carbon (AC) with specific surface area of $\sim 769 \text{ m}^2 \text{ g}^{-1}$ was used as additive to encapsulate sulphur within the pores and improve the conductivity. The AC and sulphur composites (AC/S) were prepared by a melt-infiltration method. The electrochemical performance of AC/S composite was investigated in coin-cell configuration (CR2032), in which Zn foil, AC/S composite, and 2M $\text{ZnSO}_4 + 0.5 \text{ wt\% ZnI}_2 + \text{ethylene glycol (EG)}$ were employed as anode, cathode, and electrolyte, respectively. The AC/S composite shows a specific capacity of 450 mAh g^{-1} at 0.1 A g^{-1} of current density in the potential range of 1.4V. This work reveals the role of AC to encapsulate sulphur and hybrid electrolyte engineering to improve the electrochemical performance of AZSBs.

Keywords: Activated Carbon; Sulphur; Hybrid Electrolyte; Zinc-Sulphur Battery, Electrochemistry

P0170 • Dr. Stuti Shrivastava

ICEAM2026-POSTER-0170 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

MACHINE LEARNING BASED APPROACH FOR PREDICTING THE PERFORMANCE OF SUPERCAPACITOR FOR ENERGY STORAGEStuti Shrivastava¹, Amarish Dubey²¹*Electrical and Electronics Engineering, Rajiv Gandhi Institute of Petroleum Technology (Institute of National Importance), Amethi, Uttar Pradesh, India*

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*Keywords: Supercapacitor, Machine learning, Energy Storage, Random Forest, Feature Importance Objectives***Abstract**

The objective of this study is to predict the performance of supercapacitor produced from activated carbon electrode obtained from natural precursors that significantly influence the specific capacitance of supercapacitors. Therefore, the machine learning (ML) is used as tool to recognize the effect of physicochemical features on activated carbon-electrode for prediction the performance of supercapacitor.

Methodology

The comprehensive dataset of supercapacitors that contains important physicochemical features of supercapacitors was compiled from previously published experimental literature. The initial dataset was not in organized form, by doing feature engineering to convert the dataset into more organized form by extracting important features for the prediction. The final dataset formed was utilized to train and validate various machine learning models using train: test split. After model selection, model evaluation is performed using ML performance metrics in which error is calculated between the actual specific capacitance and predicted specific capacitance. The result obtained is used to analyse the correlation between the ML performance and its electrochemical performance

Results

ML model performance: The different ML models were used to predict the performance of supercapacitor by determining its specific capacitance. The four models were used, including Random Forest (RF), Linear regression, Gradient boost and decision tree. Among these, RF demonstrated the best performance by achieving root mean square error (RMSE) of 65.698 and correlation coefficient (R^2) of 0.716, indicating its accuracy in predicting specific capacitance. The feature importance score analysis helps to determine which input feature has the greatest influence on ML model predictions. The SSA ranked highest with the importance score of 0.59, and potential window is the lowest with the importance score of 0.02.

Correlation between prediction results with electrochemical performance: The positive correlation between SSA and specific capacitance depicts that increment in SSA provides more active sites for formation of double layer through electrolyte and electrode interface. The RF model points out that specific capacitance is governed by complex relationship between SSA, pore architecture and operating parameters and conditions

Conclusion

The implementation of ML models offers significant benefits in the field of energy storage research. These models can accelerate the innovation, fabrication and development process of making energy storage devices by reducing both cost, time and effort needed in experimental process.

P0193 • JITENDRA KUMAR YADAV

ICEAM2026-POSTER-0193 | Oral Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT4 (Best Thesis)

Boosting Iron-Ion Battery Performance with Porous Carbon Aerogel as High-Rate Charge/Discharge Cathode

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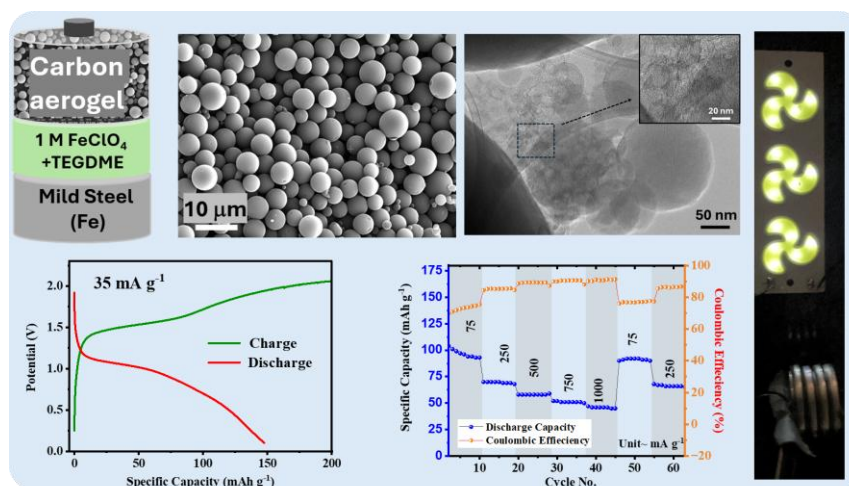
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Abstract

Iron-ion batteries are emerging as a sustainable alternative to conventional rechargeable batteries; however, their cathode development is hindered by sluggish Fe-ion diffusion, limited conductivity, and interfacial instability. Addressing these challenges requires designing cathode materials with high conductivity, large surface area, and stable electrochemical interfaces. In this work, we explore carbon aerogel-based cathodes to overcome these limitations and enhance Fe-ion storage performance. Highly porous carbon aerogel (CA) is used as the cathode material, synthesized using the sol-gel process and confirmed using Transmission Electron Microscopy, Field Emission Scanning Electron Microscopy, X-ray Diffraction, and Brunauer-Emmett-Teller measurements. Detailed cyclic voltammetry (CV) is investigated at different scan rates to understand the characteristics of the Fe-ion storage in carbon aerogel hosts during cycling. The galvanostatic charging-discharging (GCD) is determined at various current densities, showing a high discharge capacity of $\sim 150 \text{ mAh g}^{-1}$ and $\sim 45 \text{ mAh g}^{-1}$ at 35 mA g^{-1} and 1000 mA g^{-1} discharge current densities, respectively. The capacity retention is more than $\sim 60\%$, with more than 85% coulombic efficiency after 750 cycles at 1000 mA g^{-1} , and fast charge-discharge characteristics of $\sim 18\text{C}$ rate. The galvanostatic intermittent titration technique (GITT) measurements were also performed to check the diffusion characteristics of the Fe-ion during charging and discharging. A digital clock and 5V light-emitting diode are connected to CA-based Fe-ion coin cells to demonstrate the potential of iron-ion batteries. A detailed electrochemical impedance spectroscopy and post-mortem measurements before and after the GCD cycling suggest a slight degradation of electrochemical performance, which is attributed to the oxidation of the anode during cycling^{1,2}.

Keywords: Carbon aerogel cathode; Mild steel anode; Impedance analysis; Iron-ion battery; GITT analysis.

GRAPHICAL ABSTRACT



P0122 • Shashi Kant Mohapatra

ICEAM2026-POSTER-0122 | Oral Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

ANNEALING DRIVEN ALTERATION IN PHASE STRUCTURE AND MAGNETIC PROPERTY OF MECHANICALLY ALLOYED $\text{Co}_{35}\text{Fe}_{10}\text{Ni}_{30}\text{Ti}_{20}\text{Al}_5$ HIGH ENTROPY ALLOY

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Abstract

High entropy alloys (HEAs) have attracted great research interest due to their innovative compositional design strategy and extraordinary functional properties. Recently, we found an optimized $\text{Co}_{35}\text{Fe}_{10}\text{Ni}_{30}\text{Ti}_{20}\text{Al}_5$ HEA with excellent soft magnetic properties. In the present study, we have synthesized $\text{Co}_{35}\text{Fe}_{10}\text{Ni}_{30}\text{Ti}_{20}\text{Al}_5$ HEA through mechanical alloying. The as-synthesized sample possessed a major fcc and a minor bcc phase. The thermal stability of the synthesized sample was investigated through vacuum annealing the synthesized sample at different temperatures (500, 700, 900 and 1000°C) for 2 hr. After annealing, it was found that the as-synthesized phase structure remained stable up to 900°C whereas 1000°C annealed sample possessed an fcc phase while bcc phase completely disappeared. In the as-synthesized state, the value of M_s and H_c was found to be 80 emu/g and 28 Oe respectively. For 500, 700, 900 and 1000°C, the value of M_s was found to be 108, 99, 97, 94 emu/g respectively and H_c was found to be 24, 22, 3 and 1 Oe respectively. After annealing, it can be seen that the value of M_s and H_c of the as-synthesized sample changed significantly as compared to the as-synthesized sample. The discussion behind the change in the magnetic property after annealing will be discussed in detail during the presentation.

Keywords: High Entropy Alloys, Mechanical Alloying, Annealing, Magnetic properties

P0155 • Mohammed Kolo

ICEAM2026-POSTER-0155 | Oral Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Interfacial Engineering of Fe-Doped V_2O_5 @HKUST-1 MOF Nanocomposites for Enhanced Oxygen Evolution and Supercapacitive Energy Storage

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Abstract

The slow kinetics of the oxygen evolution reaction (OER) in alkaline water electrolysis remains a significant barrier for the development of this technology and low-cost non-precious metal electrocatalysts are needed. The conductivity of vanadium pentoxide (V_2O_5) is low and the number of active sites is small, although it has a layered orthorhombic structure and multivalent ($V^{5+}/V^{4+}/V^{3+}$) redox chemistry. In the present work, Fe-doped V_2O_5 was template grafted onto a Cu-based metal–organic framework (HKUST-1) at three different mass ratios (V2, V3, V4) to increase density of active site, conductivity and stability. Phase purity of the orthorhombic lattice was confirmed by XRD after Fe doping. The 1:1 Fe– V_2O_5 @MOF composite (V2) exhibited the highest OER activity of all compositions, with an overpotential of 261.4 mV at 10 mA cm⁻² and a Tafel slope of 22.59 mV dec⁻¹, which also outperformed the binary Fe– V_2O_5 and benchmark RuO₂. Cyclic voltammetry results showed quasi-rectangular cyclic voltammograms on V2 with more reversible vanadium redox characteristics and the highest voltammetric charge compared to all the samples, indicating that the charge-storage mechanism was a combination of double-layer and pseudocapacitive mechanism, which made V2 highly potential as a supercapacitor electrode. This places the optimized Fe– V_2O_5 @MOF composite to be a good bifunctional material for energy storage and water splitting.

Keywords: V_2O_5 ; Fe doping; metal–organic framework; oxygen evolution reaction; pseudocapacitance; supercapacitor



Poster Presentations

126 Papers • 4 Sessions



Poster Session I

ACS Sustainable Resource Management (Day 1, 08 Oct 2026) • 17 Posters

P0006 • Aliya Siddiqua

ICEAM2026-POSTER-0006 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

SYNTHESIS OF ANATASE TITANIUM DIOXIDE NANOPARTICLES HAVING TAILORED BAND GAP FOR VISIBLE LIGHT DRIVEN PHOTOCATALYTIC APPLICATIONSAliya Siddiqua¹, Onkar Mangla^{1,*}, Neeru Sehdev¹, Arti Jain²¹*Department of Physics, Daulat Ram College, University of Delhi, Delhi-110007, INDIA*²*Department of Chemistry, Daulat Ram College, University of Delhi, Delhi-110007, INDIA*

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Abstract

In this study, a green sol–gel approach was employed to synthesize anatase TiO₂ nanoparticles using the leaf extracts of Aloe vera (*Aloe barbadensis*), Neem (*Azadirachta indica*), and Jamun (*Syzygium cumini*) as natural stabilizing agents. Structural analysis using X-ray diffraction (XRD) and Raman spectroscopy confirmed the formation of a pure anatase phase in all three samples. XRD results further revealed that the average crystallite size was largest for Aloe vera (~35 nm) and smallest for Jamun (~20 nm) stabilized TiO₂ nanoparticles. Scanning electron microscopy revealed well-defined quasi-spherical nanoparticles with clean surfaces for the Aloe vera sample, whereas the Neem and Jamun samples exhibited highly agglomerated structures embedded in a dense amorphous organic matrix. Optical investigations using UV–Vis absorption spectra revealed an extended absorption tail into the visible region for the Neem- and Jamun-stabilized variants. Photoluminescence spectra further revealed broad defect-related emissions, with red-shifted features observed for the Neem- and Jamun-stabilized samples, suggesting the presence of surface and defect states associated with phytochemical-derived residues. The comparative analysis indicates that the phytochemical composition of the plant extracts influences the structural and optical properties of TiO₂ nanoparticles, as reflected in the observed differences in crystallite size, surface morphology, visible-light absorption, and defect-related emissions. The results therefore demonstrate that the choice of plant extract affects the characteristics of the synthesized TiO₂ nanoparticles and provides a basis for comparing different phytochemical-mediated stabilization routes. Among the three samples, Jamun-stabilized TiO₂ exhibited the most pronounced extension of absorption into the visible region, highlighting its potential for visible-light-driven photocatalytic applications.

Keywords: Green synthesis; TiO₂ nanoparticles; phytochemical stabilization; optical band gap; visible-light absorption.

P0024 • Aisha

ICEAM2026-POSTER-0024 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

The structural, spectroscopic and functional investigation of nanostructured copper sulfide-mancozeb conjugates for enhanced antifungal activity for agriculture.Aisha^{1,*}, Anil Kant², Ragini Raj Singh¹¹*Nanotechnology Laboratory, Department of Physics and Materials Science, Jaypee University of Information Technology, Waknaghat, Solan, Himachal Pradesh, India, 173234*²*Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Waknaghat, Solan, Himachal Pradesh, India, 173234*

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Abstract

The development of efficient and environmentally responsible strategies for controlling fungal diseases is essential for sustainable agriculture. This work presents a novel copper sulphide-mancozeb (CuS-M) nanoconjugate system that consists of copper sulfide (CuS) nanoparticles conjugated with the mancozeb fungicide (M) and aim is to study the change in its structural, physicochemical and antifungal changes resulting from their conjugation. CuS-M nanoconjugates were prepared by a wet-chemical method and their characterization was done by X-ray diffraction (XRD), dynamic light scattering (DLS), UV-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, and transmission electron microscopy (TEM). Characterization tests confirmed that surface modification and CuS-mancozeb interaction were successful. Zeta-potential analysis indicates that CuS-M showed better colloidal stability than bare CuS nanoparticles. The UV-visible spectroscopy showed that after conjugation the optical band gap increases from 1.94 eV to 2.08 eV indicating modification of the electronic environment. FTIR analysis indicates characteristic peak shifts and the formation of new bonding interactions between the dithiocarbamate groups of mancozeb and the surface Cu²⁺ sites of CuS. Results from TEM and DLS analyses indicate a reduced particle size and better dispersion of the nanoconjugate. Antifungal testing against *Aspergillus flavus* nanoconjugate (CuS-M) showed approximately 1.5, 2, and 2.4-fold higher efficacy than physical mixture of CuS+M, mancozeb, and CuS nanoparticles respectively. The study showed that effectiveness of nanoconjugate was significantly greater than efficacy of other treatments. As a whole, it is the interfacial interaction between CuS and mancozeb that enabled the enhanced antifungal performance and revealed CuS-M as a nano-enabled, efficient, and sustainable tool for disease management respectively.

Keywords: Copper sulfide nanoparticles; Mancozeb; Nanoconjugate; Antifungal activity; Sustainable agriculture.

P0059 • Nilam Kumari

ICEAM2026-POSTER-0059 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

GREEN SYNTHESIS OF SILVER NANOPARTICLES FOR EFFICIENT AND ULTRA-TRACE DETECTION OF Cr(VI)

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Abstract

Wastewater contamination by toxic heavy metals has become a major environmental concern due to rapid industrialization and the discharge of untreated industrial effluents into aquatic ecosystems. In the present work, silver nanoparticles (AgNPs) were synthesized through a green and eco-friendly approach using glucose as both a reducing and stabilizing agent for the efficient ultra-trace colorimetric detection of Cr(VI). The synthesized glucose-stabilized silver nanoparticles (Ag@DNPs) were characterized using Fourier-transform infrared spectroscopy (FTIR), ultraviolet-visible (UV–Vis) spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and selected area electron diffraction (SAED). The FTIR spectrum confirmed the involvement of hydroxyl and carbonyl-containing functional groups of glucose in the reduction of Ag⁺ ions and stabilization of the synthesized nanoparticles. TEM analysis revealed the formation of predominantly spherical and well-dispersed nanoparticles, while the SAED pattern confirmed their crystalline nature. SEM observations demonstrated a rough and granular morphology with nanoparticle aggregation. The UV–Vis spectrum exhibited a characteristic surface plasmon resonance (SPR) band associated with the formation of silver nanoparticles.

The synthesized Ag@DNPs were subsequently investigated as a colorimetric sensing platform for the detection of Cr(VI) ions using potassium dichromate as a model analyte exhibiting limit of detection as 160 ppm in a wide range of concentration 160 ppm to 500 nanomolar. The interaction between Cr(VI) ions and Ag@DNPs is attributed to the interaction of Cr(VI) with the AgNP surface, leading to changes in the electronic and local dielectric environment of the nanoparticles and consequent modulation of their SPR properties. These results can be used for the development of portable paper-based or smartphone-assisted sensing platforms which can enhance the practical applicability of Ag@DNPs for rapid, on-site monitoring of Cr(VI) and other hazardous pollutants.

Keywords: Wastewater treatment, Colorimetric sensing, Silver nanoparticle, Cr(VI) detection, Green Synthesis.

P0061 • Sandhya Devi

ICEAM2026-POSTER-0061 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

GREEN-SYNTHESIZED C₃N₅–ZnO HYBRID NANOPARTICLES AS EFFICIENT PHOTOCATALYSTS FOR SUNLIGHT-INDUCED DEGRADATION OF ORGANIC DYESSandhya Devi^{1,2}, Radhe Shyam³, Dhananjay^{1,2}, Nilam Kumari^{1,2}, Rajiv Prakash⁴, Akhilesh Kumar Singh⁴, Madhu Tiwari^{1*},¹*Department of Chemistry, N. S. P. S. Govt. P. G. College, Magaraha, Mirzapur-231306, India*²*Department of Chemistry, Science and Technology Centres, Mahatma Gandhi Kashi Vidyapith, Varanasi-221002, India*³*Graduate School of Science and Technology and Faculty of Engineering, Niigata University-8050 Ikarashi 2-nocho, Nishi-ku, Niigata-950-2181, Japan*⁴*School of Materials Science & Technology, IIT (BHU), Varanasi-221005, India*

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Abstract

The increasing discharge of synthetic dyes into aquatic environments has created a significant need for efficient and environmentally sustainable approaches for wastewater treatment. In the present study, C₃N₅–ZnO hybrid nanoparticles were synthesized through both green and conventional chemical approaches and investigated as sunlight-responsive photocatalysts for the degradation of Reactive Black dye in aqueous solution. The synthesized nanomaterials were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), and UV–Visible spectroscopy to investigate their crystalline structure, surface functional groups, morphology, and optical properties. TEM analysis of the green-synthesized material revealed nanoparticles morphology. The photocatalytic performance of both C₃N₅–ZnO hybrid nanoparticles were evaluated under natural sunlight, and the degradation process was monitored using UV–Visible spectrophotometry. The green-synthesized C₃N₅–ZnO hybrid nanoparticles achieved approximately 80% degradation of Reactive Black dye under the investigated conditions, whereas the chemically synthesized counterpart exhibited approximately 60% degradation. The superior photocatalytic performance of the green-synthesized material may be attributed to the synergistic interaction between C₃N₅ and ZnO, which facilitates charge separation and suppresses electron–hole recombination during solar irradiation, together with favorable surface characteristics imparted by the green synthesis route. The comparative results demonstrate that the green synthesis approach provides a more environmentally sustainable route for preparing C₃N₅–ZnO hybrid nanoparticles and results in enhanced photocatalytic degradation efficiency compared with the conventional chemical synthesis route. These findings highlight the promising potential of green-synthesized C₃N₅–ZnO hybrid nanoparticles for effective sunlight-assisted treatment of dye-contaminated wastewater.

Keywords:

C₃N₅–ZnO hybrid nanoparticles; Green synthesis; Reactive Black dye; Photocatalytic degradation; Sunlight irradiation; Nanoparticles; Wastewater treatment; Solar photocatalysis.

P0063 • Sarita singh

ICEAM2026-POSTER-0063 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

AGROWASTE-BASED HYBRID CARBON NANOSTRUCTURES FOR HIGHLY EFFICIENT REMOVAL OF DYES FROM CARPET INDUSTRY WASTE WATERSarita Singh^{1,2}, Nilam Kumari^{1,2}, Dhananjay^{1,2} Madhu Tiwari^{1,2*}, Rajiv Prakash³, Rajesh Kumar Upadhyay⁴¹*Department of Chemistry, N. S. P. S. Govt. P. G. College Magaraha, Mirzapur, Uttar Pradesh-231306, India*²*Department of Chemistry, Science and Technology Centres, Mahatma Gandhi Kashi Vidyapith, Varanasi-221002, India*³*School of Materials Science & Technology, IIT (BHU), Varanasi-221005, India*⁴*Department of Chemical Engineering, IIT (BHU), Varanasi-221005, India*

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Abstract

The development of sustainable adsorbent materials from agricultural waste has attracted increasing attention for wastewater remediation. In this work, two hybrid carbon nanostructures were synthesized from sugarcane bagasse; one through pyrolysis followed by alkaline activation and another surface functionalization using benzophenone-3,3',4,4'-tetracarboxylic dianhydride (BTDA). The prepared materials, including raw sugarcane bagasse (SB), BTDA-modified bagasse (BTDA-SB), and NaOH-activated biochar (SCB-BC-1), were evaluated for the removal of cationic dyes such as malachite green (MG) and crystal violet (CV) from aqueous solutions. Structural and surface properties of the adsorbents were characterized using FTIR, SEM, TEM, BET surface area analysis, XRD, zeta potential measurements, and EDX spectroscopy. The modified biochar exhibited enhanced porosity and abundant oxygen-containing functional groups, resulting in significantly improved adsorption performance. Kinetic analysis indicated that both the adsorption followed a pseudo-second-order model, suggesting chemisorption as the dominant mechanism. Isotherm analysis also demonstrated better agreement with the Langmuir model in both the adsorption, indicating monolayer adsorption behavior. Adsorption experiments revealed rapid dye uptake with equilibrium capacities reaching up to 270.31 mg g⁻¹ for MG and 150.10 mg g⁻¹ for CV with SCB-BC-1 indicating SCB-BC-1 as a superior adsorbent. Real wastewater experiments confirmed the effectiveness of the prepared adsorbents even in complex matrices. These findings demonstrate that both engineered agrowaste-derived hybrid carbon nanostructures represent promising low-cost and environmentally sustainable materials for the treatment of dye contaminated industrial waste water.

Keywords: Agrowaste valorisation; Modified biochar; Surface functionalization; Malachite green; Crystal violet; Adsorption isotherm.

P0064 • Dhananjay

ICEAM2026-POSTER-0064 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

ENHANCED SOLAR-DRIVEN PHOTOCATALYTIC DYE DEGRADATION USING ENGINEERED C_3N_5 NS @PdDhananjay^{1,2}, Sarita Singh^{1,2}, Sandhya Devi^{1,2}, Rajiv Prakash³, Akhilesh Kumar Singh³, Madhu Tiwari^{1*}.¹Department of Chemistry, N. S. P. S. Govt. P. G. College, Magaraha, Mirzapur-221306, U.P., India²Department of Chemistry, Science and Technology Centres, Mahatma Gandhi Kashi Vidyapith, Varanasi-221002, India³School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India

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Abstract

The generation and development of metal-free and metal-modified photocatalysts with enhanced activity and their efficiency in environmental remediation remains a central challenge in the scientific studies. In this study, a systematic and well organised synthesis as well as comparative evaluation of graphitic carbon nitride-based material such as pure C_3N_5 (P- C_3N_5), exfoliated nanosheet of graphitic carbon nitride (C_3N_5 NS), and palladium-doped C_3N_5 nanocomposites (C_3N_5 NS @Pd) has been carried out for the effective-efficient degradation of hazardous azo dyes (Methyl Orange and Congo Red) in aqueous systems. The Pure C_3N_5 was synthesized via controlled thermal polymerization and followed by a top-down exfoliation approach to obtain ultrathin 2D Nanosheets with increased surface area and active sites. The subsequent incorporation of Pd metal Nanoparticles was achieved through a facile chemical reduction route which ensured the uniform dispersion and strong interfacial interaction with the C_3N_5 matrix. The structural, morphological and optical analyses confirm the successfully formation of photocatalyst. The Pd NP decorated C_3N_5 Nanosheets is improved light absorption and suppressed charge carrier recombination. Amongst the synthesized material C_3N_5 NS @Pd exhibited advanced and superior photocatalytic performance which attributed to synergistic effects of Nanosheets morphology and Pd NP induced charge separation enhancement. Under the Solar irradiation the Pd doped nanocomposite demonstrated rapid and highly efficient degradation of dyes (Methyl Orange, Congo Red). This research represented the critical role of structural engineering and noble metal doping on C_3N_5 system. The specified C_3N_5 NS @Pd offering effective-efficient, robust and reusable Photocatalyst for the treatment of dye-contaminated wastewater.

Keywords: Graphitic carbon nitride; 2D Nanosheet; Nanocomposites; Nanoparticles; Thermal polymerization; Exfoliation; Degradation; Hazardous dye;

P0066 • Tagamud Tazmeen

ICEAM2026-POSTER-0066 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

TURBOSTRATIC CARBON FROM CEDRUS DEODARA CONE AS A LOW-COST MICROBIAL FUEL CELL BIOANODE FOR SIMULTANEOUS WASTEWATER REMEDIATION AND BIOELECTRICITY GENERATION

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Abstract

Deodar cone (*Cedrus deodara*) biochar (ADC) is, to our knowledge, investigated for the first time as a microbial fuel cell (MFC) bioanode. Its performance was evaluated using a mechanistic electrochemical framework. Deodar cones were pyrolyzed at 750 °C, activated with KOH, and further characterized using various physicochemical and electrochemical methods, before testing as an anode in a dual-chamber MFC. Characterization revealed a turbostratic carbon structure ($d_{002} = 0.392$ nm, $L_c = 0.91$ nm, $N_l = 2.3$ layers, $ID/IG = 0.211$) with hierarchical mesoporosity ($SBET = 92.6$ m²·g⁻¹; $V_p = 0.0615$ cm³·g⁻¹; $r_{avg} = 14.09$ Å). Three-electrode analysis yielded $C_s = 82.2$ mF·g⁻¹ (5 mV·s⁻¹), $R_s = 1.81$ Ω, $R_{ct} = 1.74$ Ω, with C' decreasing from 363.8 μF (0.1 Hz) to 22.6 μF (1 kHz; 6.2% retention). b-value analysis (mean $b = 0.791$) and Dunn-method separation indicated mixed capacitive/diffusion kinetics, the capacitive contribution rising from 53% to 76% (5-40 mV·s⁻¹). The scan-rate-independent $q_a/q_c = 6.8$ is consistent with rate-independent, surface-confined Faradaic oxidation. In a dual-chamber MFC, ADC achieved $P_{max} = 58.5$ mW·m⁻² (0.65 mW·g⁻¹), open-circuit voltage (OCV) = 0.816 V, chemical oxygen demand (COD) removal = 80.36%, Coulombic efficiency (CE) = 7.83%, normalized energy recovery (NER) = 20.5 Wh·m⁻³, and energy conversion efficiency $\eta = 1.73\%$. These results indicate the deodar cone as a viable biomass for low-cost MFC anodes.

Keywords: Microbial fuel cell; *Cedrus deodara*; KOH activation; energy conversion efficiency; biochar anode; COD removal

P0109 • Nityanutan Mohapatra

ICEAM2026-POSTER-0109 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Sustainable In-Situ Synthesis of Indian Loofah-Derived Activated Carbon/Bismuth Ferrite Composite for Enhanced Electrochemical Energy Storage

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Abstract

The development of sustainable and high-performance electrode materials is essential for advancing next-generation supercapacitor technologies. In this study, a biomass-derived activated carbon (AC)-Bismuth ferrite (BFO) composites were synthesized through an in-situ hydrothermal approach and investigated as an electrode material for supercapacitor applications. Activated carbon derived from loofah biomass was integrated with BFO at different compositions (wt %) to exploit the complementary properties of the conductive carbon framework and the redox-active BFO phase. Structural and morphological characteristics were investigated using X-ray diffraction (XRD), Raman spectroscopy, and field-emission scanning electron microscopy (FE-SEM) and X-ray Photoelectron Spectroscopy (XPS). The electrochemical behaviour was evaluated using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The incorporation of AC substantially modified the morphology and interfacial characteristics of BFO, enhanced the concentration of defect-associated oxygen vacancies, thereby resulting in enhanced electrochemical activity compared with pristine BFO. The electrochemical behaviour of BiFeO₃ improved significantly on forming composites, especially, the composite with 3 wt.% of AC (ACBFO-3). In particular, ACBFO-3 composite exhibited a higher specific capacitance of 1539 F/g (@1 mV/s) as compared to the pristine BFO i.e. 695 F/g (@1 mV/s) with enlarged CV areas, wide potential window and enhanced Bi- and Fe-associated redox responses, indicating improved charge-transfer characteristics and greater utilization of electrochemically active sites. The synergistic interaction between the conductive biomass-derived carbon and redox-active BFO provides an effective strategy for improving charge-storage performance. These findings demonstrate the potential of biomass-derived AC-BFO in-situ composites as sustainable electrode materials for high-performance supercapacitors.

Keywords: Supercapacitor, Bismuth ferrite, Biomass, Activated-carbon, Composites

P0133 • Neelesh Kumar Mishra

ICEAM2026-POSTER-0133 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Sustainable Synthesis of Graphene Nanosheets from Rice Husk Agro-Waste: Structural and Morphological CharacterizationNeelesh Kumar Mishra¹, Sandhya Devi¹, Thakur Prasad Yadav² and Kalpana Awasthi^{1*}¹*Department of Physics, Kashi Naresh University, Bhadohi-221304, India*²*Department of Physics and Astrophysics, University of Delhi, Delhi-110007 India*

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Abstract

The discovery of a new class of two-dimensional (2D) carbon-based nanomaterials has brought together researchers from chemistry, physics, materials science, and engineering to explore their remarkable potential for a wide range of modern technological applications. Among these materials, the graphene family has attracted considerable attention owing to its unique structural, electronic, optical, mechanical, and physicochemical properties, as well as its broad applicability in areas such as electronics, energy storage, catalysis, sensing, and biomedical devices. Recently, considerable efforts have been devoted to developing green and sustainable approaches for the synthesis of graphene-based materials using environmentally friendly and renewable biomass resources. In this context, agricultural wastes represent promising precursors because of their abundance, low cost, renewability, and potential to address environmental challenges associated with waste disposal. In the present study, rice husk agro-waste was employed as a renewable precursor for the eco-friendly synthesis of graphene nanosheets. The utilization of rice husk not only provides a cost-effective and sustainable carbon source but also contributes to agricultural-waste management, resource conservation, and the development of value-added materials from waste biomass. Graphene nanosheets were synthesized through the carbonization of rice husk, followed by pyrolysis treatment with ferrocene at 350 °C under a muffle furnace atmosphere. The structural, morphological, and vibrational characteristics of the as-prepared graphene nanosheets were investigated using Fourier-transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), transmission electron microscopy (TEM), and Raman spectroscopy. The combined characterization results provide insights into the structural features and morphology of the synthesized graphene nanosheets. This study demonstrates the potential of agro-waste-derived graphene nanosheets as sustainable and versatile carbon nanomaterials for a variety of emerging technological applications. The proposed approach offers an environmentally responsible route for converting abundant agricultural waste into value-added nanomaterials, thereby contributing to both resource conservation and the advancement of sustainable nanotechnology.

Keywords: Graphene nanosheets, Rice Husk, Pyrolysis, Cost-effective.

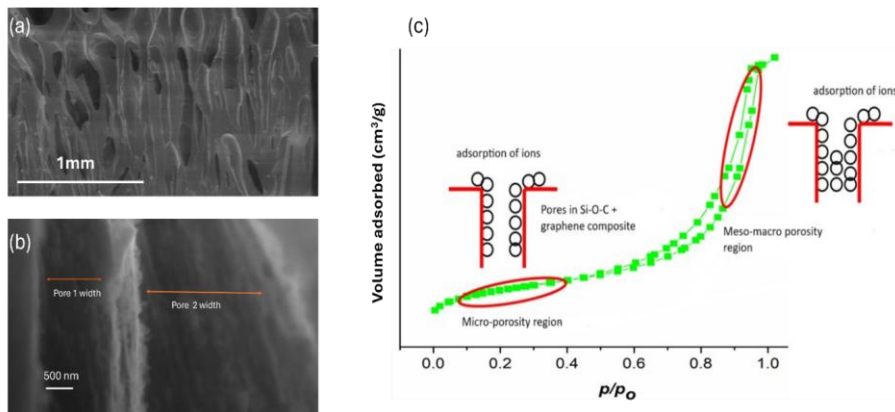
P0160 • Pawan Kumar Chauhan

ICEAM2026-POSTER-0160 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

HOUSEHOLD WATER PURIFICATION VIA CAPACITIVE DEIONIZATION: ROLE OF Si–O–C/GRAPHENE COMPOSITE ELECTRODESPawan Kumar Chauhan¹, Abhinav Adarsh², Raju Patel^{3*}^{1,2}*Department of Advanced Computer Science and Engineering, Vignan's Foundation for Science, Technology and Research (Deemed to be University), Yadadri Buvanagiri, Hyderabad, Telangana- 508284, India*³*School of Electronics Engineering, Vellore Institute of Technology, Chennai, India-600127**Corresponding author email-raju.patel@vit.ac.in**Abstract**

The contamination of fresh drinking water has become a major global challenge. It has been driven primarily by the rapidly growing population and unregulated industrial activities, which eventually leads to unacceptable rise in total dissolved solids (TDS) levels. In the present work, we review various household water purification technologies currently available in the market like Reverse Osmosis (RO), activated carbon filters technology and Ultraviolet disinfection. Further, we examine the status of a potentially sustainable, drinking water purification technology called Capacitive Deionization (CDI), focusing on its operational requirements and the challenges hindering its widespread adoption. Further, in response to the challenges being faced by CDI, we propose a novel hierarchically porous composite material based on silicon oxycarbide (Si–O–C) and graphene, which offers excellent thermal and chemical stability. Also, strategies to enhance performance of Si–O–C-based material, its tentative working methodology and its long-term sustainability in household water purification application have been discussed.

Keywords: Capacitive Deionization, Porous Silicon Oxycarbide Ceramics, Graphene, Electrode Materials



P0165 • AMIT TIWARI

ICEAM2026-POSTER-0165 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Eco-Friendly Synthesis of Eucalyptus-Mediated Silver Nanoparticles: Physicochemical Characterization and Potential ApplicationsAmit Tiwari¹, J. P. Singh¹, Sweta Shukla², Dharendra Kumar Sharma²¹*Uttar Pradesh Textile Technology Institute, Souterganj, Kanpur, INDIA*²*Krishna institute of Engineering & Technology (KIET), Ghaziabad, Delhi-NCR, Uttar Pradesh, INDIA***Abstract**

The plant-derived approach to green synthesis of metallic nanoparticles has become an alternative sustainable and cost-effective approach to the conventional chemical and physical synthesis routes. In this study, silver nanoparticles (AgNPs) were synthesized with the aim of using Eucalyptus leaves as a natural reducing and stabilizing agent. The phytochemicals in Eucalyptus leaves, such as phenolics, flavonoids, terpenoids and other bioactive compounds, promote the reduction of Ag⁺ ions and stabilization of the resulting nanoparticles. Presence of AgNPs were initially suggested by the colour of the reaction mixture, supported by spectroscopic and structural characterization. The presence of AgNPs was confirmed by the appearance of a characteristic surface plasmon resonance band at ~ 440 nm with the aid of UV–Visible spectroscopy. The crystallinity of the prepared nanoparticles was confirmed by X-ray diffraction analysis, which showed strong diffraction peaks at 38.1°, 44.3° and 64.4° 2θ, typical of the crystal planes of face-centered cubic (FCC) silver. Scanning electron microscopy showed the size of the particles to be mostly in the nanoscale range (32-80 nm) with relative uniformity. Energy-dispersive X-ray spectroscopy (EDX) also verified that the main element was silver, which was further confirmed by the presence of carbon linked to the phytochemical residues of the plant extract. The results show that the synthesized AgNPs using the Eucalyptus leaf extract are an efficient and environmentally friendly method that does not involve the use of conventional chemical reducing agents for crystalline AgNPs. The synthesized nanoparticles have potential applications in antimicrobial coatings, functionalized textiles, environmental remediation, wastewater treatment, and biomedical technologies, which can be evaluated further for specific applications.

Keywords: Green synthesis; Silver nanoparticles (AgNPs); Eucalyptus leaf extract; Surface plasmon resonance; Nanomaterials characterization

P0173 • Yash Srivastava

ICEAM2026-POSTER-0173 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Sustainable Valorization of Biomass Waste into Activated Carbon for Supercapacitor Applications: Integrated Electrochemical, Life-Cycle, and Techno-Economic AssessmentYash Srivastava¹, Prasenjit Mondal¹¹ *Department of Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand 247667, India***Abstract**

This study investigates the conversion of algae, waste pine needles, and spent coffee grounds into activated carbon for sustainable supercapacitor applications. The biomass-derived chars were pyrolyzed and chemically activated to develop porous carbon electrodes, followed by electrochemical evaluation using cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. A life-cycle assessment (LCA) was performed to quantify the environmental impacts associated with biomass conversion, activation, washing, and electrode fabrication, while techno-economic analysis (TEA) was used to evaluate process costs and economic feasibility. The integrated assessment compares the three biomass-derived activated carbons based on their electrochemical performance, environmental footprint, and economic viability, providing insights into the development of sustainable and cost-effective biomass-based supercapacitor electrodes.

Keywords: Supercapacitors; Life cycle assessment, Technoeconomic assessment;

P0176 • NITESH KUMARI

ICEAM2026-POSTER-0176 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

PREPARATION OF TiO₂/MoS₂ NANOHYBRID FOR EFFICIENT REMOVAL OF ORGANIC POLLUTANT UNDER VISIBLE LIGHTNitesh Kumari¹, Jaspal Singh¹¹ *Department of Physics, Akal University, Talwandi Sabo, Bathinda, Punjab, India*

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Abstract

Designing semiconductor heterostructures with improved optical response and interfacial charge-transport characteristics is a promising approach for developing photocatalytic materials. In this work, anatase TiO₂ nanostructures and their MoS₂-incorporated heterostructures were synthesized using a hydrothermal synthesis method to produce MoS₂/TiO₂ nanohybrid and then studied the effect of two-dimensional MoS₂ addition on the structural and optoelectronic properties of TiO₂. Anatase TiO₂, MoS₂ and TiO₂/MoS₂ nanohybrid samples were characterized using Raman spectroscopy, SEM and TEM to investigate their structural and morphological properties. The coupling of MoS₂ with TiO₂ and the morphology of the resulting nanohybrid were further examined using microscopic and spectroscopic techniques. UV-Visible spectroscopy was performed to study the optical response of the materials, while photoluminescence measurements were used to understand the behaviour of photoinduced charge carriers and their recombination rate. The incorporation of MoS₂ influenced the light-harvesting ability of TiO₂ and promote interfacial charge transfer within the heterostructure. Thus, the TiO₂/MoS₂ nanohybrid almost diminished the rhodamine dye in 120 min under visible light source as compared to the pristine samples.

Keywords: MoS₂; TiO₂; Heterostructures; Nanohybrids; Photocatalysis

P0183 • Nikhil Ashok Bodhare

ICEAM2026-POSTER-0183 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

BLACKMASS COMPOSITE MATERIAL AS AN EFFICIENT OER CATALYST IN ALKALINE MEDIUMNikhil Bodhare¹, Neetu Jha²,¹ *Institute of Chemical Technology, Matunga, Mumbai*

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Abstract

Water splitting has emerged as the promising method for generating hydrogen, however there is a need to develop low cost non-noble electrocatalyst to reduce the cost. Here we have used the battery waste material as the catalyst and prepared composite material with biomass derived carbon to reduce the cost and improve the performance of Oxygen Evolution Reaction. The composite of black mass and activated carbon derived from biomass shows improved OER performance and lower tafel slope indicating improved kinetics. The results will be discussed in the manuscript.

Keywords: Black mass; Activated Carbon; Electrocatalyst; Oxygen Evolution Reaction;

P0184 • Abdullahi Abdulkadir

ICEAM2026-POSTER-0184 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Sonocatalytic Performance of a Plant Based-Derived Biochar/ZnO Composite: pH-Dependent Kinetics and Degradation Mechanism of Dye Pollutants*Abdullahi Abdulkadir^{1,3}, Lavi Aluna¹, Har Mohan Singh^{1,2}*¹*Department of Physics & Environment Sciences, Sharda School of Engineering & Science, Sharda University, Greater Noida, Uttar Pradesh 201310, India*²*Centre of Excellence in Solar Cell & Renewable Energy, Sharda University, Greater Noida, Uttar Pradesh 201310, India*³*Department of Biological, Kashim Ibrahim University, P.M.B. 1122, Njimitilo, Kano Road, Maiduguri, Nigeria***Abstract**

The escalating discharge of dye-laden textile effluents poses a persistent threat to aquatic ecosystems and human health, necessitating cost-effective and sustainable remediation strategies. In this study, a biochar/ZnO composite was synthesized using plant biomass and zinc acetate as precursors. UV, FTIR, XRD and SEM analyses were carried out to assess the characteristics of the materials. The sonocatalytic degradation efficiency was tested against Methyl Orange (MO) and Crystal Violet (CV) under varying pH. The biochar/ZnO characterization revealed Zn–O vibrational bands and a rougher, granular surface morphology relative to pristine biochar. Under ultrasonic irradiation at near-neutral pH (6.5), the composite achieved degradation efficiencies of 97.01% for CV and 95.96% for MO within 60 minutes, substantially outperforming plain sonolysis. Degradation followed pseudo-first-order kinetics, with an apparent rate constant of $k = 0.0516 \text{ min}^{-1}$ for MO ($R^2 \geq 0.99$). The degradation efficiency declined under both acidic and alkaline conditions, identifying slightly acidic-to-neutral pH as optimal for the sonocatalytic process. The possible degradation mechanism involves ultrasound-induced cavitation, which excites electrons in ZnO from the valence to conduction band, while the biochar matrix suppresses charge recombination and facilitates the generation of reactive oxygen species ($\bullet\text{OH}$, $\bullet\text{O}_2^-$, H_2O_2) that degrade the dye chromophores. These findings demonstrate that Biochar/ZnO is an efficient, low-cost sonocatalyst, offering a sustainable route for biomass valorization and the remediation of dye-contaminated wastewater.

Keywords: Pyrolysis; Biochar; Sonocatalytic Degradation; Reactive Oxygen Species; Dyes

P0210 • Manendra Verma

ICEAM2026-POSTER-0210 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

Removal of Microplastics from Natural Freshwater Systems: Conventional and Green Technologies with Special Emphasis on Adsorption-Based RemediationMohini Singh^{1*}, Shruti Gupta¹, Manendra Verma¹, Pushpa Sahn¹*¹Department of Chemistry, Faculty of Science,
Dayalbagh Educational Institute, Agra-282005***mohinisingh0862@gmail.com***Abstract**

Microplastics (MPs) have emerged as persistent contaminants of freshwater ecosystems, including rivers, lakes, ponds, and groundwater, owing to their widespread occurrence, environmental persistence, and continuous input from domestic wastewater, stormwater runoff, agricultural activities, industrial discharge, textile fibres, and degradation of plastic products. Their heterogeneous characteristics, including variable polymer composition, size, shape, density, surface charge, and degree of environmental weathering, make their removal considerably more challenging than that of conventional dissolved pollutants. The review critically discussed the occurrence, migration and removal of microplastics from natural freshwater systems, focusing on adsorption-based and environmentally sustainable remediation technologies. Conventional treatment approaches, including coagulation–flocculation, sedimentation, sand filtration, dissolved-air flotation, membrane filtration, and electrocoagulation, are evaluated in the terms of their removal mechanisms, performance, operational requirements, and limitations. Although these technologies can achieve substantial MPs separation, rather than destroying them. Emerging green technologies based on biochar, activated carbon, algal biomass, chitosan, cellulose-based materials, magnetic biochar, and magnetic composite adsorbents are therefore receiving increasing attention. Adsorption-based removal is governed by a combination of hydrophobic interactions, electrostatic attraction, hydrogen bonding, π – π interactions, surface complexation, physical interception, and entrapment. Recent studies indicate that engineered and magnetically recoverable bioadsorbents can provide high removal efficiencies and adsorption capacities while facilitating post-treatment separation and adsorbent reuse. However, substantial research gaps remain regarding the behaviour of environmentally aged and mixed-polymer microplastics, nanoplastics, natural organic matter, competing ions, and complex freshwater matrices. Moreover, aspects such as regeneration, secondary pollution, adsorbent stability, life-cycle impacts, and economic feasibility require additional work before large-scale implementation. Over all the information available indicates that integrated treatment trains comprising source control, physical separation, filtration, sustainable adsorption and magnetic recovery may be a more efficient and environmentally acceptable way of freshwater microplastic remediation. Future research should focus on the continuous-flow systems, real freshwater validation, standardized analytical protocols, complete microplastic mass balances, regeneration studies, and field-scale verification in order to facilitate the transition of adsorption-based technologies from laboratory scale to practical freshwater management.

Keywords: Microplastics; freshwater ecosystems; adsorption; biochar; magnetic biochar; green remediation; magnetic adsorbents; rivers; lakes; groundwater; microplastic removal; sustainable water treatment.

P0213 • Aditi Das Talukdar

ICEAM2026-POSTER-0213 | Poster Presentation | Day 1, 08 Oct 2026, 3:30-4:00 PM, Tea Break & Poster Session

COMPARATIVE TECHNO-ECONOMIC AND LIFE CYCLE ASSESSMENT OF DIRECT LITHIUM EXTRACTION TECHNOLOGIES FOR GEOTHERMAL BRINE: LAYERED DOUBLE HYDROXIDE (LDH)SORPTION, NANOFILTRATION, AND ELECTRO-DRIVEN PATHWAYSAditi Das Talukdar¹, Prof. Prasenjit Mondal²^{1,2} *Department of Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

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Abstract

Rising global demand for lithium, driven by the rapid expansion of electric vehicles and grid-scale energy storage, has intensified interest in direct lithium extraction (DLE) from unconventional resources such as geothermal brines. Compared to conventional evaporitic and hard-rock lithium production, DLE technologies offer the potential for faster processing, smaller land footprints, and reduced water consumption, but their comparative economic and environmental performance remains insufficiently characterized on a consistent basis. This work presents a combined techno-economic assessment (TEA) and life cycle assessment (LCA) of three distinct DLE technologies for lithium recovery from geothermal brine: lithium-aluminum layered double hydroxide (LDH) sorption coupled with forward osmosis, multipass nanofiltration (NF), and an electro-driven pathway integrating intercalation deionization (IDI) with bipolar membrane electrodialysis (BMED). In order to facilitate an equitable, direct comparison, all three methods were assessed on a uniform plant foundation, employing the same brine flow rate, feed concentration, operational lifespan, and financial premises, while the performance metrics specific to each technology (recovery efficiency, energy usage, material and equipment needs) were sourced from their respective peer-reviewed literature. Cost inventories for capital and operations were created for each pathway employing a uniform cost-estimation approach, while standard economic indicators such as net present value, internal rate of return, profitability index, and payback period were utilized to evaluate financial feasibility throughout the entire lifespan of the plant. Simultaneously, a life cycle evaluation was performed to analyze and contrast the environmental efficacy of the three paths across pertinent impact categories, offering insights into the material, energy, and process-related burdens linked to each extraction method. The findings offer a transferable methodological framework for evaluating emerging lithium extraction technologies in a consistent, defensible manner, and highlight the importance of evaluating both cost and environmental performance jointly, rather than in isolation, when assessing the readiness of alternative lithium recovery pathways for industrial deployment.

Keywords: Life Cycle Assessment (LCA); Techno Economic Analysis (TEA); Direct Lithium Extraction (DLE); Geothermal Brine.



Poster Session II

ACS Materials Au (Day 2, 09 Oct 2026) • 30 Posters

P0007 • Kareena Yadav

ICEAM2026-POSTER-0007 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Structural, Morphological and Temperature Dependent Electrical Investigation of Spin-Coated ZnO Thin Film for Electronic Device ApplicationKareena Yadav¹, Rashmi Singh^{2*}*Department of Physics, School of Physical Science, Starex University, Gurugram, Haryana, 122413, India***Corresponding author email: rash.pink@gmail.com***Abstract**

In the present study, Zinc Oxide (ZnO) thin film was synthesized using Spin coating technique and systematically investigated for its structural, morphological, compositional and electrical properties for potential applications. The structural properties were analysed using X-ray diffraction (XRD), confirming the formation of hexagonal wurtzite structure of ZnO with prominent reflections corresponding to the (002), (102) and (103) crystallographic planes. The crystallite size, compressive strain and dislocation density were evaluated from the XRD data to understand the structural quality and defect characteristics of the prepared material. The average crystallite size, compressive strain and dislocation density was estimated to be 133nm, 0.077% and $5.65 \times 10^{13} \text{m}^{-2}$. The electrical properties were investigated using four-probe method over the temperature ranging of 30–70°C under both heating and cooling cycles at a constant current of 6 mA. The calculated resistivity varied from 7.1–53.2 $\Omega\text{-cm}$ during heating and 21.3–60.3 $\Omega\text{-cm}$ during cooling. Arrhenius analysis yielded activation energies of 0.343 eV and 0.229 eV for the heating and cooling cycles, respectively, indicating thermally activated charge transport. The distinct resistivity and activation-energy values obtained during heating and cooling reveal a pronounced thermal-cycle dependence of charge transport in the ZnO thin film. The combined structural, optical and electrical characteristics demonstrate that the fabricated ZnO films are promising candidates for transparent electronics, UV photodetector, gas sensors and other advanced optoelectronic applications. The elemental composition was examined using energy-dispersive X-ray analysis (EDAX), confirming the presence of the constituent elements with desired compositional purity. Scanning Electron Microscopy was employed to investigate the surface morphology, grain distribution and microstructural features. The correlation between structural parameters, surface morphology, element composition and electrical resistivity demonstrates the suitability of the prepared material for applications. The observed properties indicate that ZnO thin film has promising potential for use in advanced functional electronic devices.

Keywords: Spin-coating, X-ray Diffraction, Electrical, ZnO, Thin Film, Electronic Devices.

P0033 • Neha Thakur

ICEAM2026-POSTER-0033 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

TAILORING OF SURFACE DEFECT MEDIATED BAND BENDING AND WORK FUNCTION IN ZNO NANOPARTICLES: EFFECT OF INTERFACE STRENGTH

Neha Thakur^{1*}, Sanjay Kumar Srivastava², and Sanjiv Kumar Tiwari¹¹ Department of Physics and Materials Science, Jaypee University of Information Technology, Waknaghat, Solan, H.P, India² Advanced Materials and Device Metrology, CSIR-National Physical Laboratory, New Delhi, India

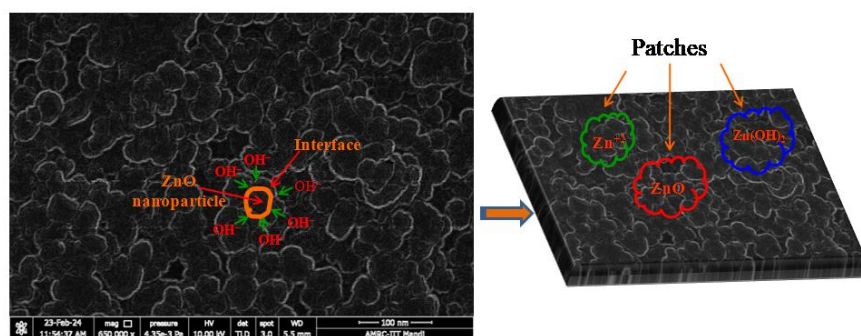
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Abstract

Zinc oxide (ZnO) is a highly transparent, II-VI group n-type for potential applications in photo-catalysis, gas sensing, transparent electronics, and optoelectronics devices. These applications require tunability of the surface electronic properties of ZnO nanoparticles, which are strongly influenced by ionic strength, surface defects, surface band bending. In the present work, ZnO nanoparticles were synthesized via a solvo-thermal method using $\text{Zn}(\text{Ac})_2 \cdot 2\text{H}_2\text{O}$ dissolved in CH_3OH and KOH as precipitating agent in the molar ratio of 1:2, 1:3, 1:4, 1:5 and 1:6 to modify the ionic strength and interfacial energy. This excess cation/anion induces variation in interfacial energy, interface strength, and local fluctuation in surface energy of nucleation center. Moreover, local fluctuation in surface energy and interfacial width decouple the growth of nanoparticle as a result small agglomerated nanoparticles formed in solution. The effect of surface morphology and surface defects on optical emission, surface band bending, work function, and valance band edge are investigated using Photoluminescence (PL), Ultraviolet photoelectron spectroscopy (UPS) respectively, whereas, structural and morphology was studied using X-ray diffraction (XRD), and Field emission scanning electronic microscopy (FESEM) respectively. The XRD shows that ZnO predominately crystallizes in wurtzite –type hexagonal crystal structure, in which Zinc (Zn) and Oxygen (O) atoms are tetrahedrally coordinated. FESEM analysis reveals the spherical type particles size of 17.5nm, 22.4nm, 25.4nm, 12.8nm and 15.5nm respectively, with enhanced defects related PL emission states. The variation in spectral width of PL induces potential fluctuations from 0.750eV to 0.917eV, and band tailing from 0.9eV to 1eV, respectively. UPS reveal the increase in work function from 4.72eV to 5.22eV, and surface band bending from 1.281eV to 0.634eV respectively.

Keywords: Defects, UPS, Band bending, Photoluminescence.

GRAPHICAL ABSTRACT:



P0034 • Pradyumn

ICEAM2026-POSTER-0034 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Influence of Ag-rich $\text{Pd}_x\text{Ag}_{1-x}$ nano-alloys on the gas sensing characteristics of rGO Schottky devices

Pradyumn.^{1*}, Partha Bir Barman¹, Anjan Sil^{2,3}, Surajit Kumar Hazra¹¹Department of Physics and Materials Science, Jaypee University of Information Technology, Waknaghat, Solan, Himachal Pradesh 173234, INDIA²Department of Metallurgical and Materials Engineering, Indian Institute of Technology Roorkee, Roorkee-247667, INDIA³Center for Sustainable Energy, Indian Institute of Technology Roorkee, Roorkee-247667, INDIA

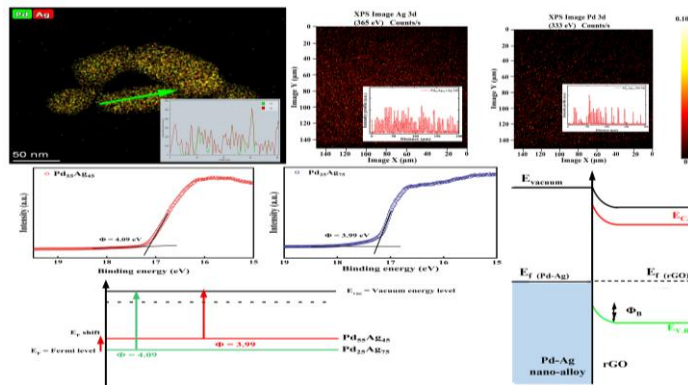
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Abstract

This work investigates the impact of Ag-rich composition and lattice strain induced in the $\text{Pd}_x\text{Ag}_{1-x}$ nano-alloy (NA) on the gas sensing characteristics of $\text{Pd}_x\text{Ag}_{1-x}$ /rGO Schottky devices in order to reduce the use of Pd without compromising sensing characteristics. $\text{Pd}_{55}\text{Ag}_{45}$ and $\text{Pd}_{25}\text{Ag}_{75}$ NA were synthesized and integrated with rGO in Schottky diode configuration to examine the $\text{H}_2/\text{CO}/\text{CH}_4$ sensing behaviour. The structural, morphological, compositional, surface and electronic properties of the NA were systematically investigated by XRD, HRTEM-EDS, XPS, and UPS. It was observed that Ag gets redistributed towards the NA surface due to the out-diffusion tendency of Ag, as evidenced by HRTEM-EDS and surface-sensitive XPS mapping. This led to the modification of the surface composition and electronic structure of NA. UPS-derived work-function variation further indicates composition-dependent changes that modulate the Schottky barrier and associated charge transport upon integration with rGO, which influence the gas sensing behaviour. The distinct sensing characteristics are governed by the coupled effects of alloy composition, surface states and elemental redistribution, and interfacial electronic structure. The findings demonstrate the potential of Ag-rich $\text{Pd}_x\text{Ag}_{1-x}$ nano-alloys as stable and Pd-efficient alternatives for rGO Schottky diode gas sensors, providing a pathway for reducing the dependence on Pd through composition and interface engineering.

Keywords: Ag out-diffusion; Ag-rich; Work function; Nano-alloy; Gas sensors



P0042 • Narendra Chhetri

ICEAM2026-POSTER-0042 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Phase Diagram of the Two-Dimensional Random Site Coulomb Glass Model

Narendra Chhetri, Vikas Malik

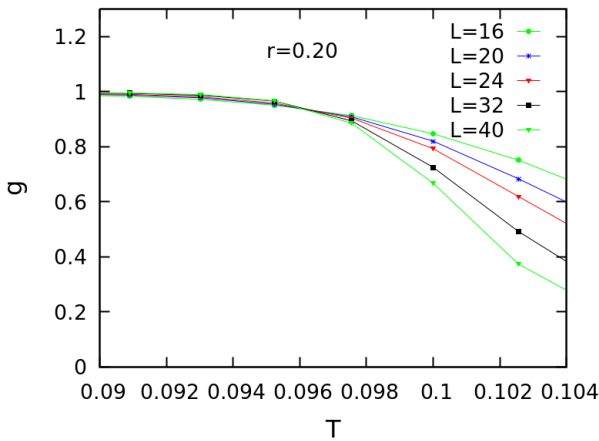
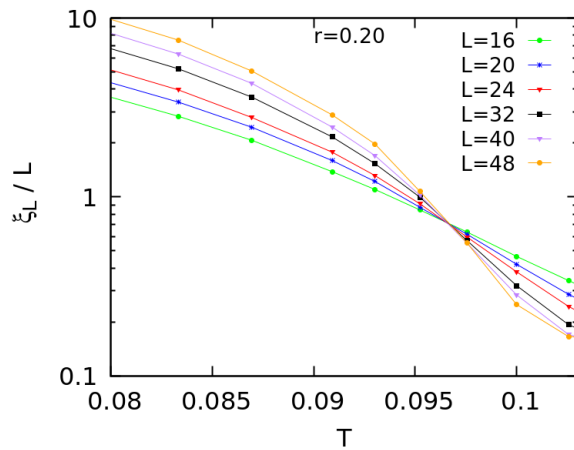
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Abstract

In this paper, we investigate the possibility of a phase transition in the two-dimensional Coulomb glass with positional disorder which is commonly known as the Random Site Model. The Coulomb glass system consists of localized electrons interacting via unscreened Coulomb interaction. The randomness in the position of sites is introduced by displacing the sites from their lattice positions by a distance r . This leads to disorder in interaction energies with the disorder increasing with the disorder parameter r . The Monte Carlo simulation is used to anneal the system from a high temperature to a very small temperature using Metropolis algorithm. For zero disorder, the Coulomb glass system has a second order phase transition from paramagnetic to antiferromagnetic phase. In this paper we show that for disorders less than the critical disorder the system exhibits a transition from paramagnetic phase to a charge ordered phase (antiferromagnet) as the temperature of the system decreases. The order parameter of the antiferromagnetic phase is the staggered magnetization and one observes that the order parameter increases from zero to its saturation value as the system temperature is decreased. The crossing of Binder cumulant and the correlation length for different system sizes at a particular temperature gives the transition temperature of the system. The transition temperature decreases as the disorder in the system increases. Finite size scaling is used to determine the critical exponents.

Keywords: Coulomb glass, Monte Carlo simulation, Metropolis algorithm, Spin-glass

Fig. Binder cumulant for different system sizes at $r=0.20$.Fig. Correlation length for different system sizes at $r=0.20$.

P0048 • Satyendra kumar satyarthi

ICEAM2026-POSTER-0048 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

DFT, MD and ML-Supported Defect Chemistry and Entropy-Stabilized Functionalities in a Novel A-Site High-Entropy ($\text{Ba}_{0.2}\text{Sr}_{0.2}\text{Na}_{0.2}\text{Ca}_{0.2}\text{Ce}_{0.2}$) TiO_3 Perovskite for Hybrid Energy StorageSatyendra Kumar Satyarthi¹, Mkrtich Yerosyan¹¹*Innovation Center for Nanoscience and Technology, A.B. Nalbandyan Institute of Chemical Physics Yerevan- 0014, Armenia*

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Abstract

High-entropy perovskite oxides offer a promising route for developing multifunctional materials with tunable defect chemistry, structural disorder, and energy-storage properties. In this work, we report a novel A-site high-entropy perovskite, $(\text{Ba}_{0.2}\text{Sr}_{0.2}\text{Na}_{0.2}\text{Ca}_{0.2}\text{Ce}_{0.2})\text{TiO}_3$ and investigate its defect chemistry and multifunctional energy-storage behavior. The material was synthesized through controlled heat treatment at 1200-1400 °C, followed by comprehensive structural, morphological, chemical, optical, dielectric, ferroelectric, and electrochemical characterization. XRD, FTIR, TGA, SEM-EDS, elemental mapping, XPS, UV-Vis, and photoluminescence analyses were used to establish the structural and defect-related features of the high-entropy perovskite. Its energy-storage performance was evaluated through dielectric and ferroelectric measurements for electrostatic capacitive energy storage, together with electrochemical characterization for supercapacitor applications. The results reveal a strong dependence of the structural characteristics, oxygen-vacancy chemistry, dielectric response, polarization behavior, and charge-storage performance on heat-treatment temperature. Thus, the material demonstrates potential for combining electrostatic capacitive and electrochemical charge-storage mechanisms within a single high-entropy perovskite platform. To further understand the origin of these properties, DFT, molecular dynamics, and machine-learning approaches are being integrated to correlate oxygen-vacancy formation, electronic structure, local atomic disorder, thermal stability, and experimentally observed energy-storage behavior. This combined approach provides a pathway for rational design of high-entropy perovskites for hybrid energy-storage applications.

Keywords: High entropy oxide, supercapacitor, ferroelectric, energy storage**References:**

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P0051 • Pooja Sharma

ICEAM2026-POSTER-0051 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Optimizing Terahertz Generation from Metallic Nanoparticles Using Tapered Magnetic field and Structured Laser Beams

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Abstract

An analytical model is developed to investigate terahertz radiation generation from spherical metallic nanoparticles exposed to a linearly tapered external magnetic field, $B_T = B_0(1 + \alpha z)$. The Terahertz radiation arises from the nonlinear beat-wave interaction of two intense cosh– Gaussian laser beams, whose ponderomotive force drives the collective motion of conduction electrons. The influence of the tapered magnetic field on terahertz generation is first examined by analysing its effects on electron dynamics and the resulting terahertz field. The results show that both the magnetic-field strength and the tapering parameter play important roles in controlling the amplitude and efficiency of terahertz radiation. In particular, increasing the tapering parameter α from 0 to 0.3 enhances the terahertz-field amplitude by approximately 25%, demonstrating that magnetic-field tapering can significantly improve terahertz emission. The effects of different laser-beam profiles are then investigated using four configurations: super-Gaussian, cosh-Gaussian, flat-top, and ring-shaped beams. Among these profiles, the ring-shaped beam produces the strongest THz emission, with an enhancement of approximately 30% compared with the other beam types. This improvement is attributed to its favourable spatial intensity distribution. The effects of other important parameters, including nanoparticles radius, interparticle separation, incident laser-field strength, and beam waist, are also analysed. The generated Terahertz field increases substantially with the nanoparticle radius and laser-field strength, whereas greater interparticle separation reduces the THz emission. Moreover, an appropriate beam waist improves the coupling between the laser field and the nanoparticles, resulting in more efficient Terahertz generation. These findings provide useful guidance for developing efficient nanoparticle-based THz sources with potential applications in photonics, biomedical imaging, sensing, and next-generation wireless communication.

Keywords: Tapered magnetic field, Spherical nanoparticles, Ponderomotive force, cyclotron frequency, Terahertz radiation, laser beam profiles.

P0057 • Prashant Chauhan

ICEAM2026-POSTER-0057 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

TERAHERTZ RADIATION GENERATION VIA MODULATED ELECTRON BEAM TRANSMISSION USING SPHERICAL NANOPARTICLES

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Abstract

This work presents a theoretical approach for terahertz (THz) radiation generation from an array of spherical nanoparticles (SNPs) driven by a modulated electron-sheet beam. The electron-sheet pulse exerts a Coulomb repulsive force on the free-electron clouds of the SNPs, displacing them relative to their positively charged ion backgrounds. Following the passage of the electron sheet, the displaced electron clouds undergo oscillations at their characteristic plasma frequency, resulting in THz radiation. The oscillating electron clouds of the SNPs collectively act as nanoscale dipole radiators, while the modulation of the electron-sheet beam enables coherent excitation of the nanoparticle (NP) array. An analytical expression for the THz conversion efficiency is derived, incorporating the modulation index of the electron-sheet beam, SNP radius, and interparticle separation. The results show that the emitted THz power increases with increasing SNP radius, owing to the enhanced dipole moment of the NPs. In addition, reducing the interparticle separation leads to an increase in THz conversion efficiency due to stronger collective and coherent radiation from the NP array. The proposed electron-sheet-driven SNP array provides a potential route for efficient and tunable THz radiation generation through controlled electron-beam modulation and NP-geometry.

Keywords: Terahertz radiation; Electron-sheet beam; Spherical nanoparticles; Dipole array.

P0069 • Sanjay Kumar

ICEAM2026-POSTER-0069 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

ANTIBACTERIAL PERFORMANCE OF ELECTROLESS Ni-P-TiO₂-SiO₂ PLATINGS AGAINST *KLEBSIELLA PNEUMONIAE* BACTERIUMSanjay Kumar¹, Sulaxna Sharma², Awanish Sharma³¹*Department of Physics, Graphic Era Deemed to be University, Dehradun, India*²*Assistant Professor, Department of AS&H, THDC IHET, Bhagirathi Puram Tehri, India*³*Professor, Department of Physics, Graphic Era Deemed to be University, Dehradun, India*

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Abstract

In present experimental work, the Ni-P/Ni-P-TiO₂-SiO₂ nanocomposite deposits were developed on the mild-steel (MS, AISI 1040 grade) substrate through the alkaline electroless method. Further, the surface morphology of the developed deposits was analyzed by means of SEM, EDAX and XRD physical methods. The results of these studies confirmed that the TiO₂ and SiO₂ nanoparticles are consistently embedded into electroless Ni-P matrix. Moreover, the as-plated Ni-P/Ni-P-TiO₂-SiO₂ nanodepositions had revealed the amorphous structures, while the heated depositions transitioned from amorphous to crystalline structure. The glowing developed Ni-P/Ni-P-TiO₂-SiO₂ nanoplatings were also tested for the antibacterial resistance against a gram-negative strain named as Klebsiella pneumonia. The antibacterial results revealed that the Ni-P-TiO₂-SiO₂ nanoplatings exhibited the significant antibacterial resistance against the Klebsiella pneumonia bacterium.

Keywords: electroless, titania, silica, Klebsiella pneumonia, antibacterial.

P0071 • Akanksha Priya

ICEAM2026-POSTER-0071 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Annealing-Induced Allotropic Phase Formation and its Correlation with Magnetic Properties for $\text{Co}_{35}\text{Cr}_5\text{Fe}_{10}\text{Ni}_{30}\text{Al}_{20}$ High Entropy Alloys

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Abstract

Present investigation focuses on the effect of annealing induced allotropic phase formation and its correlation with the magnetic properties of $\text{Co}_{35}\text{Cr}_5\text{Fe}_{10}\text{Ni}_{30}\text{Al}_{20}$ High entropy alloy (HEA). The selected HEA synthesized through mechanical alloying followed by vacuum annealing at 500, 800, 900 and 1000°C for 2h. The XRD analysis reveals the formation of mixture of fcc and bcc along with minor amount of σ -phase for the as synthesized HEA. For 500°C annealed HEA similar phase is maintained, only volume phase fraction of bcc increased and fcc phase was decreased, for 800°C annealed HEA, the fcc phase transformed to new allotropic L_{10} phase along with increase in volume phase fraction of bcc phase. However, 900 and 1000°C annealed HEA new ordered B2 phase formed along with the initial phases. The value of saturation magnetization of the as-synthesized sample is found to be 52.4 emu/g. With increase in annealing temperature the value of magnetization increased to 54.5, 76, 83 and 85 emu/g for 500, 800, 900 and 1000°C annealed HEAs. The study systematically discusses the effect of annealing temperature on the phase evolution and its correlation with magnetic properties of $\text{Co}_{35}\text{Cr}_5\text{Fe}_{10}\text{Ni}_{30}\text{Al}_{20}$ HEA.

Keywords: - High Entropy Alloy; Annealing; Magnetic properties; Allotropic phase; Phase evolution.

P0078 • aditi bhardwaj

ICEAM2026-POSTER-0078 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

A Compact Double Cylindrical Dielectric Resonator Antenna Employing Defected Ground Structure for Ultra-Wideband High-Efficiency ApplicationsAditi Bhardwaj¹, Sabatini Tyagi¹, Supratim Mitra¹, Mohd Gulman Siddiqui^{1*}, Alkesh Agrawal²¹*Department of Physical Sciences, Banasthali Vidyapith, Rajasthan-304022, India*²*Department of Electrical & Electronics Engineering, Shri Ramswaroop Memorial University, Barabanki, U.P.-225003, India*

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Abstract

For wireless communication, radar imaging, satellite communication, and Internet of Things (IoT) applications, ultra-wideband (UWB) antennas with high radiation efficiency, small size, and integrated interference suppression are becoming more and more necessary. This work describes a compact double-cylindrical dielectric resonator antenna (DCDRA) that employs a slot-loaded planar radiator and a defected ground geometry (DGG). In a small footprint of $20 \times 18 \times 0.8 \text{ mm}^3$, the electromagnetic coupling between two high-permittivity alumina dielectric resonators ($\epsilon_r = 9.9$) excites several hybrid resonant modes, leading to improved impedance matching and broadband performance. The suggested coupling-driven arrangement, in contrast to traditional single-resonator dielectric resonator antennas, concurrently increases bandwidth, radiation efficiency, and interference suppression without adding further structural complexity. In order to reduce narrowband interference, the constructed antenna uses six integrated band-notched frequencies at 1.71, 4.14, 7.72, 8.16, 10.18, and 11.41 GHz. Its measured impedance bandwidth is 0.97–12.09 GHz. Over most of the operating band, a peak realised gain of about 6.8 dBi and radiation efficiency ranging from 80% to 97% are achieved. The efficiency of the proposed design is confirmed by the close agreement between the measured and simulated results. For next-generation UWB wireless communication, radar sensing, satellite communication, and Internet of Things applications, the suggested DCDRA offers a small, easily fabricated, and high-performing solution.

Keywords: Cylindrical Dielectric Resonator, Microstrip Patch, Defected Ground Structure, Wireless Communication, Super Wideband, C/X/Ku bands.

P0084 • PRITAM KUMAR NATH

ICEAM2026-POSTER-0084 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

NiO@NiMoO₄-BASED EFFICIENT GAS SENSOR FOR TRIETHYLAMINE DETECTION

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Abstract

Volatile organic compounds (VOCs) have been suggested to pose significant environmental threats and health risks, which necessitate the development of highly sensitive and selective sensors. The fabrication of these sensors is still a critical task for on-field applications. The active materials play a very important role in high sensitivity, selectivity, and room-temperature operation. Metal nanoparticles, oxide semiconductors, polymers, etc., have been studied in recent years, exhibiting enhanced sensitivity, responsivity and selectivity. However, several drawbacks in these materials hinder their on-site practical applications. To be mentioned, various applications, namely sensors, water purification, and energy storage devices, etc. have been studied in the recent past. Here, NiMoO₄ have been synthesized using the well-known hydrothermal method and tested in a custom-made gas sensing setup to test its gas sensing ability and selectivity. This work explores the fabrication of highly sensitive sensing materials for enhanced VOC(Triethylamine) sensing. The fabricated NiMoO₄ sensor shows a responsivity as high as 12.6, having a response time of ~124.5 sec and a recovery time of ~16.89 sec for 10ppm of TEA vapour at a temperature of around 30°C. Furthermore, the sensor also exhibited the highest selectivity towards TEA compared to other VOCs (Formaldehyde, Acetone, Ethanol, Ammonia). The high responsivity of the NiO@NiMoO₄ based sensor to TEA can be due to several factors, such as the catalytic properties of the composite materials and the high specific surface area. The results may have immense scope and potential for efficient detection of VOCs to ensure biosafety and environmental remediation.

Keywords: Gas sensing; Volatile Organic Compounds; Nickel molybdate; Surface-to-volume; Environmental monitoring

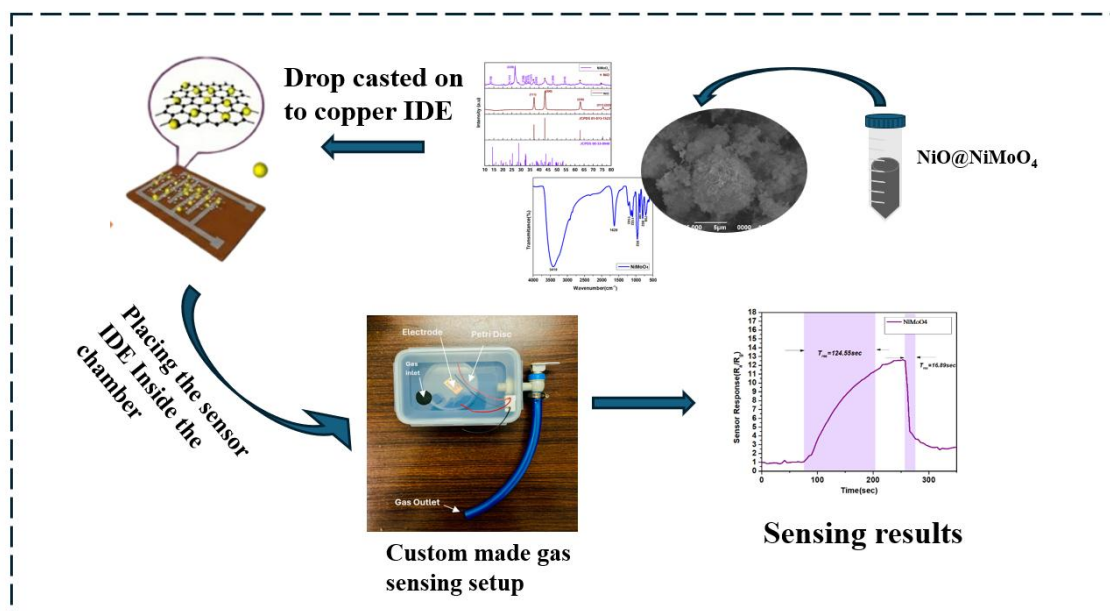


Figure 1 Graphical Abstract

P0089 • Muskan Garg

ICEAM2026-POSTER-0089 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

BACTERIAL CELLULOSE AS A TUNABLE NANOMATERIAL: MEDIA-DEPENDENT CRYSTALLINITY AND PHYSICAL PROPERTIESMuskan Garg ¹, Garima Mathur ^{2*}^{1,2} Centre of Excellence in Plant & Microbial Biotechnology
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Abstract

Bacterial Cellulose, a nanostructured cellulose material, is well recognized for its high purity, nanofibrillar structure, excellent mechanical strength, high crystallinity & water-holding capacity and remarkable biocompatibility, making it an excellent choice of material for biomedical, pharmaceutical and other industrial applications.

The media components play a critical role in bacterial growth, biopolymer production and its physicochemical properties. This study aimed at exploring the role of culture media components on BC yield and resulting changes in physicochemical and structural properties, produced by *Komagataeibacter saccharivorans* BC-C1 under static culture condition. The synthesized cellulose pellicles were purified by alkaline treatment followed by extensive washing to remove bacterial cells and residual medium components. The influence of culture media on BC production was assessed for BC yield, physicochemical and structural characteristics. Chemical characteristics, structural features & crystallographic analysis were performed using Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). FTIR analysis revealed the presence of characteristic cellulose peaks corresponding to hydroxyl groups (-OH), C-H stretching, and β -1,4 glycosidic bonds in the obtained BC across different culture media. However, the shifts in the O-H stretching band (3200-3400 cm^{-1}) and changes in the relative intensities of the 1160 cm^{-1} (C-O-C glycosidic) and 1430 cm^{-1} (CH_2 scissoring, crystalline band) peaks indicated media-dependent variation in intramolecular hydrogen-bonding density and degree of order. The findings highlight a structure–property relationship in BC samples, where media component induced variations altered the hydrogen-bonding, crystallite size, and fibrillar packing. These findings highlight the potential of optimizing the composition of culture media to enhance BC yield without affecting its physicochemical properties.

Keywords: Bacterial Cellulose; Culture Media; Physicochemical characteristics; FTIR; XRD

P0093 • Akanksha Kumari

ICEAM2026-POSTER-0093 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Grain and Grain-Boundary Contributions to Electrical Transport and Relaxation Dynamics in $\text{La}_{1-x}\text{Pr}_x\text{CrO}_3$ Perovskites

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Abstract

Polycrystalline $\text{La}_{1-x}\text{Pr}_x\text{CrO}_3$ perovskites ($x = 0.0, 0.2, \text{ and } 0.4$) were synthesized via a conventional solid-state reaction method using high-purity precursors. The precursors were preheated at 180 °C for 12 h, homogenized by grinding for 8 h, calcined at 1250 °C for 12 h, and subsequently sintered at 1350 °C for 12 h. The electrical transport and relaxation characteristics were investigated using temperature-dependent impedance spectroscopy and complex electric modulus analysis over the frequency range of 100 Hz–1 MHz and the temperature range of 30–90 °C. Nyquist plots revealed pronounced temperature- and composition-dependent impedance responses, indicating significant contributions from both grain and grain-boundary regions. The evolution of the impedance response with Pr substitution reflects changes in electrical heterogeneity and charge-carrier dynamics. An intermediate Pr concentration enhances dielectric polarization, whereas further Pr incorporation results in a decrease in the dielectric response, which is attributed to Pr-induced structural distortion and modified charge-carrier localization. The frequency-dependent Z'' and M'' spectra exhibit thermally activated relaxation, with the relaxation frequencies shifting towards higher frequencies with increasing temperature. To elucidate the temperature-dependent electrical dynamics, relaxation times and activation energies were determined. The electric modulus formalism, defined as the reciprocal of the complex relative permittivity, effectively suppresses the effects of large permittivity values associated with electrode polarization and long-range charge transport, thereby facilitating the identification of relaxation processes that may remain obscured in conventional dielectric representations. The observed evolution of grain and grain-boundary resistance and relaxation behavior is attributed to Pr-induced lattice distortion, modifications in the mixed-valence $\text{Cr}^{3+}/\text{Cr}^{4+}$ states, and changes in the Cr–O–Cr network. Overall, the results establish a clear correlation between Pr-induced structural modifications, electrical heterogeneity, localized charge transport, and thermally activated relaxation in $\text{La}_{1-x}\text{Pr}_x\text{CrO}_3$ perovskites.

Keywords: Perovskites; Impedance spectroscopy; Electric modulus; Dielectric relaxation; Charge transport

P0105 • Vandana Tyagi

ICEAM2026-POSTER-0105 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Dopant-Engineered Graphene for Selective Isoprene and Toluene Detection: A DFT–NEGF StudyVandana Tyagi^{1,*}, Anurag Srivastava¹¹ *Advanced Materials Research Group, Department of Engineering Sciences, ABV-Indian Institute of Information Technology and Management, Gwalior, Madhya Pradesh 474015, India*

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Abstract

Volatile organic compounds (VOCs) in exhaled breath is a promising non-invasive method for early disease screening. But specific detection of biomarkers in humid condition has still not studied. Here, the adsorption and sensing characteristics of isoprene and toluene on pristine graphene (PG), nitrogen-doped graphene (NG), and boron-doped graphene (BG) were investigated using density functional theory (DFT) and non-equilibrium Green's function (NEGF) calculations. Both dry and water co-adsorbed conditions were investigated. The adsorption energies of isoprene on PG, NG, and BG were -1.34 , -1.34 , and -1.27 eV, respectively, while those of toluene were -1.61 , -0.76 , and -1.52 eV. The equilibrium adsorption distances varied between 2.31 and 2.77 Å, while the charge transfer ranged from 0.001 to 0.016 e, with BG–isoprene exhibiting the highest charge transfer. Doping significantly modified the electronic properties, with clean-surface work functions ranging from 4.00 eV for NG to 5.27 eV for BG. The adsorption-induced work-function modulation was strongly analyte dependent, with NG exhibiting shifts of 12 meV for isoprene and 1.24 eV for toluene, indicating its potential for selective discrimination between the two VOCs. Quantum-transport analysis demonstrated contrasting electrical responses of NG and BG to isoprene adsorption, emphasizing the role of heteroatom doping in modulating sensor response. The recovery analysis revealed that the NG shows rapid desorption for toluene, with a recovery time of about 6.9 s at 298 K, while other configurations require external input. In conclusion, heteroatom doping is an effective way to control the interactions between the VOCs and graphene, and hence, doped graphene can be used for selective VOC detection in breath analysis.

Keywords: Doped graphene; DFT; NEGF; Isoprene; Toluene; Breath analysis; VOC sensing

P0107 • Roshni Tarai

ICEAM2026-POSTER-0107 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

EASY SYNTHESIS OF BANDGAP TUNABLE ZINC-TIN-OXIDE THIN FILMS BY SPIN COATING

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Abstract

Zinc tin oxide (ZTO) thin films are of intense interest as transparent semiconductors with a variable band gap, high optical transparency, and the ability to be processed in solution at low cost. The ZTO is a hard amorphous semiconductor prepared by the physical deposition method using high-end instruments, *e.g.* reactive ion sputtering etc. In this study, ZTO thin films were prepared on glass substrates by spin-coating a mixture of precursor chemicals with ease of processing, compositional adjustment and feasibility. The deposited films were heat-treated to obtain homogeneous and adherent coatings. The structural and optical characteristics were analysed by ultraviolet visible (UV–Vis) spectroscopy, and Raman spectroscopy. The UV–Vis analysis demonstrated a good level of transparency in the visible spectrum, alongside a tunable optical band gap that is affected by variations in the composition of zinc and tin. The Raman spectra validated the establishment of zinc–tin–oxygen networks and reveal insight of the as-prepared films. Detailed characterisation results of ZTO thin films from UV-Vis Absorption, Raman Scattering, conductivity measurements etc will be presented.

Keywords: Zinc tin oxide (ZTO), Thin-film, Spin coating, Optical properties

P0114 • Renu mamgai

ICEAM2026-POSTER-0114 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Structural, Microstructural and Dielectric Evolution of Sm/Fe modified NaNbO₃ Lead-Free Ceramics

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*Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, 201309, India***Abstract**

Lead-based perovskites have been used for capacitors and energy storage for a long time, but environmental concerns have motivated the search for lead-free alternatives, of which NaNbO₃ is one of the strongest candidates. In this study, Sm and Fe were simultaneously co-doped into NaNbO₃ at the A and B sites; a typical composition with $x = 0.07$ was prepared by the conventional solid-state reaction route. X-ray diffraction pattern confirmed single-phase formation. FTIR spectra have shown a distinct absorption band at 540–580 cm⁻¹, which corresponds to Nb-O bond stretching in the NbO₆ octahedra. SEM micrographs showed that the grain size decreased drastically upon substitution with Sm/Fe, which may be attributed to the segregation of the dopant ions at the grain boundaries, restricting grain growth during sintering. Dielectric constant vs temperature plots at 1,10,100 kHz have shown that a sharp anomaly for $x=0$, corresponding to the ferroelectric-antiferroelectric transition, has been found to collapse upon doping with Sm-Fe for $x=0.07$, and a diffuse-type frequency-dependent behaviour is seen. No anomalies in dielectric loss have been observed for the doped composition. Overall, the flattening of the dielectric response and retention of the NbO₆ framework suggest that the Sm/Fe co-doping transforms NaNbO₃ into a more temperature-stable, lead-free dielectric candidate with interesting properties for further investigation.

Keywords: Lead-free perovskites; Ferroelectric; Antiferroelectric; Dielectric Polarization; Microstructure.

P0121 • RAJ VEER SINGH

ICEAM2026-POSTER-0121 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Improvement in Electrical Transport Properties of CsSnBr₃ Nanocrystal Incorporated P3HT Thin FilmsR. V. Singh¹, A. Vishwakarma², S. P. Singh¹ and L. Kumar²¹ *Department of Physics, D. J. College, Baraut, India*² *Molecular Electronics Research Laboratory, Physics Department, University of Allahabad, Prayagraj-211002, India*

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Abstract

Metal halide perovskite (MHP) nanocrystals (NCs) have emerged as advanced material in the field of energy and display technology owing to its outstanding optoelectronic properties. Their excellent charge carrier mobility and energy level alignment with conjugated polymers makes them suitable to improve the charge transport properties of conducting polymers. In this work we have synthesized lead-free all-inorganic CsSnBr₃ perovskite NCs by conventional Hot Injection Method. Transmission electron microscopy (TEM) shows that the average particle size of CsSnBr₃ perovskite NCs is 32 nm with blue photoluminescence emission peak at 425 nm when excited by 385 nm. These CsSnBr₃ perovskite NCs are incorporated into conjugated polymer P3HT thin films and its charge transport properties have been explored by fabricating Schottky diodes. Barrier height of CsSnBr₃ incorporated P3HT thin films shows a continuous increase and decrease in reverse saturation current. CsSnBr₃ perovskite NCs tunes the energy level of conjugated polymer P3HT and improves the charge transport properties of P3HT thin films.

Keywords: Perovskite Nanocrystal; Conjugated Polymer; Charge Transport; Schottky Diode

P0128 • Naman Patel

ICEAM2026-POSTER-0128 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Engineered Ion Gradient Piezoionic Interface for Deformation Controlled Robotic ActuationNaman Patel¹¹ *Computer Science & Engineering, Rajiv Gandhi Institute of Petroleum Technology, Amethi, Uttar Pradesh, India*

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Abstract

Converting mechanical motion into digital control signals is important to designing robots and technologies that respond naturally to human touch. Piezoionic materials, which translate mechanical deformation into electrical output via stress driven ion transport, offer a compelling route toward soft, deformable control interfaces, yet poor ion redistribution and unstable signal output have limited their real world deployment. Here, we present a robotic control system built around an ion gradient piezoionic interface, engineered from an ionic liquid infused polymer, and demonstrate its direct use as a flexible steering medium for a mobile robotic car.

The interface is designed with a built-in ionic gradient that drives selective, directional ion migration under applied strain, allowing it to produce spatially distinct electrical signatures depending on where and how it is deformed. At an optimized ionic liquid loading, the material delivers a piezoionic sensitivity of 100 mV kPa⁻¹ and an areal power density of 54 mW m⁻², reflecting efficient and high fidelity ion based transduction.

Moving beyond characterization alone, we embedded this interface directly into a robot's control architecture. Touch based deformation of specific zones on the interface is decoded into electrical commands governing the car's forward, reverse, left, and right motion, enabling real time, gesture like operation. This demonstration positions the ion gradient interface as a viable substitute for rigid mechanical switches and electronic controllers, pointing toward mechanically compliant and intuitive human machine interfaces. More broadly, the work establishes a materials to robotics pipeline in which gradient engineered piezoionic materials function as integrated sensing and control elements, laying the groundwork for interactive mobile robots, soft robotics, wearable controllers, and next generation human machine interaction systems.

Keywords: Piezoionic Interface; Engineered Ion Gradient; Ionic Liquid; Deformation Sensing; Robotic Actuation; Human Machine Interface

P0139 • Dr Nidhi Dua

ICEAM2026-POSTER-0139 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Orthorhombic CsPbBr₃ Nanocrystal Films for Near-Infrared-to-Visible Upconversion PhotodetectionNidhi Dua¹, Sandeep Kumar², Madhusudan Singh³¹ *Department of Electrical Engineering, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi – 110016, Delhi, India*² *Department of Chemistry, Motilal Nehru College, Benito Juarez Marg, University of Delhi South Campus, New Delhi – 110021, India*³ *Department of Electrical Engineering, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi – 110016, Delhi, India*

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Abstract

The study investigates the synthesis, structural, and optical characterization, and near-infrared (NIR) photoresponse of CsPbBr₃ perovskite nanocrystals integrated as a photoactive coating on a low-cost photodetector. The primary objective was to examine the potential of CsPbBr₃ nanocrystal films for infrared-to-visible upconversion-assisted photodetection and to evaluate their influence on the wavelength-dependent responsivity of a low-cost (~\$5) photodetector (Electronicspices, purchased from Amazon.in; spectral response peaks at 3.705%; SpeQuest Rera solutions). Powder X-ray diffraction (XRD, Rigaku Miniflex benchtop X-ray diffractometer), recorded over a 2θ range of approximately 10–70°, confirmed the formation of crystalline CsPbBr₃ with a predominantly orthorhombic crystal structure at room temperature. The narrow and intense peaks indicate good crystallinity. The splitting or closely spaced doublet-like features between 15° and 30° indicate reduced crystal symmetry, supporting an orthorhombic crystal structure rather than a purely cubic phase. Using the Debye-Scherrer equation for the diffraction peak near 2θ ≈ 30.6°, with a fitted full width at half maximum of 0.50°, the average crystallite size was estimated to be approximately 16.5 nm. High-resolution transmission electron microscopy (HRTEM, FEI Tecnai TF20) revealed uniformly distributed, well-defined CsPbBr₃ nanocrystals with cube-like morphology and an average particle size of approximately 14 nm (in close agreement with XRD crystallite size). UV-visible absorption spectroscopy (Perkin Elmer Lambda 1050) showed a strong absorption in the visible region, with an absorption edge near 510–520 nm, corresponding to an estimated direct optical band gap of 2.41 eV. Under near-infrared excitation from 700–850 nm, the CsPbBr₃ nanocrystal film exhibited visible photoluminescence (emission peak at 525 nm, recorded on Edinburgh Instruments FLSP920), indicating NIR-to-visible anti-Stokes or upconversion-related emission. The current-voltage measurements showed that the light-induced current exceeded the dark current and increased with increasing negative bias, demonstrating field-assisted photocarrier generation and extraction. The maximum photocurrent at the highest applied negative bias was obtained under 700 nm excitation (–2.90×10^{–6} A/cm²), followed by 750 nm (–2.77×10^{–6} A/cm²) and 800 nm (–2.59×10^{–6} A/cm²) illumination. Spectral responsivity measurements further showed that the CsPbBr₃-coated low-cost photodetector exhibited a responsivity of approximately 0.006 A/W at 400 nm, followed by a pronounced increase from about .010 A/W near 500 nm to 0.024–0.025 A/W between 540 and 600 nm, corresponding to the CsPbBr₃ absorption edge region; the device retained a measurable responsivity of ≈ 0.032 A/W at 800 nm. Overall, the results demonstrate that orthorhombic CsPbBr₃ nanocrystal films are promising low-cost photoactive coatings for broadband near-infrared-to-visible upconversion-assisted photodetection.

Keywords: CsPbBr₃ nanocrystals, orthorhombic perovskite, near-infrared-to-visible upconversion, low-cost photodetector, spectral responsivity

P0157 • R. Veerapandiyan

ICEAM2026-POSTER-0157 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Mining for New Metal-Organic Frameworks (MOFs) by Graph Neural Networks for High-Throughput Screening

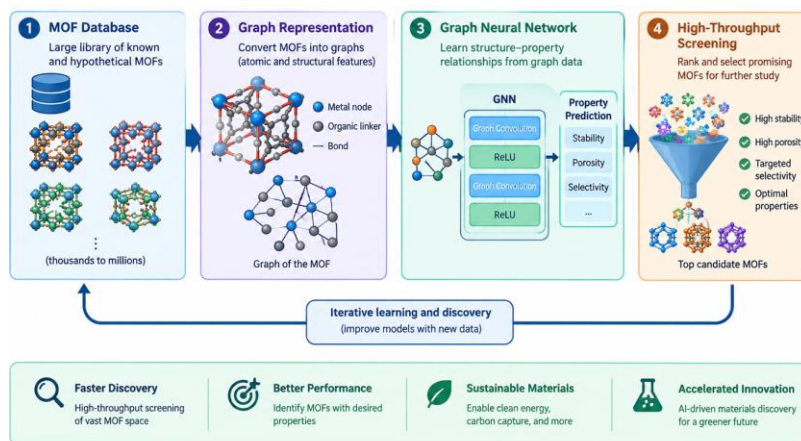
R. Veerapandiyan¹Dr S Thaiyalnayaki²¹ Department of Computer Science and Engineering, Bharath Institute of Higher Education and Research, Chennai-600073, Tamil Nadu, India.² Department of Computer Science and Engineering, Bharath Institute of Higher Education and Research, Chennai-600073, Tamil Nadu, India.

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Abstract

Metal-Organic Frameworks (MOFs) are one of the most promising classes of porous materials in the field of carbon capture because of their tunable topology, ultra-high surface area and chemical tunability. Nevertheless, the computational challenge of identifying optimal structures out of the many millions of possible candidate materials by the traditional atomistic simulation techniques (e.g., DFT and GCMC) is a significant bottleneck. In this paper, a novel deep learning framework based on Graph Neural Networks (GNNs) is proposed to rapidly and high throughput screen MOFs for efficient post-combustion carbon capture. The GNN model is learned from large computational datasets of simulated gas adsorption properties, such as the uptake capacity for carbon dioxide (CO₂), Henry's constants, and the selectivity for adsorption of CO₂ over nitrogen (N₂). The model's training is done directly from the atomic coordinate data, which enables it to deliver the metrics related to target gas separation in milliseconds instead of hours. The GNN framework achieves high predictive accuracy when evaluated on large, out-of-sample MOF databases, and also decreases the computational cost by several orders of magnitude. This strategy allows for the complete screening of large chemical spaces to identify the best candidate compounds for synthesis and implementation in industrial decarbonization projects.

Keywords: Graph Neural Networks, Metal-Organic Frameworks (MOFs), High-Throughput Screening, Materials Discovery, Deep Learning



ML-ASSISTED PAIRWISE SYMMETRIC FOUR-CHANNEL HYBRID GOLD–GRAPHENE COATED PCF-SPR SENSOR

Vikas Chandra Maurya^a, Anshu D Varshney^a and Suneet Kumar Awasthi^{a*}

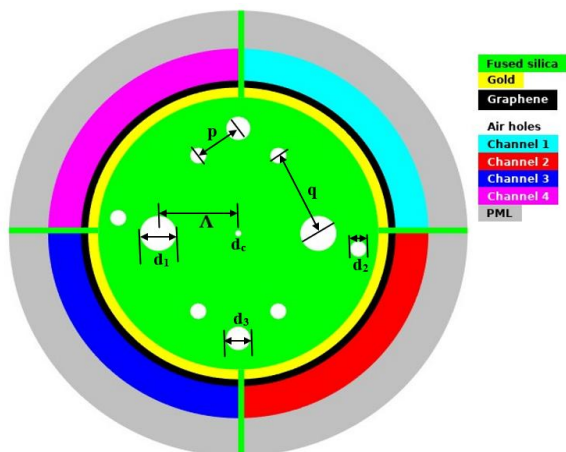
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Abstract

A single-core surface plasmon resonance (SPR) driven photonic crystal fiber (PCF) sensor coated with gold (Au) and graphene is proposed for multi-channel refractive index (RI) sensing. Four sensing channels are introduced at different coordinates around the PCF structure. Keeping to the symmetric air-hole arrangement, Channels 1 and 3 show identical responses, while Channels 2 and 4 show similar sensing results. Under y-polarization case, when the analyte RI of Channels 2 and 4 is fixed at 1.33 and Channels 1 and 3 is loaded from 1.33 to 1.39, a maximum wavelength sensitivity (WS) of 16,000 nm/RIU is achieved at RI of 1.38 by channels 1 and 3. Conversely, when Channels 1 and 3 are fixed at RI of 1.33 and the RI of Channels 2 and 4 is varied from 1.33 to 1.39, a maximum WS of 10,000 nm/RIU is achieved by channels 2 and 4. The proposed multi-channel SPR driven PCF sensor enables the simultaneous testing and comparison of healthy and infected samples, thus reducing the overall detection time. Additionally, different machine learning (ML) models are optimized to predict the confinement loss (CL) of the proposed PCF sensor, significantly reducing the requirement for computationally expensive numerical simulations. The proposed hybrid coated multi-channel SPR driven PCF sensor combined with ML-assisted prediction provides an efficient platform for high-sensitivity and computationally optimized multi-analyte sensing. The proposed work is totally based on numerical simulation. Which has been carried out in COMSOL Multiphysics 6.0 and MATLAB software.

Keywords: Photonic crystal fiber; surface plasmon resonance; refractive index; Machine learning; confinement loss; sensor.



P0167 • Karuna Kumari

ICEAM2026-POSTER-0167 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

TRANSFERRIN SURFACE FUNCTIONALIZED NANOSTRUCTURED LIPID CARRIERS OF BERBERINE FOR TARGETED GLIOBLASTOMA THERAPY: DEVELOPMENT, CHARACTERIZATION, AND IN-VITRO ANALYSIS

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Abstract

Glioblastoma multiforme (GBM) is highly aggressive and invasive primary brain tumor with poor prognosis and limited therapeutic outcomes. The major challenges in GBM treatment includes the presence of blood-brain barrier, tumor heterogeneity, and lower accumulation of therapeutic agents at the tumor site. Berberine, a natural alkaloid has been proved to have anti-cancerous properties, but its therapeutic activities get restricted because of poor solubility and limited bioavailability. Transferrin receptors are overexpressed on the surface of GBM cells to meet the high requirement of iron, necessary for rapid proliferation. These receptors can be exploited for receptor-mediated targeted drug delivery for cancer therapy. In this study, transferrin-coated berberine-loaded nanostructured lipid carriers (Tf-Berb-NLCs) were developed to facilitate an enhanced brain delivery and targeted therapy. The developed NLCs were surface-functionalized with transferrin and subsequently characterized to confirm the successful development of nano-particles and further in-vitro analysis were performed. The DLS analysis of developed formulation showed particle size and PDI of 97.05nm and 0.234 respectively for uncoated NLCs, and 158.3nm and 0.243 respectively for transferrin coated NLCs. The entrapment efficiency of berberine for the developed formulation was calculated to be 97.56%. Transmission electron microscopic analysis confirmed the development of spherical and uniform nanoparticles, while in-vitro drug release study confirmed a sustained and controlled drug release profile. Cytotoxicity analysis by MTT assay showed an enhanced toxicity of Tf-Berb-NLCs as compared to berberine and uncoated NLCs on U87-MG cell line. The qualitative analysis by confocal microscope and quantitative analysis by flow cytometry showed a better cellular uptake of transferrin coated NLCs as compared to uncoated NLCs. Overall, these findings suggest that Tf-Berb-NLCs represents an effective strategy for GBM treatment.

Keywords: glioblastoma multiforme, transferrin, nanostructured lipid carriers, brain tumor, blood brain barrier, surface modifications, targeted drug delivery.

P0168 • Divya sharma

ICEAM2026-POSTER-0168 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Development and Pharmacodynamics Evaluation of Venlafaxine-Hesperidin Loaded Lipid-Polymer Hybrid Nanoparticles for Nose -to Brain Deliver in Depression.Divya Sharma, Shweta Dang¹¹Email of corresponding author: shweta.dang@mail.jiit.ac.in**Abstract**

Depression is a prevalent neuropsychiatric disorder characterized by persistent low mood, loss of interest, and disturbances in emotional and behavioural function, while conventional antidepressant therapy may be associated with limitations such as inadequate brain delivery and adverse effects. The present study aimed to develop and evaluate venlafaxine and hesperidin co-loaded lipid-polymer hybrid nanoparticles (VLF-HES-LPHNPs) as an intranasal (nose to brain) delivery system for the management of depression. The lipid-polymer hybrid carrier was designed by integrating a lipid component with a biodegradable polymeric matrix to improve drug encapsulation, formulation stability, sustained release and potential brain delivery through intranasal route. The optimized VLF-HES-LPHNPs exhibited a particle size of 119.8 nm, PDI of 0.16 and zeta potential -19.2 mV, with high entrapment efficiency of 96.3% for venlafaxine and 89.7% for hesperidin. Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) analysis confirmed the formation of nanosized, predominantly spherical nanoparticles, while Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared Spectroscopy (FTIR) studies supported the successful incorporation of both drugs within hybrid nanocarrier. In vitro drug release studies demonstrated sustained release of both drugs, with cumulative release of approximately 97% for venlafaxine and 78% for hesperidin. The optimized formulation showed good biocompatibility, with 97.99% cell viability, and demonstrated enhanced cellular uptake in Neuro-2a cells. Cytokines analysis in RAW264.7 macrophages indicating modulation of inflammatory mediators, supporting the potential anti-inflammatory activity of the formulation. Furthermore, pharmacodynamics evaluation was performed in a corticosterone induced depression model, where treatment with VLF-HES-LPHNPs improved depression associated behavioural responses, as evidence by changes in forced swim test, tail suspension test and locomotor activity parameters compared with corticosterone-induced group. Overall, the findings demonstrate that VLF-HES-LPHNPs possess favourable physicochemical characteristics, high drug entrapment, sustained drug release, good biocompatibility, enhanced cellular uptake, and promising antidepressant pharmacodynamic activity, highlighting their potential as an intranasal nano-formulation for improved therapeutic management of depression.

Keywords: ; Venlafaxine; Hesperidin; Lipid-polymer hybrid nanoparticles; Intranasal delivery; Nose-to-brain delivery; Depression; Pharmacodynamics; Corticosterone-induced depression; Neuro-2a cells.

P0171 • Divya Singhal

ICEAM2026-POSTER-0171 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

MYRICETIN-LOADED LIPID NANOSTRUCTURES: AN IN-VITRO INVESTIGATION FOR ADVANCED WOUND HEALINGDivya Singhal¹, Shweta Dang^{*}*Department of Biotechnology, Jaypee Institute of Information Technology, Noida, India*

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Abstract

Myricetin is a naturally occurring flavonoid with favorable antioxidative and anti-inflammatory characteristics and a long history of relevance to traditional Chinese medicine. However, the poor aqueous solubility and physicochemical stability of myricetin pose a major problem for its effective delivery. In this study, the development of a nanostructured lipid carrier (NLC), which are second-generation lipid-based nanocarriers consisting of both solid and liquid lipids, has been done for enhanced myricetin delivery. A systematic screening process comprising myricetin solubility assessment in selected lipidic excipients, surfactant screening, and UV-visible spectrophotometric analysis, established Gelucire 50/13, Labrafac MC60, and Tween 80 as promising lipid and surfactant components for MYR-NLC formulation. The prepared MYR-NLCs were systematically characterized to understand their physicochemical, drug encapsulation, and performance properties. Physicochemical properties of optimized batches were evaluated in terms of particle size, zeta potential, drug loading, and encapsulation efficiency. In vitro drug release studies were carried out to find out release pattern of myricetin from the lipid matrix, and stability studies were conducted to check the stability of the developed nanocarrier during storage. Biological performance of the prepared nanocarriers was determined using in vitro wound-scratch healing assay taking free myricetin and blank NLCs as control groups on selected cell lines. Overall, this study used a systematic formulation comprising of lipid materials to develop a nanostructured lipid carrier, which could overcome the drug delivery issues associated with myricetin for effective wound healing.

Keywords: Nanostructured lipid carriers; Lipid nanomaterials; Biomedical materials; Myricetin; Localized drug delivery, Functional nanomaterials

P0178 • Rituparna Deo

ICEAM2026-POSTER-0178 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

NON-ENZYMATIC ELECTROCHEMICAL SENSOR FOR SELECTIVE DETECTION OF DOPAMINE IN THE PRESENCE OF ASCORBIC ACID USING CuO/rGO NANOCOMPOSITE

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Abstract

The concentration of the neurotransmitter dopamine in human blood serum is 10^{-8} M. Numerous neurological conditions, including schizophrenia and Parkinson's disease, are caused by its dysregulation. Therefore, early identification of these disorders depends on accurate and sensitive detection of dopamine. An electrochemical sensor using CuO/rGO nanocomposite was developed for the sensitive and selective detection of dopamine. The composite was prepared by the ultrasonication process, and resulted nanocomposite was characterized by X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM), Uv-Vis spectroscopy. From XRD the phase was confirmed and the FESEM image shows the presence of CuO in rGO sheet, which confirms the nanocomposite formation. The phase was verified by XRD, and the presence of CuO in the rGO sheet is visible in the FESEM image, confirming the formation of the nanocomposite. Faster electron transfer rates at the electrode surface are made possible by the UV-Vis's lower band gap value of 2.1 eV. The detection technique for dopamine includes Cyclic voltammetry (CV), which shows the enhanced catalytic activity due to the synergistic effect of rGO and CuO. The selectivity of the electrode for dopamine was also demonstrated in the presence of ascorbic acid. The sensor also shows long-term stability, which proves its efficiency as an electrochemical sensor for the detection of dopamine.

TI-INDUCED ENHANCEMENT OF FERROELECTRICITY AND STABILIZATION OF THE METASTABLE STATE IN TETRAGONAL ZnZrO_3 THIN FILMS

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Abstract

Stabilizing metastable ferroelectric states is essential for realizing negative-capacitance (NC) behaviour in low-power electronic devices. Here, we investigate the effect of Ti substitution on the structural, dielectric, ferroelectric, electronic, and energy-landscape characteristics of tetragonal ZnZrO_3 thin films. ZnZrO_3 (ZZO), $\text{ZnZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ (ZZT1) and $\text{ZnZr}_{0.5}\text{Ti}_{0.5}\text{O}_3$ (ZZT2) films were fabricated by sol-gel spin coating. XRD confirms that Ti incorporation modifies the lattice while preserving the tetragonal structure, accompanied by composition-dependent microstructural evolution. Ti substitution improves dielectric stability and reduces dielectric loss, with ZZT2 exhibiting the most favourable response. Ferroelectric measurements reveal enhanced polarization and improved switching characteristics with Ti incorporation, with ZZT2 exhibiting the optimum ferroelectric response. Landau–Khalatnikov analysis reveals a pronounced modification of the double-well free-energy landscape, accompanied by an S-shaped polarization–electric-field response associated with the metastable NC region. Electronic-structure analysis further indicates enhanced charge polarizability following Ti incorporation. PUND and leakage-current measurements support the improved switchable polarization and electrical performance of ZZT2. These findings demonstrate that optimized Ti substitution provides an effective route for engineering the coupled structural, electronic, and ferroelectric energy landscape of ZnZrO_3 toward metastable-state stabilization and NC-based low-power electronic applications.

Keywords: Ferroelectricity, Metastable state, Landau–Khalatnikov theory, Energy landscape; Thin films.

P0212 • V. Bhasker Raj

ICEAM2026-POSTER-0212 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

Hybrid PCA–ANN Framework for Hazardous Vapor Classification Using an Electronic Nose

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Abstract

Air pollution from hazardous vapors/gases and volatile organic compounds (VOCs) causes many environmental and health problems, thus requiring robust smart gas detection systems. In this study, an E-nose device was designed employing a four-channel Surface Acoustic Wave (SAW) sensor array, where each channel is functionalized with metal oxide sensors. The purpose of this work is the differentiation of simulants of hazardous vapors of CW agents (Dibutyl sulfide (DBS), diethyl chlorophosphate (DECP), and chloroethyl phenyl sulfide (CEPS)), fuels and volatile organic compounds. For data analysis, the Principal Component Analysis (PCA) was applied to reduce dimensionality while preserving the essential information. Afterward, Artificial Neural Network (ANN) models were trained on the original sensor data as well as on PCA-derived features. The performance of these models was evaluated on the basis of training and testing datasets in terms of the Root Mean Square (RMS) error. Comparative results proved that the PCA-ANN hybrid model is capable of efficient vapor classification utilizing a smaller number of hidden neurons than the traditional ANN model. The proposed methodology is a promising solution for smart hazardous vapors classification.

Keywords: - Air Pollution Detection, Metal Oxide (MOX) Sensors, Neural network, Volatile Organic Compounds (VOCs), PCA, ANN.

P0220 • Dr. Mirza Samiulla Beg

ICEAM2026-POSTER-0220 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

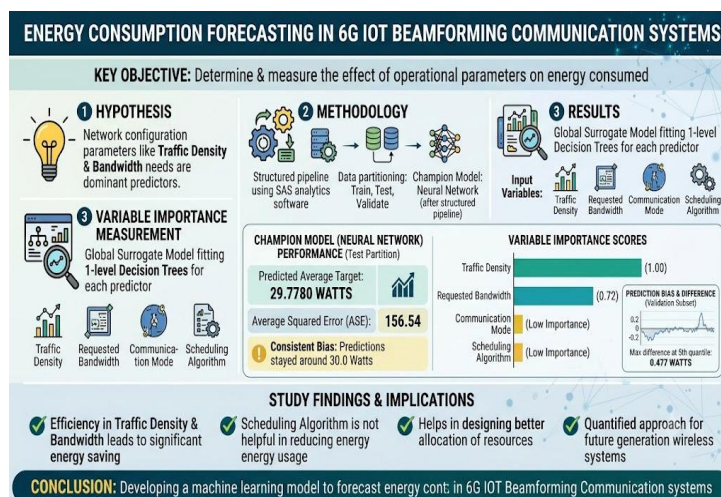
PREDICTIVE MODELING OF ENERGY CONSUMPTION IN 6G IOT BEAMFORMING SYSTEMS: IDENTIFYING KEY OPERATIONAL DRIVERS VIA NEURAL NETWORKSDr. Mirza Samiulla Beg¹, Author Name², Author Name³¹ Department Computer Science and Engineering, Poornima University, Jaipur, Rajasthan, India

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Abstract

This report provides the development of a predictive machine learning model to forecast the consumption of energy in 6G IoT Beamforming Communication Systems where our key objective is to determine and measure the effect of the most important influencing factors or operational parameters with respect to the energy consumed. Our hypothesis was that the network configuration parameters such as the density of traffic and the bandwidth needs will be the dominant predictors of the consumption of energy and our methodology involved the use of a Neural Network model as the selected champion model after running a structured pipeline using SAS analytics software. We partitioned the data set into train, test, and validate partitions and performed variable importance measurement through the use of a Global Surrogate Model that fitted one-level Decision Trees for each predictor. The input variables used include Traffic Density, Requested Bandwidth, Communication Mode, and Scheduling Algorithm. The champion model predicted an average target value of 29.7780 watts and an average squared error of 156.54 on the test partition. Traffic Density and Requested Bandwidth were the two main predictors with scores of 1.00 and 0.72 respectively, while the other two had very low importance scores. However, the prediction was consistently biased with the predictions staying around 30.0 Watts but varying mean in real, with the maximum difference observed at 0.477 watts in the validation subset at the 5th quantile of the depth. This study has provided a quantified approach to understanding the important factors influencing energy consumption in future generation wireless systems and helps in designing better allocation of resources. The findings clearly show that the efficiency in traffic density and bandwidth can lead to significant energy saving, whereas the schedule algorithm is not helpful in reducing energy usage.

Keywords: 6G Internet of Things (IoT), Beamforming, Energy Consumption Prediction , Neural Networks , Operational Driver Analysis



PHYSICAL PROPERTIES OF SAMARIUM DOPED ALUMINIUM BORATE GLASSES**Payal, Rajni Bala**

Department of Physics, Maharshi Dayanand University, Rohtak, Haryana, 124001, India

Corresponding Author Email: payalmalik0940@gmail.com**Abstract**

Samarium doped aluminium borate glasses were synthesized using the melt-quenching technique. The X-ray diffraction pattern shows a broad hump rather than sharp peaks, confirming the non-crystalline nature of the prepared series. The incorporation of samarium ions was found to influence the physical parameters like density (ρ), molar volume (M_v), crystalline volume (M_c), oxygen packing density (OPD) interionic distance (R_i), polaron radius (R_p), and field strength (F) of the host glass. With the increase in Sm^{3+} ion concentration, increase in density showed the replacement of lighter host ions by heavier samarium ions and the molar volume, crystalline volume, and oxygen packing density (OPD) of the prepared glass samples increase. The findings demonstrate that Sm^{3+} doping systematically modifies the physical framework of oxide glasses, with the simultaneous increase in OPD and molar volume offering new insights into their structural behaviour and potential for photonic applications.

P0225 • RADHIKA

ICEAM2026-POSTER-0225 | Poster Presentation | Day 2, 09 Oct 2026, , Tea Break & Poster Session

PHYSICAL PROPERTIES OF LITHIUM MODIFIED TITANIUM BISMUTH BORATE GLASSES

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Abstract

A series of $\text{Li}_2\text{O} \cdot \text{TiO}_2 \cdot \text{Bi}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$ glass varying concentrations of lithium was prepared using melt-quench technique. The non-crystalline nature of the prepared series is confirmed by the X-ray diffraction spectra. To evaluate the effect of Li_2O , parameters like density (ρ), molar volume (M_v), interionic distance (R_i), polaron radius (R_p), oxygen packing density (OPD), and field strength (F) were calculated. The decrease in density and molar volume with composition, indicating that structural changes in glass network. The decrease in interionic distance indicates that the ions move closer shows stronger interaction among neighbouring ions.



Poster Session III

ACS Applied Energy Materials (Day 2, 09 Oct 2026) • 58 Posters

P0003 • Vipin Kumar Gupta

ICEAM2026-POSTER-0003 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

ENHANCED THERMOELECTRIC PERFORMANCE AND CARRIER-TYPE TRANSITION IN Ce-MODIFIED TiNiSn HALF-HEUSLER ALLOYS: A FIRST-PRINCIPLE APPROACHVipin Kumar Gupta¹, Raj Kumar¹, Nidhi Mani Tripathi¹, Upendra Kumar^{1*}¹*Advanced Functional Materials Laboratory, Department of Applied Sciences, Indian Institute of Information Technology Allahabad, Prayagraj, Uttar Pradesh, India*

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Abstract

Half-Heusler alloys are the most promising candidate for large-scale thermoelectric power generation. TiNiSn-based half-Heusler alloys are promising thermoelectric materials due to their excellent thermal stability and favorable electronic transport; however, their relatively high lattice thermal conductivity challenges their energy conversion efficiency. In this work, we accomplished a systematic study of the structural, electronic, and thermoelectric properties of TiNiSn $Ce_{0.125}Ti_{0.875}NiSn$, and $Ce_{0.25}Ti_{0.75}NiSn$ based on density functional calculation (WIEN2k), the quasi-harmonic Debye model, the Slack model, and semiclassical Boltzmann transport theory. Structural optimization confirms the stability of all studied compositions. The Ce substitutions alter the electronic structure and profoundly reduce the band gap from 0.451 eV for pristine TiNiSn to 0.165 eV for 12.50% Ce substitution, whereas a slightly larger band gap of 0.340 eV is achieved for 25% Ce doping. The prominent band gap reduction at moderate Ce doping concentration is due to the Ce-induced electronic states and orbital hybridization enhanced close to the Fermi level, whereas the partial recovery of the band gap at higher Ce doping concentration is attributed to the altered electronic structure and symmetry of the doped supercell. The incorporation of Ce also led to a large lattice distortion and mass fluctuation, thereby enhancing phonon scattering and effectively suppressing the lattice thermal conductivity. Furthermore, the transport calculation reveals a carrier-type transition from p-type conduction in pristine and 12.5% Ce-doped TiNiSn to n-type conduction in $Ce_{0.25}Ti_{0.75}NiSn$ which suggests an effective carrier engineering by rare-earth substitution. The concurrent optimization of electronic and photonic transport leads to a significant enhancement of the thermoelectric figure of merit (zT) reaching 0.87 for $Ce_{0.125}Ti_{0.875}NiSn$ and 1.13 for $Ce_{0.25}Ti_{0.75}NiSn$. The ability to achieve both p-type and n-type transport in the same TiNiSn material system offers an attractive platform for fabricating thermoelectric modules with improved material compatibility and reduced interfacial losses. These observations suggest that Ce substitution is a robust method for altering the electronic configuration, charge-transport mobility, and phonon scattering in TiNiSn, providing a practical route to fabricating high-performance half-Heusler thermoelectric materials for waste-heat recovery, automotive exhaust energy extraction, industrial heat retrieval, and high-temperature power generation.

Keywords: Half-Heusler alloys, Carrier-transition, Lattice thermal conductivity, WIEN2k, Thermoelectric material

P0009 • ILAVARASI A

ICEAM2026-POSTER-0009 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

LINKER-DEPENDENT ELECTROCHEMICAL PERFORMANCE OF METAL-ORGANIC FRAMEWORK/BIOMASS-DERIVED ACTIVATED CARBON COMPOSITES FOR SUPERCAPACITORS

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Abstract

The development of high-performance electrode materials is essential for advancing electrochemical energy-storage technologies. In this study, a metal–organic framework (MOF)/biomass-derived activated carbon composite was developed as an electrode material for supercapacitor applications. The influence of organic linker composition on the structural and electrochemical properties of the MOF was investigated by employing two different linkers individually and in combination. Biomass-derived activated carbon was prepared through hydrothermal treatment and subsequently incorporated into the MOF matrix using a solvothermal synthesis approach. The integration of activated carbon was intended to enhance electrical conductivity, surface area, and accessibility of electrochemically active sites while providing a porous conductive network for efficient ion transport. The synthesized materials were systematically characterized to evaluate their structural, morphological, and surface properties. Their electrochemical performance was investigated using cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. The MOF/activated carbon composite exhibited improved electrochemical characteristics compared with the individual components, demonstrating the complementary contribution of the porous MOF framework and biomass-derived carbon. These findings highlight the potential of MOF/biomass-derived activated carbon composites as promising electrode materials for high-performance supercapacitor applications.

Keywords: Metal–organic framework (MOF); Biomass-derived activated carbon; Supercapacitor; Linker engineering; Porous electrode; Electrochemical energy storage.

P0010 • Vishnu, Musammimul, Abhishek

ICEAM2026-POSTER-0010 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Enhanced β -Phase and Dielectric Properties in SnO_2 -hBN/PVDF Flexible Piezoelectric Nanocomposite FilmsVishnu Prajapati¹, Musammimul Hoque¹, Abhishek Kumar¹, Savita Sharma², Nitin K. Puri^{1,3}, Shailesh N. Sharma^{1,*}¹Department of Applied Physics, Delhi Technological University, Shahbad Daulatpur, Delhi, 110042, India²Department of Physics, Kalindi College, University of Delhi, New Delhi, Delhi, 110008, India³National Institute of Electronics and Information Technology (NIELIT) Patna, Amhara, Bihta, Bihar, 8010116, India

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Abstract

Flexible piezoelectric nanogenerators (PENGs) have attracted great attention as potential devices for scavenging mechanical energy from low-frequency and human-induced motions. In the present study, synthesis of hBN doped SnO_2 ceramic powder by hydrothermal method and preparation of SnO_2 -hBN/PVDF composite films were done and their structural and phase characteristics were studied. Initially, hBN and SnO_2 ceramic powders were prepared separately and then mixed to obtain hBN-doped SnO_2 ceramic powder. The SnO_2 -hBN ceramic powder containing 7% hBN was characterised by X-ray diffraction (XRD) to investigate its crystalline structure and phase formation. Moreover, SnO_2 -hBN was embedded into a PVDF polymer matrix to prepare flexible composite films with various filler contents of 0%, 3%, 6%, 9%, and 12% in polymer matrix. The prepared composite films were systematically characterised by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) and field emission scanning electron microscope (FE-SEM). The crystalline structure and phase formation of the composites were investigated by XRD, while the structural and molecular interactions between PVDF and the ceramic filler were investigated by FTIR. The surface morphology and distribution of the SnO_2 -h-BN filler in PVDF matrix were studied using FE-SEM. Among the investigated compositions, the 6% SnO_2 -hBN/PVDF composite showed a relatively enhanced β -phase related peak, indicating the enhancement in the β -phase content of PVDF. The observed structural and morphological changes reveal the influence of the incorporation of SnO_2 -hBN on the properties of PVDF-based composite films. These results indicate that SnO_2 -hBN/PVDF composites have potential for functional flexible material applications, especially for piezoelectric and energy-harvesting devices.

Keywords: Flexible energy harvesting, β -phase, PENG, Dielectric permittivity

P0011 • Mayank Lokesh Abhishek

ICEAM2026-POSTER-0011 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Flexible Piezoelectric Nanogenerators Based on Sol-Gel Synthesized TiO₂-Doped V₂O₅/PVDF Nanocomposite Films for Energy Harvesting ApplicationsMayank Pareek¹, Lokesh Kumar¹, Abhishek Kumar¹, Savita Sharma², Nitin K. Puri^{1,3}, Vinod Singh^{1,*}¹Department of Applied Physics, Delhi Technological University, Shahbad Daultapur, Delhi, 110042, India²Department of Physics, Kalindi College, University of Delhi, New Delhi, Delhi, 110008, India³National Institute of Electronics and Information Technology (NIELIT) Patna, Amhara, Bihta, Bihar, 8010116, India

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Abstract

Rising demand for sustainable energy harvesting and flexible wearable electronics necessitates functional materials that convert low-frequency mechanical stimuli into electrical energy. Here, a flexible piezoelectric nanogenerator (PENG) was fabricated by incorporating sol-gel-synthesized 10% TiO₂-doped V₂O₅ (VT10) nanofillers into a PVDF matrix at 0, 4, 8, 12, and 16 wt% loadings, with films prepared on glass substrates via drop-casting. XRD confirmed phase purity and crystallinity of the ceramic powder and composite films. FTIR analysis showed a marked increase in electroactive β -phase and reduced α -phase content at optimal filler loading, while FESEM confirmed uniform nanoparticle dispersion within the polymer matrix. Under mechanical deformation, the device exhibited significantly enhanced electrical output, confirming VT10's role in strengthening PVDF's piezoelectric response. In comparison to pristine PVDF, impedance analysis showed that 12 weight percent VT10/PVDF had the highest dielectric permittivity and the lowest dielectric loss, which correlated with β -phase enhancement. The manufactured PENG successfully harvested useful electrical energy while exhibiting exceptional flexibility and sensitivity to human biomechanical actions, such as finger tapping and hand movement. These results make VT10/PVDF nanocomposites viable alternatives for wearable energy-harvesting and motion-sensing systems.

Keywords: PVDF, VT10/PVDF composite films, Piezoelectric nanogenerator (PENG)

P0012 • ATUL KUMAR VERMA

ICEAM2026-POSTER-0012 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

HIGH TEMPERATURE EFFECT ON SURFACE MORPHOLOGY AND ELECTRICAL PROPERTIES OF MAGNESIUM FERRITE BASED HYDRO ELECTRIC CELL (HEC)Atul Kumar Verma¹, Satish Kumar¹*¹Department of Physics and Computer science, Dayalbagh Educational, Institute, Agra 282005
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Abstract

Magnesium ferrite (MgFe_2O_4) was synthesized by the solid-state reaction method at 850 °C for 5 hours. Synthesized material was converted into a pellet of size (2 cm × 4 cm × 0.5 cm). Pellet sintered at 850 °C for 2 hours for hardening. The surface morphology of the material involves nucleation taking place at high temperature, which was observed by FESEM, and alters the size and shape of grains into nano flakes, spheres, and pores created on the surface of the material. The change in grain size was clearly calculated by XRD and visible in FESEM, which is nearly 72 -80 nm. This hardened pellet was converted into HEC (AJ102) by attaching a Zn thin plate (anode) and comb-patterned Ag paste (cathode). The open-circuit voltage 974mV and a short-circuit current of 739 mA were produced with the cement matrix by water dissociation at the surface of HEC in nano pores.

Keywords: HEC, Physioabsorption, Chemidissociation, Nanopores etc.

P0013 • Sreya Das

ICEAM2026-POSTER-0013 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Porous Halide Double Perovskite $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ for High-Capacitance Energy Storage and Prospective Photo-Assisted Applications

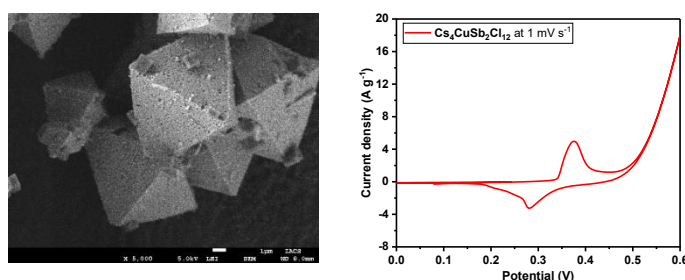
Sreya Das¹, Abhirup Chatterjee¹, Soumen Maiti² and Kalyan Kumar Chattopadhyay^{1,3*}¹Department of Physics, Jadavpur University, Kolkata 700032, India²Department of Physics, St. Thomas College of Engineering & Technology, Kolkata 700023, India³School of Materials Science and Nanotechnology, Jadavpur University, Kolkata 700032, India

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Abstract

The growing demand for high-performance, rapid, and sustainable energy-storage technologies has stimulated extensive research into advanced electrode materials. While carbon nanostructures, transition-metal oxides, conducting polymers, and two-dimensional MXenes have attracted considerable attention, Cu-based halide double perovskites remain largely unexplored despite their structurally diverse frameworks, compositional tunability, defect tolerance, and versatile electronic properties. In this work, we report the synthesis of the halide double perovskite $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ through a facile solution-based approach and demonstrate its viability as an electrochemical electrode. Structural phase purity was confirmed by XRD, while FESEM imaging revealed a porous surface morphology favorable for electrolyte penetration. Electrochemical measurements in a three-electrode configuration (1 M KOH, 0-0.6 V vs Ag/AgCl) revealed a vacancy-assisted charge-storage mechanism. The presence of halide vacancies provides favorable sites for OH^- interaction/intercalation, while reversible Cu-based redox reactions contribute to faradaic charge transfer. Consequently, $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ exhibits a remarkably high specific capacitance of $\sim 4384 \text{ F g}^{-1}$ at 1 mV s^{-1} , alongside excellent cycling stability, retaining $\sim 70\%$ of its initial capacitance after a prolonged charge–discharge cycle. Furthermore, we explore the intrinsic photo-responsive nature of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$, which demonstrates potential in photodetection and provides an opportunity to couple light-induced charge generation with electrochemical energy storage. This photo-response could potentially be utilized to develop photo-induced supercapacitors, where photogenerated charge carriers may influence the charge-storage kinetics and electrochemical response. These findings establish halide double perovskites as an emerging class of multifunctional electrode materials and highlight $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ as a promising candidate for next-generation electrochemical and photo-assisted energy-storage technologies.

Keywords: $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$, halide double perovskite, pseudo-capacitance, photo-assisted energy storage.

Figure 1: FESEM image and CV profile of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ 

P0014 • Abhirup Chatterjee

ICEAM2026-POSTER-0014 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Jahn-Teller mediated Piezoelectricity in Lead-Free CsCuX_3 ($\text{X}=\text{Cl}, \text{Br}$) for Efficient Energy Harvesting Application

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Abstract

Lead-free halide perovskites have emerged as promising candidates for next generation energy harvesting applications, offering exceptional environmental stability. The structural flexibility and Jahn-Teller active Cu^{2+} centers in copper-based halide perovskites provide an excellent opportunity to harness their piezoelectric characteristics through halide substitution. To address the structural and functional factors driving piezoelectricity in copper-based halide perovskites, we investigated piezoelectric characteristics of CsCuX_3 ($\text{X} = \text{Cl}, \text{Br}$) with particular emphasis on the role of Jahn-Teller distortion and structural dimensionality. CsCuX_3 ($\text{X} = \text{Cl}, \text{Br}$) crystals were synthesized via a facile slow-evaporation method having hexagonal and orthorhombic structures respectively. The cooperative Jahn-Teller distortion of Cu^{2+} ions facilitate the formation of a macroscopic non-centrosymmetric lattice, while the larger, more polarizable Br^- ions form softer Cu-Br bonds enabling enhanced lattice deformation. The piezoelectric behavior of the sample was investigated using piezoresponse force microscopy. We utilized density functional theory (DFT) calculations to evaluate the electronic band structure and density of states for CsCuBr_3 . Furthermore, a CsCuBr_3 and PVDF composite was fabricated to investigate its potential for energy harvesting applications as a piezoelectric nanogenerator. Under an optimized applied pressure of ~ 25 kPa, the fabricated nanogenerator device delivered instantaneous output values of ~ 100 V and ~ 9.5 μA . The device also exhibited stable output performance under various mechanical stimuli- such as heel pressing, knee bending, and finger tapping- demonstrating its practical applicability for wearable energy harvesting. Our findings reveal new insights into the origin of piezoelectricity in all-inorganic lead-free copper-based halide perovskites and provide a viable strategy to tailor their properties for next-generation self-powered electronics and energy harvesting applications.

Keywords: Lead-free halide perovskite; Jahn-Teller distortion; Halide substitution; piezoelectricity; Energy harvesting.

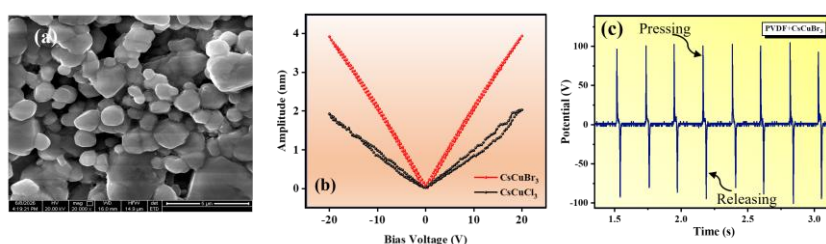


Fig 1: (a) FESEM of CsCuBr_3 (b) PFM amplitude of CsCuX_3 (c) Nanogenerator output of PVDF/ CsCuBr_3 composite film.

P0017 • DIPTI MEENA

ICEAM2026-POSTER-0017 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Engineering a polyvinyl alcohol polymer gel electrolyte with CeP_2O_7 and MXene for enhanced ionic transport and supercapacitorDipti Meena¹, Jay N. Mishra^{1,2}, Akash Patel¹, Prabhakar Singh^{1*}¹*Department of Physics, Indian Institute of Technology (BHU) Varanasi, 221007, Uttar Pradesh, India*²*Research Centre for Electronic and Optical Materials, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan*

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Abstract

The development of highly ion-conducting and thermally stable gel polymer electrolytes is crucial for advancing efficient and reliable electrochemical energy-storage systems. Herein, a CeP_2O_7 /MXene-modified poly(vinyl alcohol) (PVA) gel electrolyte is developed for symmetric supercapacitor applications by integrating cerium pyrophosphate and two-dimensional MXene within a PVA polymer matrix followed by KOH loading. Structural analysis confirms the formation of phase-pure cubic CeP_2O_7 with an $\text{Fm-}3m$ space group and a lattice parameter of 8.338 Å, with crystallite sizes of 42.6 nm and 40.22 nm obtained from Scherrer and Williamson-Hall analyses, respectively. Incorporation of CeP_2O_7 into PVA decreases the crystallinity of the polymer matrix, whereas subsequent MXene incorporation increases the crystallinity from 53.29% to 65.38%, indicating improved structural organisation of the composite. Morphological and elemental analyses confirm the formation of a relatively homogeneous composite membrane, while FTIR and thermal analyses reveal strong filler–polymer interactions and enhanced thermal stability, with the CeP_2O_7 /PVA/MXene membrane exhibiting a degradation temperature of approximately 270 °C. Electrochemical impedance spectroscopy demonstrates enhanced ionic transport following MXene incorporation, with the conductivity increasing progressively with temperature up to 180 °C. Further KOH loading substantially enhances the ionic conductivity of the composite membranes, enabling their application as gel electrolytes in symmetric supercapacitors. The CeP_2O_7 /PVA/MXene-based gel electrolyte exhibits improved capacitive characteristics, higher specific capacitance over the investigated current-density range, and enhanced energy-storage capability compared with the CeP_2O_7 /PVA counterpart. The improved electrochemical response is attributed to the combined contribution of the CeP_2O_7 -modified PVA matrix and the functionalized two-dimensional MXene network, which facilitates ion transport while improving the structural and thermal stability of the electrolyte. These findings demonstrate that CeP_2O_7 /MXene dual modification provides an effective strategy for engineering PVA-based gel polymer electrolytes for advanced symmetric supercapacitor applications.

Keywords: PVA/ CeP_2O_7 /MXene, Gel polymer electrolyte, supercapacitor

P0018 • Jadav Hetvi Bharatkumar

ICEAM2026-POSTER-0018 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

FIRST-PRINCIPLES STRAIN MANIFESTATIONS ON h -Be₂C MONOLAYER FOR LI-ION BATTERY APPLICATION USING DFTHetvi Jadav^a, Aditya Patel^b, Himanshu Pandey^{a*}^a*Condensed Matter & Low-Dimensional Systems Laboratory, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat, 395007, India*^b*Materials and Biophysics Group, Department of Physics, Sardar Vallabhbhai Institute of Technology, Surat, Gujarat, 395007, India*

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Abstract

To systematically modify the structural, electrical, and electrochemical properties of 2D materials without changing their chemical composition, strain engineering has become an efficient and adaptable approach. In this work, we perform a detailed first-principles study using density functional theory (DFT) to examine the impact of biaxial strain on the major battery-relevant parameters of a hexagonal beryllium carbide (h -Be₂C) monolayer using Quantum Espresso software packages [1]. Both compressive and tensile deformation regimes were covered by the systematic application of biaxial strain ranging from –5% to +5%. Van der Waals dispersion corrections were added to the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) [2] parameterization of the exchange–correlation functional in order to precisely describe interlayer and adsorption interactions. Lithium-ion adsorption energetics were evaluated across multiple high-symmetry adsorption sites. Applied strain functions as an efficient modulator of the electronic characteristics that directly affect the electrode's electrical conductivity, according to electronic structure calculations, covering band structure and density of states (DOS). The diffusion energy barrier is calculated using the nudged elastic band (NEB) approach [3], which shows a dependence on the applied strain: compressive strain increases the barrier and restricts ion mobility, whereas tensile strain gradually reduces the barrier and improves ionic transport. In addition, the theoretical specific capacity and average open-circuit voltage were measured as functions of strain. Thus, strain engineering can be used as a tunable knob to optimize various battery performance metrics.

Keywords: Lithium-ion battery; Strain engineering; 2D material; density functional theory**References:**

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P0020 • ABHISHEK KUMAR

ICEAM2026-POSTER-0020 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Flexible SnS₂ NS/PVDF Piezoelectric Nanogenerator for Wearable Sensing and Sustainable Energy Harvesting

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Abstract

Tin disulfide (SnS₂) nanosheets were synthesized via a hydrothermal method and characterized using XRD, FESEM, HRTEM, and Raman spectroscopy, confirming their layered hexagonal morphology. SnS₂ NS /PVDF composite films with varying filler content (0–12 wt%) were fabricated by drop-casting to evaluate concentration-dependent structural and dielectric behavior. FTIR and XRD analyses revealed that the 9 wt% SnS₂ NS/PVDF film exhibited the maximum electroactive β -phase fraction (80.38%), attributed to favorable interfacial interactions between SnS₂ and PVDF dipoles. FESEM and AFM confirmed uniform nanosheet dispersion, while dielectric studies showed this composite possessed the highest dielectric constant ($\epsilon \sim 51.7$) at low frequency (100 Hz) and elevated temperature (~ 97.2 °C), along with reduced dielectric loss. The optimized 9 wt% film was used to fabricate a piezoelectric nanogenerator (PENG), yielding higher open-circuit voltage and short-circuit current than pristine PVDF, with consistent durability. The device effectively sensed human body motions such as finger bending, punching, heel tapping, and twisting, and demonstrated energy-harvesting capability by powering LEDs, charging–discharging a capacitor, and operating a digital stopwatch and wristwatch, with corresponding power density evaluated. These results establish SnS₂ as an efficient nucleating agent for β -phase PVDF and highlight its potential for flexible, self-powered sensing and energy-harvesting devices. Future studies may explore scalability and the integration of hybrid energy harvesting.

Keywords: PVDF, SnS₂ NS/PVDF, composite films, Piezoelectric nanogenerator (PENG)

P0026 • Sadhana Matth

ICEAM2026-POSTER-0026 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

HIGH-PERFORMANCE THERMOELECTRIC PROPERTIES OF HALF-HEUSLER COHFZ (Z=SI/SN/SB): A FIRST-PRINCIPLES STUDY WITH TEMPERATURE-DEPENDENT RELAXATION TIME

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Abstract

In the ongoing search for innovative thermoelectric (TE) materials with superior TE performance globally, we aim to investigate the possible use of *half*-Heusler alloy CoHfZ (Z=Si/Sn/Sb) in TE applications. The structure stability, thermodynamic inertia, and electrical and thermal transport properties are analyzed using density functional formalism and semi-classical Boltzmann transport theory. Positive phonon frequencies confirm these alloy's dynamical stability, and the Born-Huang stability criterion is also satisfied, confirming the robust mechanical stability. A large Seebeck voltage between 110.56 $\mu\text{V/K}$ to 264.61 $\mu\text{V/K}$ is estimated, an essential and typical requirement for improved heat-to-electricity conversion efficiency. This Seebeck voltage can be further increased by an order of magnitude with suitable doping. The Slack's model are used to compare the lattice thermal conductivity. Despite the commonly used constant relaxation time approximation to estimate the TE performance, we adopt the temperature-dependent relaxation time and found a clear drop in figure-of merit (zT) from those estimated without considering the lattice thermal conductivity and relaxation time both, still, the zT values are remarkably more than two, for the temperatures above 500 K, which is a striking numeral in the field of TE materials.

Keywords: Half-Heusler Alloys; Mechanical properties; First-Principle; DFT; Thermoelectric Properties

P0036 • Anvi

ICEAM2026-POSTER-0036 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

SYNTHESIS AND CHARACTERISATION OF BIOCHAR-REDUCED GRAPHENE OXIDE (rGO) COMPOSITE ELECTRODES FOR SUSTAINABLE BATTERY APPLICATIONS

Anvi*, Mukesh Kumar

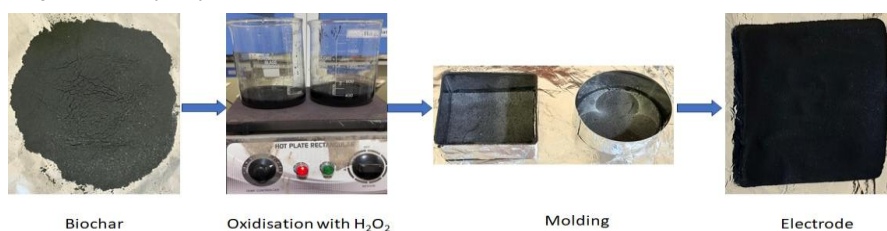
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Abstract

The growing demand for sustainable and cost-effective energy storage systems has intensified research into biomass-derived carbon materials as alternatives to conventional graphite and metal-based electrodes. This study focuses on the synthesis and characterisation of biochar-based electrodes for battery applications, with particular emphasis on surface functionalisation using hydrogen peroxide (H_2O_2) oxidation and composite engineering with reduced graphene oxide (rGO). Biochar was synthesised by pyrolysis of biomass precursors under controlled temperature and inert atmosphere, followed by oxidative treatment with H_2O_2 to introduce oxygen-containing functional groups, including hydroxyl, carboxyl, and carbonyl groups, onto the carbon surface. This modification is expected to enhance hydrophilicity, ion accessible active sites, and pseudocapacitive contribution. The oxidised biochar was subsequently combined with rGO through solution mixing to develop hybrid electrode architectures that integrate the enhanced surface chemistry and porosity of oxidised biochar with the high electrical conductivity and mechanical stability of rGO. Structural and morphological properties were investigated using XRD, FTIR, Raman spectroscopy, and SEM/TEM. Electrochemical performance was evaluated using cyclic voltammetry (CV), Galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) to determine specific capacitance/capacity, weight capability, and long-term cycling stability. The H_2O_2 -oxidised biochar/rGO composite electrodes exhibit improved wettability, higher specific capacitance, reduced charge-transfer resistance, and enhanced cycling stability compared with pristine and oxidised biochar electrodes. The synergistic interaction between oxygen-rich surface functionalities and a conductive rGO network highlights the potential of these composites as low-cost, sustainable electrode material for next-generation eco-friendly energy storage applications.

Keywords: Pyrolysis; Biochar; rGO; electrodes



DEVELOPMENT OF Li⁺ IONS INCORPORATED PVdF-HFP/PMMA GEL POLYMER ELECTROLYTE FOR MXENE- BASED SOLID-STATE SUPERCAPACITORS.

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Abstract

Gel polymer electrolytes (GPEs) are attracting significant attention as safer, flexible alternatives to liquid electrolytes for next-generation energy storage devices. In this study, poly(vinylidene fluoride-co-hexafluoropropylene)(PVDF-HFP) and poly(methyl methacrylate) (PMMA) polymer blend, 1-ethyl-3-methylimidazoliumbis(trifluoromethylsulfonyl)imide (EMIMTFSI) ionic liquid and LiBF₄ salt were co-incorporated into a GPE using a and The PVdF-HFP/PMMA combination has been chosen for its favourable electrochemical stability, mechanical integrity, and thermal stability while EMIMTFSI and LiBF₄ were introduced to enhance ionic conductivity, provide additional charge carriers, suppress crystallinity, and improve the thermal and dimensional stability of the film. Structural and morphological analyses (XRD, FTIR, SEM) confirmed effective polymer blending, reduced crystallinity, and uniform distribution of the ionic liquid and salt within the polymer network, while TGA verified improved thermal stability of the electrolyte. The optimized GPE exhibited an ionic conductivity of $1.12 \times 10^{-3} \text{ S cm}^{-1}$ and a wide electrochemical stability window of 5.2 V, indicating efficient ion transport pathways and suitability for high-voltage devices. The GPE was integrated into a solid-state supercapacitor employing an MXene-based electrode, delivering a specific capacitance of $\sim 80 \text{ F g}^{-1}$.

Keywords: Gel polymer electrolyte, PVDF-HFP/PMMA blend, Ionic liquid (EMIMTFSI), MXene (Ti₃C₂Tx), and Solid-state supercapacitor.

P0044 • Akash Patel

ICEAM2026-POSTER-0044 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Ni-doped MnCo₂O₄ spinel structured nanoparticles for supercapacitor electrode materialAkash Patel¹, Hemant Kumar¹, Jay N Mishra^{1,2}, Dipti Meena¹, Samriddhi Pathak¹, Prabhakar Singh^{1*}¹ Department of Physics, Indian Institute of Technology (BHU), Varanasi, UP, India² Research Centre for Electronic and Optical Materials, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan

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Abstract

The increasing population causes the extreme demand of renewable and sustainable energy technologies. The intermittent nature of renewable energy sources creates opportunity to develop efficient energy storage technology. Among the energy storage technologies, supercapacitors have emerged as next generation energy storage technologies due to its numerous advantages. Such as simple and safe device configuration, rapid charging and discharging enable it to deliver energy quickly, making them perfect for instant power delivery. In this study Ni-doped MnCo₂O₄ electrode material with different levels of Ni doping were analyzed for the supercapacitor application. All materials were synthesized by co-precipitation method. The level of doping start with 0%, 5%, 10%, and 15% which is named as MCO, 5NMCO, 10NMCO, and 15NMCO, respectively. The structural confirmation was done by X-ray diffraction technique. Where no secondary phases were observed. Also, the Raman analysis shows the characteristic spinel structure peaks. Morphological analysis was performed by field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). Where, all samples have particle size in nano range of about 50 nm. Specific surface area of doped material was found as increased as compare to the bare material. The electrochemical measurements were analyzed by cyclic voltammetry (CV), galvanostatic charge discharge (GCD), and electrochemical impedance spectroscopy (EIS). Where the 10NMCO showed the highest specific capacitance of 512 Fg⁻¹ at current density of 0.5 Ag⁻¹ as compared to bare MCO of 181 F g⁻¹. Also, the impedance decreases with increasing Ni-doping, where the equivalent series resistance (ESR) obtained 0.48 Ω for 10NMCO. Therefore, 10NMCO nanomaterial found as considerable electrode material for the supercapacitor application.

Keywords: Ni-doping; MnCo₂O₄; co-precipitation; Spinel; Nanoparticles

P0045 • Akshay Yadav, Abhishek Kumar

ICEAM2026-POSTER-0045 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Effect of KNN-LiSb Filler Concentration on the Piezoelectric Performance of Flexible PVDF-based Composite Films for Energy Harvesting Applications

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Abstract

In this work, we have fabricated a KNN-LiSb/ PVDF based piezoelectric generator (PEG). To construct PEG a piezoelectric filler material is added in PDVF matrix in varying ratio from 0 wt % to 20 wt%. The phase and structural analysis of the fabricated composite films are investigating using XRD (X- Ray Diffraction) and FTIR (Fourier Transform Infrared Spectroscopy). SEM (Scanning Electron Microscopy) analysis of the composite films revealed that the ceramic particles are dispersed uniformly throughout the PVDF matrix. Furthermore, the piezoelectric output performance was tested by applying on the surface of the composite film. The composite film consisting of 15 wt% ceramic filler in the PVDF matrix generating maximum open circuit voltage of 15.47 V. The current work showed that LiSb doped KNN ceramic is a promising filler to enhance the performance of PVDF based piezoelectric generator. Lead-free piezoelectric ceramics can be modified with suitable dopants to provide high-performance PEG. Ultimately, the synthesized flexible piezoelectric generator's outputs indicate that there are significant possibilities for application in wearable and self-powered electronics.

Keywords: Piezoelectricity, PVDF, Flexible, KNN-LiSb, Ceramic.

P0046 • Pallavi Gupta

ICEAM2026-POSTER-0046 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

INTERFACE ENGINEERED NITROGEN-DOPED HIERARCHICAL POROUS CARBON/MOS₂ HETEROSTRUCTURE FOR ENERGY STORAGE APPLICATIONPallavi Gupta¹, Sandeep Chhoker^{1*}¹*Department of Physics and Materials Science, Jaypee Institute of Information Technology, Noida- 201309, Uttar Pradesh, India*

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Abstract

Developing high performance, sustainable electrode materials are critical for advanced electrochemical energy storage system. Therefore, an interface engineered nitrogen doped hierarchical porous carbon/molybdenum disulfide (N-HPC/MoS₂) heterostructure was successfully synthesized via a facile hydrothermal approach utilizing biowaste rice husk as a green, low cost carbon precursor. The initial chemical activation and nitrogen doping yield a robust, high surface area porous framework, while the subsequent hydrothermal growth of MoS₂ on the porous carbon matrix effectively buffers volume expansion, facilitates fast ion/electron transport and prevent the restacking of MoS₂ nanosheet. Synergistic interface engineering between the nitrogen doped carbon substrate and hydrothermal derived MoS₂ created abundant electrochemically active sites and accelerates charge transfer kinetics. As a result, the optimized N-HPC/MoS₂ composite exhibits superior specific capacitance/capacity, excellent rate capability, and outstanding cycling stability. This work highlights a scalable approach for transforming agricultural waste into high value heterostructure materials for next generation energy storage application.

Keywords: *N-HPC/MoS₂ heterostructure; Biomass-derived carbon; Rice husk biowaste; Electrochemical energy storage*

P0050 • Abhimanyu Abhimanyu

ICEAM2026-POSTER-0050 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

METALLIC 1T-MOS₂ AS A CATALYTIC PLATFORM FOR ACCELERATED SULFUR REDOX IN HIGH-PERFORMANCE LI-S BATTERIES

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Abstract

The 1T phase of molybdenum disulfide (1T-MoS₂) has emerged as a promising electrocatalyst for lithium–sulfur batteries (LSBs) owing to its excellent physicochemical characteristics, including high electrical conductivity, abundant catalytically active sites, and strong affinity toward lithium polysulfides (LiPSs). These intrinsic properties can effectively address several critical limitations of Li-S batteries, including polysulfide shuttling, sluggish sulfur redox kinetics, poor rate capability, and inadequate cycling stability. In this work, a simple and scalable approach was employed to utilize 1T-MoS₂ as a catalytic sulfur host for LSBs, thereby enhancing the overall electrochemical activity of the cathode. The results demonstrate that 1T-MoS₂ promotes the adsorption and catalytic conversion of LiPSs while effectively suppressing their shuttle effect, leading to substantially improved electrochemical performance compared with the 2H-MoS₂ counterpart. The S/1T-MoS₂ cathode delivered an initial discharge capacity of **920 mAh g⁻¹** and maintained **750 mAh g⁻¹ after 200 cycles at 1C**, corresponding to a high-capacity retention of **81.5%**. Furthermore, density functional theory (DFT) calculations, including **density of states (DOS) and Bader charge analysis**, were performed to elucidate the underlying mechanisms responsible for the enhanced electrochemical behavior. Overall, these findings demonstrate the potential of **1T-MoS₂ as an efficient electrocatalytic sulfur host** for mitigating key challenges associated with LSB technology.

Keywords: Lithium sulfur batteries, electrocatalyst, polysulphides adsorption, shuttle effect, pouch cell.

P0053 • BITHIKA PATI

ICEAM2026-POSTER-0053 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

NiMoO₄@POLYINDOLE COMPOSITE FOR HIGH-PERFORMANCE SOLID-STATE SYMMETRIC SUPERCAPACITORS**Bithika Pati, Swetapadma Praharaj*, Dibyaranjan Rout****Functional Materials Lab, Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar 751024, Odisha, India*

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Abstract

The development of high-performance electrodes is essential for next-generation electrochemical energy storage technologies [1,2]. In this study, nickel molybdate@polyindole (NiMoO₄@PIN) composite electrodes were successfully synthesized through an in situ oxidative polymerization method. To optimize the electrochemical performance, a series of composites with different weight ratios was systematically prepared. Detailed structural, morphological, and compositional characterizations demonstrate that the incorporation of polyindole induces a distinct morphological evolution in NiMoO₄, generating more accessible channels for efficient ion transport. The electrochemical performance was analyzed using cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The optimized NiMoO₄@PIN composite exhibits a high specific capacitance of 646.6 F/g at a current density of 0.5 A/g. The material also exhibits a high energy density of about 151.7 Wh/kg at a power density of 649.63 W/kg. The superior electrochemical performance is attributed to the synergistic interaction between the pseudocapacitive NiMoO₄ framework and the conductive polyindole network, which collectively enhances charge transfer kinetics and accommodates structural changes during cycling. Further, a solid-state symmetric supercapacitor device was successfully fabricated using PVA/H₂SO₄ gel electrolyte. The all-solid-state symmetric supercapacitor powered a red LED, demonstrating its potential for energy-storage applications.

Keywords: Polyindole; Nickel molybdate; Supercapacitor; Energy storage**REFERENCES**

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P0055 • Pooja Attri

ICEAM2026-POSTER-0055 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

NiCoZn-LDH/1T-2H MoS₂/N-rGO TERNARY COMPOSITE COUPLED WITH BIOMASS-DERIVED ACTIVATED CARBON FOR HIGH PERFORMANCE ASYMMETRIC SUPERCAPACITORS

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Abstract

Nickel-cobalt-Zinc layered double hydroxides (NiCoZn-LDHs), as potential electrode materials for supercapacitors, have unique layered structures and high theoretical specific capacitance. Unfortunately, NiCoZn-LDHs often suffer from inherent low electrical conductivity and their unsatisfactory cyclic stability, hindering their practical applications. In this study, a hybrid electrode material was developed by integrating transition-metal layered double hydroxide (LDH), 1T-2H MoS₂, N-doped reduced graphene oxide (N-rGO). A ternary NiCoZn-LDH/1T-2H MoS₂/N-rGO composite was subsequently synthesized via a hydrothermal route, in which NiCoZn-LDH and 1T-2H MoS₂ were maintained at a 1:1 ratio and the N-rGO content was varied to optimize the synergistic interaction among the components. The NiCoZn-LDH provides abundant redox-active sites, 1T-2H MoS₂ contributes additional electrochemically active sites and facilitates charge transfer, while N-rGO enhances electrical conductivity, ion transport, surface accessibility, and structural stability. The morphology and structure were analyzed using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), and the specific surface area and pore-size distribution were calculated using N₂ adsorption-desorption isotherms (BET method). An asymmetric supercapacitor (ASC) was fabricated using the optimized NiCoZn-LDH/1T-2H MoS₂/N-rGO composite as the positive electrode and corn-husk derived porous activated carbon as the negative electrode. The complementary pseudocapacitive and electric double layer charge-storage mechanisms of the two electrodes are expected to provide an extended operating voltage window and enhanced energy-storage characteristics. This provides new insights for the design of next-generation ASC active materials and is beneficial for the development of new energy storage devices.

Keywords: Supercapacitor; Layered double hydroxide; Biomass; Activated carbon; Energy Storage

P0060 • AMIT KUMAR

ICEAM2026-POSTER-0060 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Non-aqueous gel polymer electrolyte with dual cations for high-performance zinc-sodium hybrid battery

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Rechargeable zinc-ion batteries (ZIBs) are considered as the prominent alternative of lithium-ion batteries (LIBs) because of their considerable energy density, high safety, environment friendly nature and, less toxicity and low-cost of zinc-sheets. However, the uncontrollable dendrite growth and low reversibility of zinc (Zn) electrode are the challenging issues related to the development of high-performance ZIBs. To tackle these issues, various approaches have been adopted including the fabrication of dual-ion hybrid batteries based on the electrolytes with dual cations. Herein, we report the zinc-sodium hybrid battery (ZNHB) fabricated with a non-aqueous hybrid gel polymer electrolyte (hGPE) comprising liquid electrolyte containing dual (Zn and Na) salts dissolved in high flash point solvent adiponitrile (ADN), entrapped a polymer PVdF-HFP. The morphological and structural studies were carried out via field emission scanning electron microscopy and X-ray diffraction respectively, whereas, Fourier transform infra-red spectroscopy was used to confirm the ion-solvent-polymer interactions in hGPE-composition. The thermal stability of hGPE-film was tested by thermogravimetric analysis and differential scanning calorimetry. The gel-films shows good ionic conductivity $\sim 1 \text{ mS cm}^{-1}$ and high thermal stability up to $\sim 150^\circ\text{C}$. The Zn-electrode/hGPE-film interfaces show excellent stability and reversibility of Zn-ions as evident from the long-term electrochemical impedance spectroscopy (EIS) and stripping/plating measurements. A ZNHB-cell has been assembled using Zn-sheet as anode and $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP) added with super-P and electrolyte composition as cathode, separated by the flexible hGPE-film. The charge/discharge measurements of the ZNHB-cell have been performed at different C-rates. The ZNHB-cell exhibits stable discharge capacity of $\sim 100 \text{ mAh g}^{-1}$ at 0.1 C-rate for 100 GCD cycles ($1\text{C} = 117 \text{ mAh g}^{-1}$). The cell has ability to deliver Coulombic efficiency (CE) $\sim 99\%$, indicating its excellent cyclic stability.

Keywords: Gel polymer electrolyte; Electrochemical stability window, Transport number; zinc-sodium hybrid battery; Galvanostatic Charge-discharge

P0062 • Sonu Ghanghas

ICEAM2026-POSTER-0062 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

SUGARCANE BAGASSE-DERIVED POROUS CARBON/RGO INTEGRATED WITH NICKEL-MANGANESE SULFIDE HETEROSTRUCTURES AS AN ELECTRODE MATERIAL FOR SUPERCAPACITOR APPLICATIONSSonu Ghanghas^{1*}, Tanu Bhar¹, Ishu Khatri¹, Latisha Gaba¹, Priya Siwach¹, Kuldeep Singh², Anil Ohlan^{1*}¹ *Department of Physics, Maharshi Dayanand University, Rohtak-124001, Haryana, India*² *Surface Engineering Division (SED), CSIR - National Aerospace Laboratories, Bangalore-560017, Karnataka, India*

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Abstract

Developing supercapacitors that deliver both high energy density and fast power discharge relies heavily on active electrode materials with enhanced chemical and physical properties. In this work, we present an eco-friendly strategy for synthesizing porous activated carbon (AC) from waste sugarcane bagasse using KOH as an activating agent. Furthermore, a ternary composites have been synthesized by in situ growth of nickel-manganese sulfide (NMS) on porous activated carbon and reduced graphene oxide (rGO) at varying weight ratios of rGO via a facile hydrothermal method. Comprehensive structural, morphological, and characterizations including X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Fourier-Transform Infrared Spectroscopy (FTIR), and Brunauer–Emmett–Teller (BET) surface area analysis, have been performed. The high-surface-area biomass-derived porous carbon provides abundant ion-reservoir channels, while rGO serves as a highly conductive backbone that prevents agglomeration of the NMS nanostructure and improves structural stability. The strong synergistic interaction among AC, rGO, and electrochemically active NMS yields a robust three-dimensional conductive network with enhanced Faradaic redox-active sites. On evaluation as a supercapacitor electrode, the optimized composite demonstrates excellent specific capacitance, superior rate capability, and good cycling stability over repeated charge-discharge cycles. This study provides an efficient strategy for utilizing sustainable biomass waste to construct high-energy hybrid electrode materials for next-generation supercapacitors.

Keywords: Biomass; Reduced graphene oxide; Composites; Electrode materials; Supercapacitor

P0068 • Bhuvan Singh Bhandari

ICEAM2026-POSTER-0068 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

MoS₂/Nitrogen-Doped Biomass-Derived Carbon Composite for Enhanced Zn²⁺ Storage in Aqueous Zinc-Ion BatteriesBhuvan Singh Bhandari¹, Sanjeev Kimothi¹, Navinchandra G. Shimpi³,Naveen Chandra Joshi^{*2}¹ *Department of Allied Sciences-Physics, Graphic Era Deemed to be University, Dehradun, 248002, Uttarakhand, India*² *Department of Allied Sciences-Chemistry, Graphic Era Deemed to be University, Dehradun, 248002, Uttarakhand, India*³ *Department of Chemistry, University of Mumbai, Santacruz, Mumbai, 400098, Maharashtra, India*

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Abstract

The design of sustainable and high-performance cathode materials plays an important role to bring ahead aqueous zinc-ion batteries (AZIBs) as safe and low-cost energy-storage devices. In this work, MoS₂/nitrogen-doped carbon (MoS₂/NC) composite were prepared, where MoS₂ was prepared by simple hydrothermal method and the nitrogen-doped carbon was prepared from conventional natural resources *Ficus religiosa*. Structural/morphological, elemental and chemical analyses of the synthesized materials were done by XRD, FESEM, EDX, elemental mapping, and FTIR technique, while, structural and surface analyses of MoS₂/NC composite were performed by HR-TEM, BET and XPS studies. Furthermore, the electrochemical behaviour of prepared materials was characterized by cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), rate capability, long-term cycling and electrochemical impedance spectroscopy (EIS) measurements. It was observed from the GCD that the MoS₂/NC composite showed a superior specific capacity of 552.43 mAh g⁻¹ at 0.25 A g⁻¹, when compared to pure MoS₂ (226.67 m Ah g⁻¹) and Nitrogen-doped carbon (233.08 mAh g⁻¹). Furthermore, the MoS₂/NC composite shows long-term cycling stability of 94.1% retention after 1000 cycles. The enhanced electrochemical behaviour of MoS₂/NC cathode is mainly mediated by the efficient charge migration at the mixture/whole electrode interface along with the charging/discharging kinetics of the Zn²⁺ ions in the composite cathode. This work provides an innovative biomass-assisted approach for high-performance AZIBs energy storages.

Keywords: MoS₂, NC, AZIBs, specific capacity, Zinc-Ion Batteries, CV, GCD, EIS.

P0073 • USHNA AFREEN

ICEAM2026-POSTER-0073 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

NANOPOROUS NiCo_2S_4 @MWCNT HYBRID CATHODE MATERIAL FOR ADVANCED SUPERCAPATTERY DEVICE

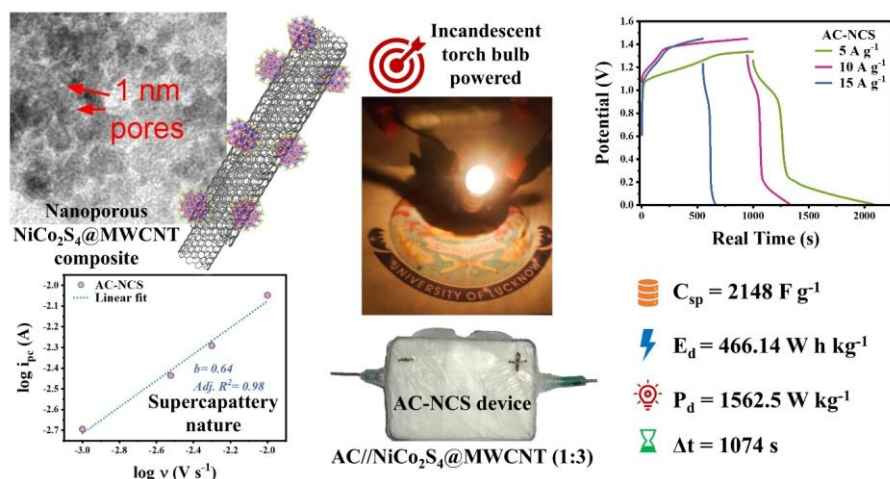
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Abstract

The urgent need to switch to sustainable energy alternative has promoted intense research in this field. Our aim behind this work is to contribute to the growing body of research in the energy storage realm. This work encompasses the development of composites of hydrothermally synthesized nickel thiocobaltite (NiCo_2S_4) and multiwalled carbon nanotubes (MWCNT) for advanced electrochemical energy storage (EES). The NiCo_2S_4 @MWCNT (1:3) nanoporous composite demonstrated the best performance towards EES in half-cell measurements. In a full-cell supercapattery configuration, with NiCo_2S_4 @MWCNT (1:3) as the cathode material and activated carbon (AC) as the anode material, an outstanding energy density (E_d) of $466.14 \text{ W h kg}^{-1}$ for a 1562.5 W kg^{-1} power density (P_d), at a current density of 2.5 A g^{-1} was achieved. The specific capacity of the device at 2.5 A g^{-1} is $746.43 \text{ mA h g}^{-1}$, which is highly appreciable. With a total device mass loading of 20 mg , the fabricated supercapattery device (AC-NCS) shows impressive performance towards advanced EES. The exceptional spike in the E_d is attributed to the average pore size of $\sim 1 \text{ nm}$, as observed in the HRTEM images of NiCo_2S_4 @MWCNT (1:3) composite. The nanometer confinement compels the partial de-solvation of the migrating electrolyte ions, drastically minimizing the charge-separation distance and unlocking maximum active mass participation in charge-storage. Real-world testing revealed a wide operating potential window of 1.63 V for the device. Two such devices, connected in parallel, powered an incandescent torch bulb for 12 seconds, which is a great proof of concept.

Keywords: NiCo_2S_4 ; MWCNT; supercapattery; electrochemical energy storage; high energy density**GRAPHICAL ABSTRACT**

P0075 • Latisha Gaba

ICEAM2026-POSTER-0075 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

NANOFLOWER-SHAPED Ni-Co-Mn LAYERED DOUBLE HYDROXIDE ANCHORED ON CUCUMBER PEELS-DERIVED POROUS CARBON AND N-DOPED GRAPHENE AS A DURABLE ELECTRODE MATERIAL FOR SUPERCAPACITORS

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Abstract

The surge in demand for highly efficient energy storage systems (ESSs) has elicited attention on supercapacitors (SCs), dominantly on account of their outstanding power capabilities and remarkable cycle longevity. In this context, trimetallic layered double hydroxides (LDHs) are a promising choice as electrode material for advanced SCs. However, the poor stability of LDHs during redox reactions and their low conductivity constrain their practical electrochemical performance. To enhance practical performance, various strategies, such as structural modification and nanocomposite formation, have been extensively employed. In the present work, nickel cobalt manganese LDH (NCM) is integrated with cucumber peels-derived porous carbon (CPC) and N-doped graphene (NG) via an in situ hydrothermal technique, resulting in a ternary composite named LCN. The ternary composite exhibits a unique architecture comprising NCM nanoflowers anchored on porous CPC and NG nanosheets. A conductive network of CPC and NG considerably stabilizes the redox-active NCM. The composition LCN3 exhibits an impressive specific capacitance (C_s) of 2293 F/g at a current density (I_d) of 1 A/g. Further, LCN3 and CPC have been utilized as positive and negative electrodes to fabricate an asymmetric supercapacitor device (ASD). The assembled LCN3//CPC device evinces a considerable specific energy (E_s) of 59.7 Wh/Kg, along with a specific power (P_s) of 770.5 W/Kg. The device operates reliably for 24000 cycles, maintaining 91% of its capacitance. The real-time suitability of LCN3//CPC was demonstrated by operating an LED and a multifunctional display. Consequently, the multidimensional and porous nanocomposite electrode underscores its potential for practical energy storage applications.

Keywords: Layered double hydroxides; N-doped graphene; Biocarbon; Supercapacitors; Asymmetric device

P0076 • Ishu Khatri

ICEAM2026-POSTER-0076 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

TERNARY HYBRID COMPOSITES BASED ON PSEUDOCAPACITIVE MELAMINE-TEREPHTHALDEHYDE COF INFUSED WITH LDH AND rGO FOR HIGH-PERFORMANCE SUPERCAPACITORS

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Abstract

For the development of efficient SC electrodes, ternary Covalent Organic Framework (COF) based composites with Ni-Mn LDH and GO, named as MTLG x, have been synthesized using a facile hydrothermal approach. The structural, morphological and compositional details were captured using physical characterization techniques such as XRD, FTIR, FESEM, EDS and XPS. Electrochemical investigations have been conducted in three- and two-electrode setups using CV, GCD, and EIS techniques. MTLG 2 nanocomposite performed best as the electrode material, delivering an excellent specific capacitance (C_s) of 3703.28 F/g at a current density (I_d) of 0.5 A/g. The synergistic layered combination of active COF sites, LDH and GO as the conductive filler have contributed towards the high-electrochemical performance of the nanocomposite. MTLG 2 retained 95% of its initial capacitance after 4800 continuous GCD cycles, indicating optimum cyclic stability. The MTLG 2-based symmetric SC device delivered a maximum C_s of 440.71 F/g at 0.25 A/g in 2-E mode, with over 98% capacitance retention over 10k GCD cycles. This high-performance hybrid ternary formulation has surpassed the performance of other COF-based composites in terms of charge storage abilities. This work would further catalyse research into hybrid COF- based composites for application as high-performance SCs.

Keywords: Covalent Organic Framework; Reduced Graphene Oxide; Electrode Materials; Supercapacitors

P0079 • SABATINI TYAGI

ICEAM2026-POSTER-0079 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

MULTIFUNCTIONAL PVDF–COBALT FERRITE SMART NANOCOMPOSITE: HIGH-PERFORMANCE SUPERCAPACITORS AND ENERGY HARVESTINGSabatini Tyagi¹, Gourav Paliwal², Divya Chauhan¹, Gyan Singh², Samina Husain², Manish Kumar Srivastava^{1*}¹*Department of Physics, Banasthali Vidyapith, Rajasthan-304022, India*²*Centre of Nanoscience and Nanotechnology, Jamia Millia Islamia, Delhi- 110025, India*

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Abstract

This study introduces a nanocomposite separator based on polyvinylidene fluoride (PVDF–cobalt ferrite (CoFe₂O₄; CFO), which uniquely integrates storage functionalities and energy harvesting. The PVDF-CFO nanocomposite films were made by using the solution casting method. FE-SEM results confirm that filler nanoparticles are evenly spread throughout the PVDF matrix. FTIR reveals the enhancement from α to β phase of the PVDF. The CV curves of the fabricated devices exhibit well-preserved quasi-rectangular shapes across various scan rates (10–100 mV/s), indicating excellent capacitive behaviour of the PVDF-CFO nanocomposite films as a separator. Among all compositions, the P5CFO separator exhibited the most balanced and superior performance, achieving the lowest bulk resistance ($R_b = 8 \Omega$), which is very lower than for commercially available non-porous Celgard™ 2500 (88.2 Ω) and micro - porous Celgard Ez 2090 (47.1 Ω). Furthermore, a symmetric supercapacitor was fabricated using the best-performing P5CFO separator to evaluate its practical applicability, delivering a high specific capacitance of 245 F g⁻¹ and retaining ~82% of its initial capacitance after 1000 GCD cycles. This enhanced performance is attributed to efficient electrolyte wettability and rapid ion transport through the hierarchical porous architecture, with only minor degradation arising from graphitic edge defects. Additionally, the piezoelectric nanogenerator (PENG) fabricated using the 5 wt% PVDF-CFO nanocomposites produced an output voltage of approximately 9 V across a 10³ k Ω load under gentle fist tapping, achieving a power density of 15 μ W/cm². These findings highlight the potential of PVDF-CFO for advanced supercapacitor and energy harvesting applications.

Keywords: Flexible Separator, PVDF/CFO nanocomposites, Energy harvesting, Symmetric Supercapacitor.

P0086 • Princy

ICEAM2026-POSTER-0086 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

AMMONIA-ASSISTED Nb₂CT_x MXENES WITH TUNEABLE LAYERING AND SURFACE CHEMISTRY FOR SUPERIOR LI AND NA-ION ENERGY STORAGE

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Abstract

MXenes are widely recognized for battery applications due to their rapid ion-intercalation capability and excellent cycling stability. However, conventional synthesis methods often involve hazardous HF, prolonged reaction times, and complex procedures, limiting their practical implementation. Here, we present an efficient and sustainable ammonia-assisted hydrothermal strategy for synthesizing Nb₂CT_x MXene from the Nb₂AlC MAX phase using a mild etchant, providing a safe, cost-effective, and scalable route. The as-prepared MXene was further delaminated via probe sonication, yielding an expanded interlayer spacing of ~9.7 Å and optimized surface functionalities. XPS reveals an oxygen-rich (-O/-OH) surface that promotes Li⁺/Na⁺ interaction and ion diffusion, consistent with the enhanced reversibility observed in CV and GCD profiles. As an anode, Nb₂CT_x delivers a high reversible discharge capacity of 484 mAh g⁻¹ at 0.1 A g⁻¹ with stable cycling over 100 cycles in lithium-ion batteries, and 198 mAh g⁻¹ at 0.1 A g⁻¹ over 100 cycles in sodium-ion batteries. Ex-situ post-mortem XRD confirms that Nb₂CT_x retains structural integrity and electrochemical stability after 100 cycles. Importantly, hydrothermal etching eliminates concentrated HF while producing well-exfoliated flakes. Combined structural, surface, and electrochemical analyses reveal the origins of its performance, providing a blueprint for next-generation sustainable MXene electrodes.

Keywords: 2D Nb₂CT_x MXene; Anode material; Interlayer spacing modulation; Lithium/Sodium-ion batteries

P0088 • Divya Gupta

ICEAM2026-POSTER-0088 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

SYNERGISTIC EFFECT OF HETEROATOM DOPED $g\text{-C}_3\text{N}_4$ /MoO₃ NANOCOMPOSITE FOR ENHANCED ENERGY STORAGE AND ELECTROCATALYTIC WATER SPLITTING APPLICATIONS

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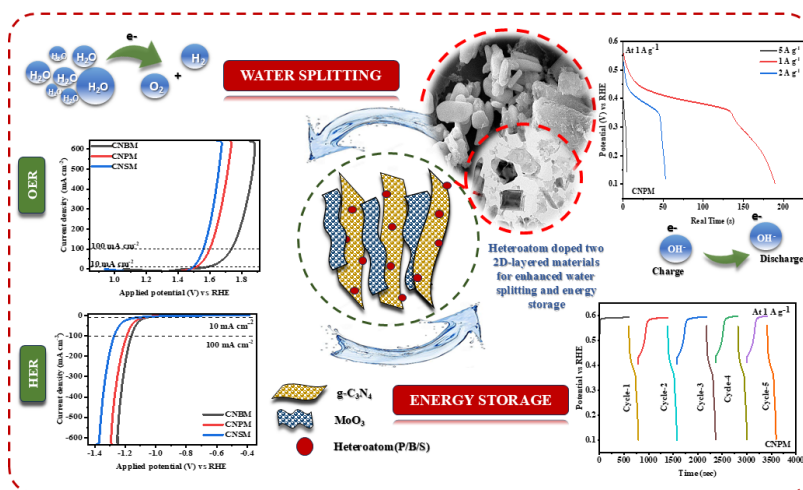
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Abstract

This study investigates the synergistic effects of heteroatom-doped graphitic carbon nitride ($g\text{-C}_3\text{N}_4$) coupled with molybdenum trioxide (MoO₃) for enhanced electrocatalytic activity and energy storage performance. Pristine $g\text{-C}_3\text{N}_4$ was synthesized via thermal polymerization of melamine, while boron (B), phosphorus (P), and sulphur (S) heteroatoms were individually introduced through *in-situ* polymerization. The modified sheets were subsequently hybridized with MoO₃ via physical mixing to construct layered hetero-structured nanocomposites. Comprehensive structural and morphological characterizations (FTIR, XRD, FESEM-EDX, and HRTEM) confirmed successful heteroatom incorporation into the triazine framework and intimate interfacial entanglement between the layered materials. Among synthesized nanocomposites, the P-doped composite (CNPM) exhibited exceptional supercapacitor performance, delivering a high value of specific capacitance of 412.89 F g⁻¹ and a power density of 228.13 W Kg⁻¹ at a current density of 1 A g⁻¹. Furthermore, the S-doped composite (CNSM) demonstrated superior performance towards oxygen evolution reaction (OER), delivering low values of overpotential of 270.9 mV (vs RHE), while B- doped composite (CNBM) exhibited best performance with the overpotential of 129.2 mV (vs RHE) for hydrogen evolution reaction (HER) at 10 mA cm⁻². Furthermore, impedance analysis revealed with the superior performance of CNSM and CNBM were possessing the lowest charge transfer resistance and superior ion diffusion kinetics, supporting it enhanced water splitting efficiency.

Keywords: Heteroatom doped $g\text{-C}_3\text{N}_4$, supercapacitor, water splitting, electrochemical energy storage.

GRAPHICAL ABSTRACT



P0091 • Parika Mahajan

ICEAM2026-POSTER-0091 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Synergistic Integration of Sm_2O_3 -modified $\text{Ti}_3\text{C}_2\text{T}_x$ MXene Electrode and PVA/ H_2SO_4 /KNN-based Gel Electrolyte for Flexible Quasi-Solid-State Supercapacitors

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Abstract

In the modern era of advanced wearable and flexible energy storage devices, quasi-solid-state supercapacitors (QSSSCs) have attracted considerable attention owing to their long-term stability, reduced risk of short circuit, and high specific power as well as energy. However, its performance is highly governed by the synergistic integration of a suitable electrode material with the electrolyte that ensures efficient ion transport, mechanical flexibility and structural integrity. Herein, motivated by the excellent properties of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene including, excellent electrical conductivity, high surface area, abundant redox-active sites, and tunable surface functional groups, a $\text{Ti}_3\text{C}_2\text{T}_x$ MXene/ Sm_2O_3 based composite was synthesized as an efficient electrode material for QSSSCs. The 1D nanorod morphology of Sm_2O_3 not only mitigated the restacking of MXene sheets and provided additional electroactive sites but also enhanced ion accessibility and charge transfer kinetics, thereby, contributing significantly to the improved electrochemical performance of the composite. The electrochemical behaviour of the electrodes was systematically optimized using different aqueous electrolytes, namely, KOH, Na_2SO_4 , and H_2SO_4 and among which, MXene/ Sm_2O_3 composite with H_2SO_4 based device was found to exhibit the highest specific capacitance of 430.66 F/g at 10 mV/s. Nevertheless, to omit leakage issue associated with the aqueous electrolyte, a PVA/ H_2SO_4 gel polymer electrolyte (GPE) was developed which helped in improving the mechanical stability and safety of the device but also resulted in a slight reduction in electrochemical performance (385.13 F/g at 10 mV/s). To address this limitation, potassium sodium niobate (KNN) was incorporated into the PVA/ H_2SO_4 gel polymer matrix, leading to the development of PVA/ H_2SO_4 /KNN based GPE that not only improved the device stability and minimized the capacitance loss but also contributed to a remarkable increase in the specific capacitance of the device. Consequently, the optimized MXene/ Sm_2O_3 electrode integrated with PVA/ H_2SO_4 /KNN based GPE was found to exhibit an enhanced specific capacitance (548.24 F/g at 10 mV/s) and excellent cycling stability (95.23% capacitance retention after 10,000 cycles), thereby, demonstrating its strong potential for flexible, stable, and environment-friendly high-performing QSSSCs.

Keywords: Supercapacitor, MXene, Sm_2O_3 , KNN, PVA/ H_2SO_4 /KNN, Gel polymer electrolyte, Quasi-Solid-State.

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P0096 • Shubhanshu Bansal

ICEAM2026-POSTER-0096 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

PHYSICS-GUIDED NUMERICAL OPTIMIZATION AND LOSS-MECHANISM ANALYSIS OF ZnO/N719/CuI SOLID-STATE DYE-SENSITIZED SOLAR CELLSShubhanshu Bansal¹, Satish Kumar Yadav², Jyotsna Singh¹, Rajendra Bahadur Singh¹¹ *Department of Physics, University of Lucknow, Lucknow, Uttar Pradesh, India*² *Institute of New and Renewable Energy, University of Lucknow, Lucknow, Uttar Pradesh, India*

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Abstract

Solid-state dye-sensitized solar cells (ssDSSCs) offer a promising low-cost photovoltaic platform; however, their practical performance is strongly governed by charge transport, interfacial recombination, defect states, and contact losses. In this study, a physics-guided numerical investigation of an FTO/ZnO/N719/CuI/Pt ssDSSC is performed using the SCAPS-1D simulation framework. Rather than relying solely on unrestricted parameter optimization, the device performance is systematically evaluated by considering the effects of ZnO photoanode thickness, sensitizer-related electronic properties, defect density, acceptor concentration, back-contact work function, operating temperature, series resistance, and shunt resistance. The analysis identifies the dominant parameters controlling the photovoltaic response and provides insight into the associated charge-generation, transport, recombination, and contact-loss mechanisms. The ZnO thickness and electronic properties of the sensitizing layer are found to strongly influence the balance between photogeneration and charge collection, whereas reduced defect density and improved contact selectivity suppress recombination and resistive losses. The optimized numerical configuration demonstrates substantial improvement in power conversion efficiency compared with the initial device configuration. Importantly, the simulated results are interpreted within experimentally relevant parameter ranges to avoid overestimation arising from idealized electrical conditions. The study therefore establishes a physically consistent numerical framework for evaluating ZnO/N719/CuI, ssDSSCs and highlights the key material and device parameters that should be prioritized for experimental optimization and performance improvement.

Keywords: Dye sensitized solar Cells; N719 dye; Power conversion efficiency; Fill factor; SCAPS-1D

P0100 • Khyati Tyagi

ICEAM2026-POSTER-0100 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

ELECTROSPUN PVDF-HFP/NiO NANOCOMPOSITES FOR EFFICIENT Piezo-Tribo HYBRID ENERGY HARVESTING SYSTEMKhyati Tyagi^a, Divya Chauhan^{a,b}, Arpit Singh^c, I. A. Palani^c, Kumkum Sharma^a, Manish Kumar Srivastava^{a,*}^a Department of Physical Sciences, Banasthali Vidyapith, Rajasthan, 304022, India^b School of Basic and Applied Sciences, Anand International College of Engineering, Jaipur, 303012, India^c Mechatronics and Instrumentation Engineering Lab, Indian Institute of Technology, Indore, 452020, India

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Abstract

Electrospun PVDF-HFP/NiO nanocomposites with 0, 2, 4, and 6 wt% NiO loading were fabricated and characterized to investigate their potential for wearable devices such as piezo-tribo hybrid nanogenerators. NiO nanoparticles were synthesized via sol-gel technique using required precursors. The incorporation of 4 wt% NiO in PVDF-HFP was found to be optimized nanocomposite with enhanced electroactive β -phase content ($\sim 82\%$), improved crystallization behavior, and significant piezoelectric coefficient (d_{33}) of 40 pC N^{-1} . A hybrid nanogenerator using optimized nanofibers generated a maximum open-circuit voltage of 80 V, short-circuit current of $3 \mu\text{A}$, and peak power density of 13.65 mW cm^{-3} at an optimal load resistance of $40 \text{ M}\Omega$ under an applied force of 5 N. The improved electrical performance of the nanogenerator is attributed to synergistic contribution of enhanced β -phase formation, stronger piezoelectric polarization and effective triboelectric charge generation at the polymer-NiO interface. Moreover, the electrospun nanofibrous membranes also maintained good moisture permeability, exhibiting water vapor transmission rates (WVTR) of ~ 115 and $\sim 104.7 \text{ g m}^{-2} \text{ h}^{-1}$ for pristine PVDF-HFP and optimized composite respectively. These results confirm their effective water vapor permeability, highlighting their potential for use in breathable textile and protective clothing applications. These findings highlight the potential of NiO-reinforced PVDF-HFP nanofibers as breathable, high-performance materials for self-powered wearable energy harvesting applications.

Keywords: PVDF-HFP; Electrospun nanofibers; Piezoelectricity; Triboelectric Nanogenerator; Energy Harvesting

P0103 • Rahul Kumar Jha

ICEAM2026-POSTER-0103 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Rational Design of B/O-Doped Triazine-Based Graphitic Carbon Nitride for Supercapacitor Electrodes: Insights from Density Functional Theory

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Abstract

This study develops a rational, concentration-dependent doping strategy for triazine-based graphitic carbon nitride (t-g-C₃N₄) as a supercapacitor electrode material, using boron (B) and oxygen (O) as dopants within a density functional theory framework. By screening inequivalent substitutional sites for their stability and impact on the band gap, two specific lattice positions adjacent to the triazine cavity are identified as the most favorable locations for incorporating B and O atoms. Doping is then carried out across a range of concentrations — 3.7 to 14.8 atomic % for boron and 3.7 to 18.5 atomic % for oxygen — to probe how composition affects performance. The results show that boron doping remains thermodynamically stable only up to 11.1 atomic %; at this threshold, the quantum capacitance peaks at approximately 140 $\mu\text{F cm}^{-2}$, with an accompanying surface charge density of about 80 $\mu\text{C cm}^{-2}$. Oxygen doping, in contrast, sustains thermodynamic stability across a wider range, up to 18.5 atomic %, while progressively narrowing the band gap and reaching a maximum quantum capacitance of around 120 $\mu\text{F cm}^{-2}$. Together, these results reveal a clear relationship linking structural modification, density of states (DOS), and quantum capacitance. The findings further indicate that boron doping is best suited for boosting intrinsic capacitance — behaving in a manner more characteristic of anode materials — while oxygen doping offers enhanced structural stability and tolerates a broader compositional window, positioning oxygen-doped t-g-C₃N₄ as the more suitable candidate for cathode applications. Overall, this work lays out practical design principles for developing sustainable, dopant-engineered carbon nitride electrodes.

Keywords: g-C₃N₄; Defect Engineering; Heteroatom Doping; Quantum Capacitance; Supercapacitors

Carbon (C/ C₂) Implanted Borophene as an Efficient Electrode Material for Supercapacitor Applications

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Abstract

Supercapacitors (SCs) are promising energy storage devices for clean hydrogen production and efficient energy storage. However, limiting voltage window and inferior cycling stability impede their large scalability; necessitates proficient electrode/interfacial materials to improve their performance and stability. To this, two-dimensional (2D) Borophene with excellent intrinsic properties have been acknowledged [1-4]. Although, Borophene based electrode delivering high current/power density but their restacking and stability issues impede their scalability for electrochemical devices. So, herein, ion beam engineering of 2D Borophenes using carbon (C and C₂) implantation has been acknowledged in controlled manner at a low energy of 80 keV using 1μA current at various fluence rates into Borophene to enhance their intrinsic properties towards energy storage ability favorable for energy storage applications. Further, the electrochemical properties towards SC application was investigated using cyclic voltammetry (CV), Galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS). These findings suggests that Carbon ions insertion into Borophene interlayers helps in providing well-exposed surface active sites, facilitating rapid charge transportation, thereby enhancing the performance of energy storage devices.

P0106 • JAGANNATH PANIGRAHY

ICEAM2026-POSTER-0106 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

EXPERIMENTAL AND DFT INSIGHTS INTO PHASE-DEPENDENT CHARGE STORAGE IN POLYMORPHIC ZnS

Jagannath Panigrahy¹, Priyadarshini Parida², Swetapadma Praharaj^{1*}, Dibyaranjan Rout^{1**}¹Functional Materials Lab, Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar 751024, Odisha, India²Computational Condensed Matter Physics Lab, Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar 751024, Odisha, India

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Abstract

Exploring the polymorph-dependent properties of ZnS serves as a key approach to optimizing supercapacitor electrode performance. Herein, we report a precursor-controlled hydrothermal route to selectively synthesize hexagonal (ZS-H) and cubic (ZS-C) ZnS nanoparticles using distinct sulphur precursors. Comprehensive structural, morphological, optical, and electrochemical characterizations confirm successful phase formation, while highlighting significant phase-dependent charge storage behaviour. Compared with the cubic counterpart, hexagonal ZnS exhibits a unique microspherical morphology, smaller crystallite size, lower charge-transfer resistance, and faster ion-diffusion kinetics. Consequently, ZS-H delivered a superior specific capacitance of 334.82 F/g at 1 mV/s and a prolonged discharge time of 505 s at 0.5 A/g, maintaining an 84 % capacitance retention after 15000 cycles. In contrast, ZS-C shows a lower specific capacitance of 272 F/g, a discharge time of 425 s, and 79% cyclic stability under the same conditions. A symmetric two-electrode device constructed using ZS-H electrodes demonstrates a high specific capacitance of 217.2 F/g at 1 mV/s, an energy density of 26 Wh/kg at 5 kW/kg, and an outstanding 97 % capacitance retention after 10000 cycles. Density Functional Theory (DFT) calculations further reveal a more favourable electronic structure and higher quantum capacitance for ZS-H, corroborating the experimental findings. Overall, this work demonstrates that precursor-controlled phase engineering is an effective approach for designing advanced ZnS-based supercapacitor electrodes.

Keywords: Supercapacitor, ZnS, Phase engineering, DFT, Quantum capacitance

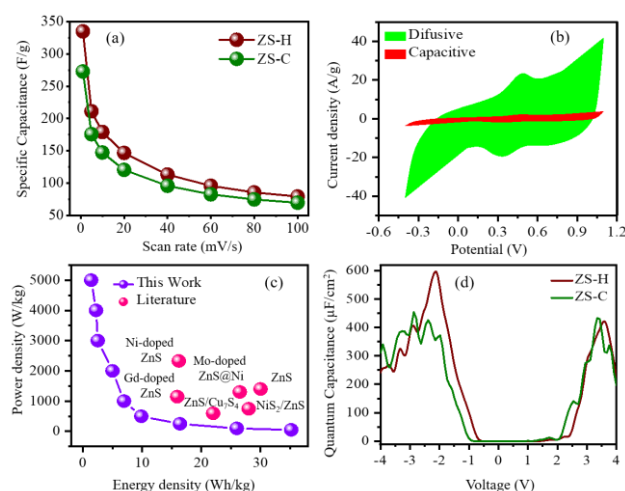


Fig. (a) Variation of specific capacitance with various scan rates; (b) Current contribution of ZS-H at 1 mV/s; (c) Ragone plot of ZS-H/ZS-H symmetric device; (d) Quantum capacitance as a function of applied voltage for hexagonal and cubic ZnS, respectively.

P0110 • ALKA SAHU

ICEAM2026-POSTER-0110 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

SYNERGISTIC $\text{MCo}_2\text{S}_4/\text{g-C}_3\text{N}_4$ (M= Ni, Co, Cu AND Zn) HETEROSTRUCTURES FOR ENHANCED ELECTROCATALYTIC WATER SPLITTING AND ELECTROCHEMICAL ENERGY STORAGE

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Presenting Author: Alka Sahu

Abstract

This work investigates the synergistic effect of MCo_2S_4 thiospinel (M= Nickel (Ni), Copper (Cu) and Zinc (Zn)) coupled with graphitic carbon nitride ($\text{g-C}_3\text{N}_4$) to enhance electroactivity for overall water splitting and electrochemical energy storage. Herein, hydrothermally synthesized thiospinels were ultrasonically integrated into thermally polymerized $\text{g-C}_3\text{N}_4$ sheets. Morphological and structural analyses (FTIR, XRD, FESEM/EDAX, and HRTEM) verified the successful anchoring of thiospinels across the $\text{g-C}_3\text{N}_4$ host. The resulting $\text{CuCo}_2\text{S}_4/\text{g-C}_3\text{N}_4$ (CUCN) hybrid exhibited outstanding electrocatalytic water-splitting activity, requiring low overpotentials of only 111 mV (vs RHE) for hydrogen evolution reaction (HER) and 308.9 mV (vs RHE) for oxygen evolution reaction (OER) respectively at 10 mA cm^{-2} , mediated by reduced charge-transfer resistance and enhanced interfacial mass transfer. In parallel, $\text{NiCo}_2\text{S}_4/\text{g-C}_3\text{N}_4$ (NICN) demonstrated high capacitive storage performance, achieving a specific capacitance of 269.59 F g^{-1} , energy density of 8.57 Wh kg^{-1} and power density of 239.24 W kg^{-1} at a current density of 1 A g^{-1} . These findings highlight the potential of thiospinel/ $\text{g-C}_3\text{N}_4$ heterostructures as robust bifunctional electrocatalysts and pseudocapacitor electrodes.

Keywords: Thiospinels, pseudocapacitor, water splitting, electrochemical energy storage.

P0111 • Ankita Nayak

ICEAM2026-POSTER-0111 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

**EXPLORING STABILITY AND THERMOELECTRIC POTENTIAL OF DEFECT CHALCOPYRITES:
A DFT-AIMD STUDY FOR SUSTAINABLE ENERGY HARVESTING**Ankita Nayak¹, Priyadarshini Parida^{1*}¹ *Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT), Deemed to be University, Bhubaneswar-751024, Odisha, India*

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Abstract

In the light of growing need for sustainable energy solution, thermoelectric materials have attracted considerable research attention due to their capacity to convert waste heat into a usable source of electrical energy. In this work, the mechanical and thermal stability, along with the thermoelectric properties of CuAl_2X_4 ($\text{X}=\text{S}, \text{Se}, \text{Te}$) defect chalcopyrites are systematically investigated using the density functional theory (DFT) within the generalized gradient approximation (GGA), combined with semiclassical Boltzmann transport theory. All investigated compounds satisfy the Born stability criteria, confirming their mechanical stability and exhibit ductile behavior with melting point exceeding 700 K. Furthermore, AIMD simulations are performed at 700 K over 6 ps, reveal only minor fluctuations in the temperature and the total energy of studied compounds, while RMSD analysis shows limited atomic displacement from the equilibrium positions, further supporting dynamical stability. Semiclassical Boltzmann transport calculations reveal enhanced thermoelectric performance under hole dominated transport, as reflected by favorable Seebeck coefficient. The maximum ZT values are achieved at an optimal carrier concentration of 10^{18} cm^{-3} and rises progressively with temperature, with CuAl_2S_4 emerging as the top performer among the series. Notably, low lattice thermal conductivity proves pivotal to this enhancement, underscoring the critical role of phonon transport in thermoelectric efficiency. As the thermoelectric performance of these compounds is modest, carrier optimization, alloying or nano-structuring may offer effective routes to enhance high temperature waste heat harvesting.

Keywords: DFT; AIMD Simulation; Carrier relaxation time; Lattice thermal conductivity; Figure of merit

P0117 • PRIYANKA NANDA

ICEAM2026-POSTER-0117 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

EXPERIMENTAL AND DFT INSIGHTS INTO PHASE-DEPENDENT CHARGE STORAGE IN POLYMORPHIC ZnS

Jagannath Panigrahy¹, Priyadarshini Parida², Swetapadma Praharaj^{1*}, Dibyaranjan Rout^{1**}¹Functional Materials Lab, Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar 751024, Odisha, India²Computational Condensed Matter Physics Lab, Department of Physics, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar 751024, Odisha, India

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Abstract

Exploring the polymorph-dependent properties of ZnS serves as a key approach to optimizing supercapacitor electrode performance. Herein, we report a precursor-controlled hydrothermal route to selectively synthesize hexagonal (ZS-H) and cubic (ZS-C) ZnS nanoparticles using distinct sulphur precursors. Comprehensive structural, morphological, optical, and electrochemical characterizations confirm successful phase formation, while highlighting significant phase-dependent charge storage behaviour. Compared with the cubic counterpart, hexagonal ZnS exhibits a unique microspherical morphology, smaller crystallite size, lower charge-transfer resistance, and faster ion-diffusion kinetics. Consequently, ZS-H delivered a superior specific capacitance of 334.82 F/g at 1 mV/s and a prolonged discharge time of 505 s at 0.5 A/g, maintaining an 84 % capacitance retention after 15000 cycles. In contrast, ZS-C shows a lower specific capacitance of 272 F/g, a discharge time of 425 s, and 79% cyclic stability under the same conditions. A symmetric two-electrode device constructed using ZS-H electrodes demonstrates a high specific capacitance of 217.2 F/g at 1 mV/s, an energy density of 26 Wh/kg at 5 kW/kg, and an outstanding 97 % capacitance retention after 10000 cycles. Density Functional Theory (DFT) calculations further reveal a more favourable electronic structure and higher quantum capacitance for ZS-H, corroborating the experimental findings. Overall, this work demonstrates that precursor-controlled phase engineering is an effective approach for designing advanced ZnS-based supercapacitor electrodes.

Keywords: Supercapacitor, ZnS, Phase engineering, DFT, Quantum capacitance

GRAPHICAL ABSTRACT

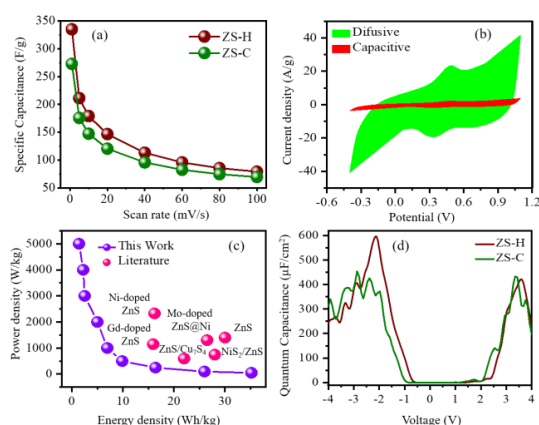


Fig. (a) Variation of specific capacitance with various scan rates; (b) Current contribution of ZS-H at 1 mV/s; (c) Ragone plot of ZS-H/ZS-H symmetric device; (d) Quantum capacitance as a function of applied voltage for hexagonal and cubic ZnS, respectively.

P0119 • Manish Jha

ICEAM2026-POSTER-0119 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Hydrothermally synthesized WS_2 @MWCNT and WS_2 @COOH-MWCNT electrodes for Supercapacitor Applications**Manish Jha¹, Sachin Pathak², Vishakha Kaushik¹**¹Materials & Nano Engineering Research Laboratory, Department of Physics, School of Physical Sciences, DIT University, Dehradun-248009, India.² Department of Physics, School of Engineering, University of Petroleum and Energy Studies, Dehradun- 248007, India.

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Abstract

The world is rapidly moving towards alternative energy storage sources to reduce the environmental damage caused by polluting fossil fuels like coal, oil and natural gas. Batteries, supercapacitors and fuel-cell technologies could greatly help in storing the electrical energy generated through hydroelectric powerplants, solar powerplants as well as wind power plants. Transition Metal Dichalcogenides (TMDs) like Tungsten disulfide (WS_2) WS_2 could be very useful for electrodes in supercapacitor applications if we make a composite of it with carbon-based nanomaterial like multi-walled carbon nanotubes (MWCNT) as WS_2 by itself offers poor conductivity and suffers from restacking issue. Here, we have examined the role of hydrothermally grown WS_2 @MWCNT and WS_2 @COOH-MWCNT in enhancing the electrochemical features of electrodes based WS_2 . The characterization techniques like Fourier-transform infrared spectroscopy (FTIR), UV-Visible Spectroscopy (UV-Vis), X-Ray Diffraction (XRD), Raman Spectroscopy and Scanning Electron Microscopy (SEM) etc. were used to confirm their successful synthesis. We prepared the electrodes by making the slurry of composites with polyvinylidene fluoride (PVDF) and deposited on Ni foam. Through the cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), electrochemical impedance spectroscopy (EIS) and cyclic stability tests, we found that the carboxyl functionalized MWCNT with WS_2 provided better specific capacitance value of 174.63 F/g as compared to that of WS_2 @MWCNT at 1 A/g as it offered lower charge transfer resistance (R_{ct}) and also offered better cyclic stability over 10,000 cycles. In this way, as COOH-functionalized MWCNTs led to better nanosheet dispersion, anchoring sites for nucleation of WS_2 as well as improved wettability of electrolyte, we got a better performance of WS_2 @COOH-MWCNT as electrodes in supercapacitors.

Keywords: Supercapacitors; Tungsten disulfide (WS_2); multi-walled carbon nanotube (MWCNT); galvanostatic charge–discharge (GCD); Specific Capacitance

P0125 • Krrish Mehta

ICEAM2026-POSTER-0125 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Source and Mitigation of capacity fade issue in all Vanadium redox flow battery: A reviewSanjay Kumar^{1*}, Krrish Parag Mehta¹, Jenius Jayesh Kerala², Ila Jogesh Ramala Sarkar¹, Ashish Bhatnagar³¹*Department of Chemical Engineering, Faculty of Technology, Marwadi University, Rajkot-360003, INDIA*²*Jubilant Agri and Consumer Products Ltd., Vadodara, India*³*Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, 201309, India***Abstract**

Vanadium redox flow batteries (VRFBs) are regarded as promising energy storage systems for industrial purposes due to their long lifespan, safety, flexible power and energy capacity, and compatibility with renewable energy systems. Regardless of this, capacity fade is an important problem that influences the battery's effective lifetime. This paper explores the main reasons for capacity fade in VRFBs and ways in which it can be reduced. The main cause of capacity fade is the passage of vanadium ions through the divider, imbalances of electrodes, water extraction, unwanted reactions, and the deterioration of electrolyte. The various methods that have been tested to minimize the loss of capacity include making ion-selective membranes, changing the electrodes, adding additives to electrolytes, changing the temperature and current density regime, and regulating electrolytes. The new types of membranes can decrease the escape of vanadium ions while contributing to stable proton conductivity. Improvement of electrodes can speed up the reactions in the electrochemical process and reduce polarizations. Apart from this, the rebalancing and mixing methods can return the needed balance of vanadium to keep the battery working longer. This review article is devoted to the analysis of the recent developments in these capacity fade reductions and the issues that still need to be solved to improve the durability and efficiency of VRFBs in energy storage.

Keywords: Redox flow battery, Capacity fade, Membrane, Vanadium, Efficiency. Corresponding Author: Dr. Sanjay Kumar, Marwadi University, Rajkot

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P0127 • Adeeba Yaqub

ICEAM2026-POSTER-0127 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

DESIGN AND MULTISCALE PERFORMANCE ASSESSMENT OF A LEAD-FREE CsSnI₂Br/FASnI₃/Cs₂AgBiBr₆ TRILAYER PEROVSKITE SOLAR CELL USING SCAPS-1D AND PVSYSAdeeba Yaqub¹, Satish Kumar Yadav², Vivekanand Yadav¹, Jyotsna Singh¹, Rajendra Bahadur Singh¹¹Department of Physics, University of Lucknow, Lucknow 226007²Institute of New and Renewable energy, University of Lucknow, Lucknow 226021

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Abstract

The development of efficient and environmentally sustainable photovoltaic technologies has intensified research on lead-free perovskite materials with complementary optoelectronic properties. In this study, a novel trilayer perovskite solar-cell architecture comprising CsSnI₂Br, FASnI₃ and Cs₂AgBiBr₆ is proposed and systematically investigated using SCAPS-1D and PVsyst. The proposed structure aims to exploit the complementary bandgaps of the three lead-free absorbers to improve solar-spectrum utilization while promoting efficient photogenerated-carrier transport and collection. SCAPS-1D simulations are employed to investigate the influence of absorber thickness, carrier concentration, bulk defect density, interface defect density, band alignment, transport-layer properties and temperature on the photovoltaic performance. Particular emphasis is placed on the CsSnI₂Br/FASnI₃ and FASnI₃/Cs₂AgBiBr₆ interfaces, where band offsets and defect-assisted recombination can significantly affect charge separation and extraction. The optimized device is evaluated through its open-circuit voltage, short-circuit current density, fill factor, power conversion efficiency, external quantum efficiency, energy-band profile and recombination characteristics. Subsequently, the optimized electrical parameters obtained from SCAPS-1D are incorporated into PVsyst to assess the practical energy-generation potential of the proposed photovoltaic technology under realistic irradiation and temperature conditions. Annual energy yield, specific energy production, performance ratio and system losses are analyzed to establish the relationship between cell-level optimization and system-level performance. The novelty of this work lies in integrating a lead-free CsSnI₂Br/FASnI₃/Cs₂AgBiBr₆ trilayer architecture with a SCAPS-1D–PVsyst simulation framework, providing a comprehensive pathway for optimizing interfaces, minimizing recombination and evaluating the practical potential of advanced lead-free perovskite photovoltaics.

Keywords: Lead-free perovskite solar cell; Trilayer perovskite; CsSnI₂Br; FASnI₃; Cs₂AgBiBr₆; Interface engineering; Defect density; SCAPS-1D; PVsyst;

P0129 • Bhubesh Joshi

ICEAM2026-POSTER-0129 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Thermal Consequences of Gate Independence in Monolithic Complementary FETs

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Abstract

The complementary FET (CFET) stacks an nFET tier above a pFET tier. One variant cuts the gate metal at the middle dielectric isolation (MDI) so the two tiers can be driven independently, and the thermal consequences of that cut remain insufficiently characterized. Self-consistent electrothermal TCAD is used to extract the full two-by-two inter-tier thermal resistance matrix for split-gate and common-gate structures. Across the cases examined, interrupting the gate produces no resolved reduction in inter-tier coupling: the power-normalized coupling resistance R_{np} agrees between the two to within 1.1 % at every bias examined, across a 25× range in gate-metal conductivity and a 4× range in dielectric conductivity. What the cut removes is an additional heat-removal path for the driven tier. At the adopted 30 nm SiO_2 conductivity the upper-tier self-heating resistance is 42 % higher and the nFET runs 36 % hotter at matched bias, so gate independence is associated with a self-heating penalty that is largest at the lower dielectric conductivities examined. The temperature-rise ratio usually quoted for crosstalk is shown to equal R_{np}/R_{nn} , so it can mislead when read as a coupling metric. R_{np} also responds far more strongly to the buried-oxide (BOX) thickness than to the MDI thickness, pointing to a substantial contribution from the substrate-side heat-removal path.

Keywords: complementary FET; CFET; thermal crosstalk; self-heating; split gate; electro-thermal TCAD; nanosheet

P0140 • Rekha kumari

ICEAM2026-POSTER-0140 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

SYNTHESIS AND ELECTROCHEMICAL CHARACTERIZATION OF MAPbI₃ PEROVSKITE COMPOSITES WITH ACTIVATED CARBON AND ZnMnW TERNARY METAL OXIDES FOR SUPERCAPACITOR APPLICATIONS

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Abstract

Supercapacitors have emerged as promising energy storage devices over the past few decades, but limitations in their charge storage capacity continue to restrict their wider application. Developing effective electrode materials is one approach to addressing these limitations. In this study, we synthesized methylammonium lead iodide (MAPbI₃) perovskite and its composites with coconut oil-derived activated carbon and ZnMnW ternary metal oxide nanoparticles. MAPbI₃ was prepared using a solution-based antisolvent precipitation method. X-ray diffraction confirmed its crystalline tetragonal structure, while Fourier-transform infrared spectroscopy identified characteristic vibrations of the methylammonium cation. The electrochemical properties of MAPbI₃ and its composites were evaluated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy. At a scan rate of 10 mV/s, CV-derived specific capacitances were 27 F/g for MAPbI₃, 17 F/g for the activated carbon composite, and 25 F/g for the ZnMnW composite. Notably, the ZnMnW composite exhibited the highest CV-derived capacitance among the three electrode systems. GCD measurements yielded maximum specific capacitances of 54, 8, and 5 F/g, respectively, at 0.3 mA/g within the potential windows investigated. Impedance measurements provided further insight into the distinct interfacial charge transport and ion diffusion behaviour of these electrodes. These findings establish the electrochemical charge storage capability of MAPbI₃-based electrodes and demonstrate how composite composition influences their capacitive response. The study provides a foundation for tailoring perovskite-based composites for further development as supercapacitor electrode materials.

Keywords: Metal halide perovskites; MAPbI₃; Activated carbon; Ternary metal oxides; Supercapacitors

P0141 • Amitabh Yadav

ICEAM2026-POSTER-0141 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Enhancing the Defect Tolerance and Stability of MAPbI₃ Perovskite Solar Cells through Interface PassivationAmitabh Yadav¹, Vivekanand Yadav¹, Satish Kumar yadav², Rajendra Bahadur Singh¹, Jyotsna Singh^{1*}¹*Department of Physics, University of Lucknow, Lucknow, India*²*Department of Renewable Energy, University of Lucknow, Lucknow, India*

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Abstract

Perovskite solar cells (PSCs) have attracted significant attention due to their excellent optoelectronic properties and potential for achieving high power conversion efficiency. However, interfacial defects and trap-assisted non-radiative recombination remain major factors limiting their efficiency and operational stability. In this study, the influence of interface passivation on the defect tolerance and performance of methylammonium lead iodide (MAPbI₃)-based PSCs is investigated using numerical simulations in the SCAPS-1D framework. A baseline FTO/TiO₂/MAPbI₃/CNT/Au device is first optimized by systematically varying the thicknesses of the absorber and charge transport layers. Subsequently, six passivation materials, namely C₆₀, PCBM, C₆₀-SAM, P3HT, graphene, and PbS quantum dots, were incorporated at the perovskite/charge-transport interface, and their thicknesses were optimized. The influence of interfacial degradation was further examined by varying the interface defect density from 10¹⁰ to 10¹⁸ cm⁻². The results demonstrate that interface passivation effectively suppresses trap-assisted recombination and improves resistance to defect-induced performance degradation. Among the investigated materials, C₆₀ and C₆₀-SAM exhibited superior photovoltaic performance and defect tolerance, with C₆₀-SAM showing particularly strong resilience under highly defective conditions. These findings provide useful guidelines for interface engineering and identify promising passivation strategies for developing efficient and stable PSCs.

Keywords: Perovskite solar cells; MAPbI₃; Interface passivation; Interface defects; Trap-assisted recombination; Defect tolerance; SCAPS-1D; C₆₀-SAM; Device optimization; Interfacial engineering.

P0142 • VIVEKANAND YADAV

ICEAM2026-POSTER-0142 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Design and Comparative Analysis of Lead-Free Perovskite 4-Terminal Tandem Solar CellsVivekanand Yadav¹, Adeeba Yakub¹, Lakshya¹, Satish Kumar yadav², Rajendra Bahadur Singh¹, Jyotsna Singh^{1*}¹*Department of Physics, University of Lucknow, Lucknow, India*²*Department of Renewable Energy, University of Lucknow, Lucknow, India*

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Abstract

The development of efficient and sustainable perovskite solar cells is essential for advancing next-generation photovoltaic technologies. In this work, three perovskite absorber materials, namely rubidium germanium tribromide (RbGeBr_3), formamidinium tin triiodide (FASnI_3), and cesium dibromodiodogermanate ($\text{Cs}_2\text{GeI}_2\text{Br}_2$), are investigated for their suitability as photovoltaic absorbers for a 4T tandem solar cell using the SCAPS-1D simulation software. Initially, Single-junction solar cells were modelled and numerically optimized under AM 1.5G sun illumination. TiO_2 is employed as the electron transport layer (ETL) in all three devices, while CuI is selected as the hole transport layer (HTL) for the RbGeBr_3 -based device and Spiro-OMeTAD is used for the FASnI_3 - and $\text{Cs}_2\text{GeI}_2\text{Br}_2$ -based devices. The optimized RbGeBr_3 , FASnI_3 , and $\text{Cs}_2\text{GeI}_2\text{Br}_2$ single-junction solar cells achieved power conversion efficiencies (PCEs) of 18.45%, 17.52%, and 19.10%, respectively, with corresponding fill factors of 81.20%, 81.19%, and 76.65%. Subsequently, four-terminal (4T) tandem solar cells are designed by employing RbGeBr_3 as the wide-bandgap top cell and FASnI_3 and $\text{Cs}_2\text{GeI}_2\text{Br}_2$ as the bottom cell. The optimized $\text{RbGeBr}_3/\text{FASnI}_3$ and $\text{RbGeBr}_3/\text{Cs}_2\text{GeI}_2\text{Br}_2$ 4T tandem configurations achieved PCEs of 35.00% and 34.28%, respectively. These results demonstrate the potential of combining RbGeBr_3 with suitable narrow-bandgap perovskite absorbers in 4T tandem architectures for achieving substantially enhanced photovoltaic performance compared with the corresponding single-junction devices. The findings provide a theoretical basis for the development and further experimental investigation of efficient, lead-free perovskite tandem solar cells.

Keywords: RbGeBr_3 ; FASnI_3 ; $\text{Cs}_2\text{GeI}_2\text{Br}_2$; SCAPS-1D; 4T tandem solar cell; Lead-free perovskite

P0145 • SALIL KUMAR

ICEAM2026-POSTER-0145 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Vacancy-Encoded High-Entropy Oxide Nano ionic Interfaces for Thermally Adaptive and Self-Healing Perovskite Solar CellsSalil Kumar^{1*}, Amit Kumar Singh²^{1,2} *National Institute of Technology Delhi, Department of Electrical Engineering, New Delhi, India, 110036*

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Abstract

Thermally induced ion migration and interfacial defect formation and microcracking are still limiting the operational durability of perovskite photovoltaic (PV) devices, although they are closing the gap to commercially significant efficiencies. A high-entropy oxide (HEO) nanoionic interface with the ability to both sense thermal history and passivate defects and recover the crack-edge in an autonomous way is herein proposed. A coupled reaction–diffusion, Arrhenius degradation, ionic-migration and photovoltaic digital-twin framework is formulated for the interface in this Ti–Sn–Zr–Hf–Ce oxide family, in the thickness range of 10–25 nm for the HEO, 0.025–0.085 for the baseline oxygen-vacancy fraction, and healing-activation temperature range of 318–345 K. The numerical experiments are carried out to compute the redistribution of vacancies on 31–61 spatial nodes, and to calculate the thermal memory, the density of defects, the migration of ions, the series resistance, the impedance response and the power conversion efficiency for different solar-thermal accelerated cycling times of 24–96 h. The model indicates that vacancy concentrations of the order of 0.06–0.09 offer the optimum memory sensitivity/recombination suppression, and that, following localized thermal stress, 80–95% of the simulated memory loss can be recovered by autonomous healing. Multi-objective optimization is also used to find composition–vacancy–thickness combinations which maximize the retained efficiency, under optical and transport penalty constraints. These findings provide a materials-level approach to self-diagnosing PVs interfaces that sense, remember, heal, and verify degradation without relying on external microsensors, paving the way to longer-lived perovskite and tandem solar technologies. Experimental testable signatures are provided in the framework for XPS, EIS, PL and J–V validation.

Keywords: Second-life electric-vehicle batteries; Physics-informed digital twins; Carbon-aware energy trading; Multi-agent reinforcement learning; Lithium-plating-aware degradation

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P0146 • Sujata Shekhawat

ICEAM2026-POSTER-0146 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

MULTISCALE COMPUTATIONAL INVESTIGATION OF PECVD-GROWN VANADIUM CARBIDE NANOFILMS FOR ELECTROCHEMICAL ENERGY STORAGE DEVICESSujata Shekhawat¹, Ravi Gupta¹¹ *Department of Physics and Material Science and Engineering, Jaypee Institute of Information Technology, 201309 Noida, Uttar Pradesh, India*

Ravi Gupta Email: ravi.gupta@mail.jiit.ac.in

Abstract

The electrode architecture plays a pivotal role in governing the lithium storage kinetics and capacity, thereby strongly influencing the power and energy densities of the lithium-ion batteries. In this study, multiscale computational framework is developed to investigate the influence of PECVD simulated vanadium carbide (VC) nanofilms, employed as anode active material, on the electrochemical performance of Lithium-ion batteries. A two-dimensional axisymmetric ICP model is developed in COMSOL Multiphysics to elucidate the growth characteristics of VC nanofilms and predicts their thickness as a function of key process parameters. The predicted VC nanofilm thickness is subsequently incorporated into lithium-ion battery model to systematically evaluate its influence on lithium-ion diffusion, energy density and power density, diffusion induced stress. This coupled Multiphysics framework establishes direct relationship between PECVD operating conditions, VC anode thickness and battery performance. The model further captures the spatiotemporal evolution of the lithium-ion concentration within the electrode for different VC thickness. Simulation results reveal that increasing the VC electrode thickness enhances the energy density owing, while simultaneously reducing the power density due to the increased lithium-ion diffusion length and associated transport limitations. The proposed framework provides a computationally efficient approach for optimizing PECVD operating conditions and VC anode thickness towards improved lithium-ion battery performance.

Keywords: COMSOL; Vanadium carbide nanofilm; ICP; Electrochemical; Anode

P0147 • Sandipan Bhattacharyya

ICEAM2026-POSTER-0147 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Cold-Sintering-Assisted Fabrication of Porous NASICON Scaffolds for High Active-Material Loading in Sodium-Ion Battery CathodesSandipan Bhattacharyya¹, Tushar Balasaheb Deshmukh¹, Sourabh Shyamal¹, Saurabh Sharma¹, Shobit Omar¹¹ *Material Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India*

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Abstract

The growing demand for sustainable energy storage has accelerated the development of alternative battery technologies beyond lithium-ion systems. Sodium-ion batteries (SIBs) have emerged as a promising energy storage technology owing to the abundance, low cost of sodium based raw material. However, achieving high active material loading ($\sim 5 \text{ mg.cm}^{-2}$) in conventional SIB electrodes remains challenging due to (1) limited electrode thickness, which restricts areal capacity and energy density; (2) poor electrolyte infiltration and long ionic diffusion pathways, which reduce active-material utilization and rate capability; and (3) particle strain during Na-ion insertion/extraction, along with parasitic reactions and gas evolution, which promote structural degradation, impedance growth, and capacity fading. This study introduces a cold-sintering-assisted (CSP) approach for designing porous NASICON-type solid-electrolyte scaffolds that enable high active-material loading through subsequent wet-chemical infiltration. The CSP process enables densification while retaining approximately 40% porosity within the electrolyte scaffold, providing an interconnected porous network for effective active-material infiltration. Mg-doped NASICON-type solid electrolyte was employed to fabricate the porous scaffold, which was subsequently infiltrated with Fe-doped sodium vanadium phosphate as the active cathode material. The resulting infiltrated composite cathode achieved a mass loading of $\sim 6 \text{ mg.cm}^{-2}$, delivering an initial discharge capacity of 66.5 mAh.g^{-1} at 0.1C. Electrochemical cycling demonstrated excellent capacity retention after 100 cycles, providing validation of the structural and electrochemical stability of the CSP-derived porous scaffold for high-loading composite cathodes. This work demonstrates a CSP-enabled strategy for engineering porous solid-electrolyte scaffolds and integrating infiltration technique, offering a promising approach for the development of high-loading composite cathodes for next-generation sodium-ion batteries.

Keywords: NASICON; Cold Sintering Process; Infiltration; Sodium Ion Battery; Keyword; Energy Density

P0148 • PRAGATI SINGH

ICEAM2026-POSTER-0148 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

UNVEILING THE IMPACT OF Na⁺ INCORPORATION ON THE ELECTROCHEMICAL PROPERTIES OF LANIO₃ NANOSTRUCTURES FOR HIGH-PERFORMANCE SUPERCAPACITOR APPLICATIONS

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Abstract

LaNiO₃ (LNO) nanostructure-based electrodes are promising for supercapacitor applications owing to their high electrical conductivity, reversible redox activity, and structural stability. However, their electrochemical performance can be limited by the availability of electrochemically active sites and charge-transfer kinetics. In the present work, pristine and Na⁺-incorporated LaNiO₃ [La_{1-x}Na_xNiO₃ with x = 0, 0.05, 0.10, and 0.15, denoted as LNO, LNNO-5, LNNO-10, and LNNO-15, respectively] nanostructures were synthesized using a simple sol-gel method. The effects of Na⁺ incorporation on the structural, morphological, electronic, and electrochemical properties of the nanostructures were systematically investigated. The synthesis conditions were optimized by sintering the as-prepared gels at different temperatures ranging from 400 to 800 °C. X-ray diffraction (XRD) analysis confirmed the formation of phase-pure, crystalline samples with a rhombohedral perovskite structure after sintering at 700 °C for 2 h. A gradual increase in crystallite size was observed with increasing Na⁺ concentration. Field-emission scanning electron microscopy (FESEM) revealed quasi-spherical, densely packed nanocrystalline particles forming interconnected cauliflower-like porous structures, with an average particle size of approximately 70 nm. X-ray photoelectron spectroscopy (XPS) analysis confirmed the presence of La³⁺ and predominantly Ni³⁺ chemical states with lattice O²⁻ as the major oxygen species in LaNiO₃. Cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) measurements demonstrated an enhancement in the charge-storage performance upon Na⁺ incorporation into the LaNiO₃ lattice. The maximum specific capacitance of 226 F g⁻¹ at a scan rate of 5 mV s⁻¹ was obtained for the LNO electrode. The LNO electrode exhibited a low charge-transfer resistance of 1.5 Ω and retained 92.4% of its initial capacitance after 10,000 charge-discharge cycles, demonstrating excellent cycling stability. The specific capacitance increased with increasing Na⁺ concentration in LNO lattice. These findings indicate that Na⁺ incorporation is an effective strategy for tailoring the electrochemical performance of LaNiO₃ and highlight its potential for the development of high-performance perovskite-based supercapacitor electrodes.

Keywords: LaNiO₃, Supercapacitor, XPS, Cyclic Voltammetry, Specific Capacitance, Electrochemical Performance.

P0151 • KUMARI DIKSHA

ICEAM2026-POSTER-0151 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Electrochemical Charge Storage in Co-sputtered Cr–W–N Thin Films Electrodes for Quasi Solid-State Supercapacitors

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Abstract

Transition-metal nitrides have attracted considerable interest as electrode materials for electrochemical energy storage because of their high electrical conductivity and chemical stability. In this work, CrN, W₂N, and co-sputtered Cr–W–N thin films were directly deposited on nickel foam by reactive magnetron sputtering and evaluated as supercapacitor electrodes. Structural and surface-chemical characterization confirms a W-rich Cr–W–N framework containing coexisting Cr–N and W–N bonding environments, with a surface elemental ratio of Cr:W:N~1:3.77:4.24. Electrochemical measurements in 1 M KOH demonstrate enhanced charge-storage capability following Cr–W coupling. At 3 mA cm⁻², Cr–W–N delivers an areal capacitance of 1138.73 mF cm⁻², compared with 948.37 and 759.38 mF cm⁻² for CrN and W₂N. Kinetic analysis reveals combined surface-controlled and diffusion-associated charge-storage processes, with the diffusion-controlled contribution reaching 96.76% at low scan rates. Cr–W–N also exhibits favourable interfacial characteristics, with a series resistance of 0.10 Ω cm² and charge-transfer resistance of 0.693 Ω cm². A Symmetric Cr–W–N | Cr–W–N solid-state device employing PVA/KOH gel electrolyte delivers an areal capacitance of 48.4 mF cm⁻², 8.13 μWh cm⁻² energy density, and 0.0266 mW cm⁻² power density. The device retains 87.80% capacitance after 10,000 cycles, demonstrating the potential of Cr–W–N thin film for durable solid-state supercapacitor.

Keywords: Cr–W–N; Transition-metal nitrides; Reactive magnetron sputtering; Symmetric supercapacitor.

P0175 • Vijay Kailas Vaishampayan

ICEAM2026-POSTER-0175 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Electrospun nanofiber-supported spinel nanomaterial for supercapacitor applicationVijay Vaishampayan¹, Nishant Chavhan¹, Pramod Junghare¹, Chandrashekhar M. Mahajan², Navin Gopinathan¹, Sarang P. Gumfekar^{1*}¹ *Department of Chemical Engineering, Indian Institute of Technology, Ropar, Rupnagar, Punjab 140001, India*² *Vishwakarma Institute of Technology, Pune, 411037, Maharashtra, India*

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Abstract

The development of electrode materials with higher power and energy densities is essential for the performance of supercapacitors. In this study, carbonized CuFe₂O₄@polysulfone (CF@PSF) nanofibers were synthesized by integrating CuFe₂O₄ nanoparticles with a polysulfone dope solution. The resultant nanofibers were carbonized at 800°C to create a conductive carbon network. The incorporation of the carbonized polymeric framework resulted in a highly microporous composite structure. The synthesized framework provided an interconnected architecture for electrolyte ion transport and electrochemical charge storage. The CF@PSF electrode exhibited a specific capacitance of 131.94 F g⁻¹, which is substantially higher than the 56.45 F g⁻¹ obtained for pristine CuFe₂O₄ under identical conditions in three electrode system. At a current density of 0.5 A g⁻¹, the CF@PSF electrode delivered an energy density of 9.5 Wh kg⁻¹ and a power density of 18,000 W kg⁻¹, compared with 3.01 Wh kg⁻¹ and 15,500 W kg⁻¹, respectively, for pristine CuFe₂O₄. The enhanced charge-storage behavior is associated with the combined contribution of the faradaic redox activity of CuFe₂O₄ and the conductive, microporous carbon framework derived from polysulfone. The CF@PSF electrode retained approximately 92% of its initial capacitance after 1000 galvanostatic charge-discharge cycles in a three-electrode configuration. The corresponding device maintained more than 85% of its initial electrochemical performance after 10,000 charge-discharge cycles. The results indicate that integrating CuFe₂O₄ with a porous carbonaceous nanofiber matrix can effectively improve the electrochemical charge-storage characteristics and cycling stability of supercapacitor electrodes.

Keywords: Supercapacitor; CuFe₂O₄@Polysulfone; Carbonization; Nanofibers; Device study

P0187 • Manu Sharma

ICEAM2026-POSTER-0187 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Improving the Thermoelectric Performance of PEDOT:PSS through DMSO/Triton X-100 modification And Hydrazine ReductionManu Sharma¹, Dinesh Tripathi²¹*Department of Physics and Materials Science & Engineering, Jaypee Institute of Information Technology, Noida, India*

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Abstract

Flexible organic thermoelectric materials are promising for low-grade and wearable energy-harvesting applications owing to their lightweight, solution processability, and mechanical compliance. In this work, the thermoelectric performance of PEDOT was systematically enhanced through a combined solvent/surfactant modification and subsequent hydrazine (HZ) treatment. DMSO was incorporated to improve the electrical transport properties of PEDOT, while Triton X-100 was introduced to enhance film processability and mechanical stability. The optimized PEDOT+DMSO+Triton-X formulation was further subjected to HZ treatment to modulate the charge-carrier concentration and optimize the balance between electrical conductivity and Seebeck coefficient. Structural, chemical, optical, and transport characteristics were investigated using UV–visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), electrical conductivity, and Seebeck coefficient measurements. The corresponding power factor was evaluated to assess the overall thermoelectric performance. The spectroscopic results revealed changes in the electronic and chemical environment of the PEDOT matrix following DMSO modification and HZ treatment, consistent with enhanced charge transport. Importantly, the incorporation of Triton X-100 helped preserve the mechanical integrity of the optimized films even after HZ treatment, addressing the mechanical degradation that can accompany strong chemical reduction of conducting polymers. The optimized treatment strategy therefore provides a route toward simultaneously improving electrical transport and maintaining mechanical robustness, making the modified PEDOT films attractive candidates for flexible and wearable thermoelectric energy-harvesting applications.

Keywords: PEDOT:PSS; Thermoelectric performance; Hydrazine treatment; Triton X-100; Flexible energy harvesting

P0195 • Riteswari Bhoi

ICEAM2026-POSTER-0195 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Hierarchical 3D MoS₂ Nanoflower/WS₂ Nanoparticle Hybrids for High-Performance SupercapacitorsRiteswari Bhoi¹, Kiran Gupta¹, Arvind Singh², Arun kumar Singh^{1*}¹*Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur (C.G.)-495009, India.*²*Department of Materials Science & Metallurgical Engineering, Indian Institute of Technology, Bhilai (C.G.)-491002*

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Abstract

Transition metal dichalcogenides (TMDs), like molybdenum disulfide (MoS₂) and tungsten disulfide (WS₂), have attracted considerable attention as electrode materials for supercapacitor applications owing to their layered structures, abundant active sites, and favorable electrochemical properties. However, their individual charge storage performance can be limited by poor electrical conductivity, and structural restacking, motivating the development of MoS₂/WS₂ hybrid material to improve electrochemical performance. In this work, we developed a MoS₂ nanoflowers (NFs)/WS₂ nanoparticles (NPs) hybrids, MoS₂ nanoflowers grown uniformly over the WS₂ nanoparticles, creating a stable and well-connected hybrid structure. The structural analysis of the MoS₂NF/WS₂NP hybrids were analysed using X-ray diffraction, and its morphology is confirmed with scanning electron microscopy. Raman and X-ray photoelectron Spectroscopy were employed to confirm the vibrational characteristics and elemental composition of the hybrids. The electrochemical performance was evaluated in a three-electrode configuration, where the MoS₂NF/WS₂NP hybrid exhibited a specific capacitance of 399 F/g. Furthermore, symmetric solid-state device fabricated using the hybrid, which delivered a specific capacitance of 86 F/g, demonstrating its potential for practical energy storage applications. The device exhibited good cycling stability, retaining 72% of its initial capacitance after 5000 charge discharge cycles. These results demonstrate the potential of the MoS₂NF/WS₂NP hybrid as an electrode material for supercapacitor applications.

Keywords: supercapacitors, molybdenum disulfide, tungsten disulfide, nanocomposites.

P0196 • Hiritika

ICEAM2026-POSTER-0196 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

NI-DOPED CO₃O₄/ MXENE NANOCOMPOSITE BASED TRIBOELECTRIC NANOGENERATOR FOR ENERGY HARVESTINGHiritika¹ and Aman Mahajan^{1*}¹ *Department of Physics, Guru Nanak Dev University, Amritsar, Punjab, India*

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Abstract

The triboelectric nanogenerators i.e. TENGs attract extensive attention as promising technologies in sustainable conversion of mechanical energy from ambient sources to electric energy. In this work, Ni-doped Co₃O₄/Ti₃C₂T_x MXene nanocomposites are designed, with Ni-doped Co₃O₄ synthesized via hydrothermal approach and subsequently combined with MXene through sonication, where Ni doping modulates Co₃O₄'s intrinsic electronic and defect-related properties and MXene provides conductive pathways and heterogeneous interfaces. This resulting nanocomposite is then incorporated into cellulose acetate (CA) matrix and electrospun to get a nanofibrous mat. The physicochemical characteristics of the composite structure were further explored using various characterization techniques and then utilized for designing and fabrication of TENG devices for mechanical energy harvesting. Collectively, this study explores the combined effects of Ni doping in metal oxides and MXene incorporation on the structural and interfacial properties of CA-based nanofibers, establishing a materials engineering approach to triboelectric energy harvesting.

Keywords: Ni doped Co₃O₄; Ti₃C₂T_x; Cellulose Acetate; Energy Harvesting; TENG

P0205 • Ankita

ICEAM2026-POSTER-0205 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Abstract

Flexible thermoelectric films based on poly (3,4- ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) were fabricated by coating PEDOT:PSS solutions containing different concentration of benzenesulfonic acid (BSA) (as a secondary dopant) onto the surface of Whatman filter paper to investigate their thermoelectric transport properties. The effect of BSA concentration (0.06, 0.08, 0.1 M) on sheet resistance and Seebeck Coefficient was systematically investigated to identify the optimize composition. Subsequently, the 0.06M BSA-treated film was further modified using dimethyl sulfoxide (DMSO) and Hydrazine (HZ) to enhance its electrical and thermoelectric performance. Temperature-dependent measurement revealed a decreasing trend in both sheet resistance and Seebeck Coefficient with increasing temperature. At approximately 40°C, the 0.06M BSA-treated film exhibited a sheet resistance of approximately 65 $\Omega \text{ sq}^{-1}$ and a Seebeck Coefficient of approximately 14.2 μVK^{-1} . Following DMSO and HZ treatment, the sheet resistance decreased to approximately 13 $\Omega \text{ sq}^{-1}$, while the seebeck coefficient remained approximately 12.8 μVK^{-1} . UV-Visible and Fourier-transform infrared spectroscopy were employed to investigated the optical characteristics and chemical interactions associated with the treatments. The results demonstrated that sequential chemical modification can substantially reduce sheet resistance while retaining a measurable thermoelectric response, highlighting the potential of flexible PEDOT: PSS films for wearable thermoelectric electronics and low-grade waste-heat harvesting applications.

STRUCTURAL, MAGNETIC AND ELECTROCHEMICAL STUDY OF W-DOPED NiCo_2O_4 MICROSPHERES FOR ENERGY STORAGE APPLICATIONS

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Abstract

In the present work, Structural, magnetic and electrochemical study of spinel- type tungsten-doped NiCo_2O_4 ($\text{W} \rightarrow \text{NiCo}_2\text{O}_4$) microspheres prepared through a facile hydrothermal and subsequent calcination route has been carried out. Structural properties were studied by using X-ray diffraction, Scanning electron microscopy, Transmission electron microscopy, BET/BJH experiments, X-ray photoelectron spectroscopy and also by Ab-Initio study. X-ray diffraction analysis confirmed the phase purity of the prepared samples. Electron microscopy revealed the 3D porous sphere-shaped microstructures built from randomly arranged nanorods and nanoparticles. The specific surface area and pore size distribution were evaluated by Brunauer–Emmett–Teller (BET) method and Barrett– Joyner– Halenda (BJH) model, respectively. SQUID testing demonstrated a change from ferromagnetic to a diamagnetic phase. The electrochemical performances of the samples as an electrode on nickel foam substrates were measured by means of cyclic voltammetry, galvanostatic charge–discharge cycling and impedance spectroscopy with a three-electrode configuration in 6M KOH electrolyte. The optimal $x=0.4$ composition showed excellent electrochemical properties in alkaline medium. The specific capacity of the electrode found to be 1116.48 Fg^{-1} at 2mVs⁻¹ and 1030.37 Fg^{-1} at 0.5 Ag⁻¹. Moreover, an asymmetric supercapacitor device built with $\text{W}_{0.4}\text{Ni}_{0.6}\text{Co}_2\text{O}_4$ as positive electrode and activated carbon (AC) as negative electrode in a 6M KOH electrolyte. Real-world usage of the asymmetric supercapacitor device is demonstrated by enlightening red light-emitting diode panel. These results indicate that the synthesized microspheres could be promising candidates for energy storage applications.

Keywords: W -doping, Structural properties, Magnetic properties, Electrochemical properties, Energy storage device.

P0219 • AKANSHA AGRWAL

ICEAM2026-POSTER-0219 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

ARTIFICIAL INTELLIGENCE-DRIVEN CATALYST DESIGN FOR ENERGY STORAGE

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Abstract

Rapid development of next generation energy-storage technologies calls for catalysts with high activity, selectivity, stability and cost-effectiveness to accelerate sluggish electrochemical reactions and improve overall device performance. The conventional way to find catalysts is usually slow and resource-intensive, relying heavily on trial-and-error experiments and simulations that require significant computational power, time and money. Artificial intelligence (AI) has emerged as a powerful approach for accelerating catalyst discovery by establishing complex relationships between composition, structure, electronic properties, catalytic activity, and electrochemical performance. This review gives a full picture of AI-driven catalyst design for energy storage, including machine learning, deep learning, graph neural networks, generative models, and physics-informed methods. Particular emphasis is placed on the representation of molecular, atomic, crystal, and catalyst–electrolyte interface structures and their integration with density functional theory and experimental data. The review discusses AI-assisted discovery and optimization of catalysts for lithium–sulfur, metal–air, lithium-ion, sodium-ion, zinc-based, and redox-flow batteries, as well as hydrogen-related energy-storage systems. Recent progress in single-atom catalysts, transition-metal compounds, carbon-based catalysts, MXenes, high-entropy materials, and heterostructured catalysts is critically reviewed from an AI perspective. Moreover, we address the importance of explainable AI, active learning, uncertainty quantification and autonomous experimentation in accelerating catalyst development. Key challenges including limited and heterogeneous datasets, transferability, interpretability, dynamic catalytic interfaces and experimental validation are highlighted.

Keywords: Artificial intelligence; Machine learning; Catalyst design; Electrocatalysis; Energy storage; Electrochemical reactions; Lithium–sulfur batteries; Metal–air batteries; Redox-flow batteries; Generative AI; Density functional theory.

P0223 • Vedika

ICEAM2026-POSTER-0223 | Poster Presentation | Day 2, 09 Oct 2026, 05:05-05:35 PM, Tea Break & Poster Session

Synthesis, Optical, and Temperature-Dependent Dielectric Properties of Praseodymium-Doped Strontium Titanate for Energy Storage Applications

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Abstract

Green nanomaterials are transforming energy storage technologies by providing sustainable and high-performance alternatives. Among these, perovskite oxides have garnered significant attention due to their outstanding structural and electronic characteristics. In this study, Praseodymium-doped strontium titanate perovskite oxides were synthesized via a solid-state reaction method, followed by heat treatment in air. X-ray diffraction (XRD) analysis confirmed the formation of a cubic crystal structure, closely resembling the ideal perovskite phase, with detailed assessments of crystallite size and microstrain. The optical properties, investigated through UV-Vis spectroscopy, indicated the presence of both direct and indirect bandgaps, offering valuable insights into the material's electronic transitions. Additionally, dielectric measurements conducted over a temperature range of 40–600°C at a 1 kHz frequency revealed significant variations in the dielectric constant and dissipation factor, demonstrating the material's tunable electrical properties. These findings highlight the potential of Praseodymium-doped strontium titanate for applications in energy storage devices, particularly in resistive random-access memory (RRAM), supercapacitors, and solid oxide fuel cells (SOFCs). The development of such perovskite-based green nanomaterials presents an environmentally sustainable pathway for advancing next-generation electronic and energy storage technologies.

Keywords: Green nanomaterials; Perovskite oxides; Praseodymium-doped strontium titanate; Energy storage devices; Dielectric and optical properties.

O0011 • Twinkle Gupta

ICEAM2026-ORAL-0011 | Poster Presentation | Day 3, 10 Oct 2026, 08:30-09:30 AM, LT5

REINFORCEMENT LEARNING ASSISTED DESIGN OPTIMIZATION OF CsFAMA-BASED PEROVSKITE SOLAR CELL WITH DUAL ETL ENGINEERINGTwinkle Gupta¹, Ankur Bhardwaj¹, Ajay Kumar¹¹ Department of ECE, Jaypee Institute of Information Technology, Noida, U.P, 201309, India**Abstract**

The relentless growth of global human activity has driven a continuous rise in energy demand. With increasing interest in Perovskite Solar cell, this study highlights optimized PCE of 32.43%. The performance of PSC is highly sensitive to the interplay between absorber and charge transport layer thicknesses. Numerical simulation exploration is computationally expensive. In this work, reinforcement learning (RL) framework has been employed, trained with proximal policy optimization (PPO) to identify the optimal layer configuration of for device FTO/Al:Mg-TiO₂/SnO₂/CsFAMA(triple-cation)/Spiro-OMeTAD/Ni solar cell, simulated in SCAPS-1D. The RL agent is trained against a fast surrogate reward function built by trilinear interpolation over a 792 full factorial dataset spanning temperature (250-500 K), absorber thickness (350-900 nm), and SnO₂ buffer thickness (5-10 nm), which enables efficient policy learning without repeated calls to the underlying physics solver. At 300 K, both the trained policy and a direct search of the interpolated design surface converge on a common optimum with 900 nm CsFAMA absorber paired with a 5 nm SnO₂ buffer, yielding Voc = 1.2764 V, Jsc = 22.42 mA/cm², FF = 83.18%, and a power conversion efficiency of 32.43%. This configuration reproduces the best-performing device identified independently within the sampled design space, cross-validating the RL-derived result against ground-truth simulation data. Efficiency is found to increase monotonically with absorber thickness and decrease with buffer thickness across the explored ranges with both trends still active at the sampled boundaries. This indicates that the reported optimum is best for device design. These findings establish RL as a computationally efficient and independently verifiable approach for guiding SCAPS-1D-based PSC device optimization.

Keywords: Co-doped Al:Mg-TiO₂, Hybrid SCAPS-AI approaches, Perovskites, Reinforcement learning (RL), SCAPS-1D.



Poster Session IV

Energy & Fuels (Day 3, 10 Oct 2026) • 21 Posters

P0005 • Pranati Sharma

ICEAM2026-POSTER-0005 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

STRONTIUM-DOPED MIEC BASED PEROVSKITE AS A PROMISING CATHODE MATERIAL FOR LT-SOFCPranati Sharma^{1*}, Amit Sarin¹, Gaurav Bhargava²¹*Department of Physics, I.K. Gujral Punjab Technical University Kapurthala- 144603, Punjab, India*²*Department of Chemistry, I.K. Gujral Punjab Technical University Kapurthala- 144603, Punjab, India*

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Abstract

In recent times, the entire world is currently working to create some novel, non-conventional energy sources that are highly efficient, reasonably priced, and eco-friendly. Solid Oxide Fuel Cell (SOFC) is one type of fuel cell which attracts research attention due to their fuel flexibility and high efficiency. A solid oxide fuel cell consists of cathode, anode and electrolytes where the cathode goes through reduction, the anode goes through oxidation [1,2]. The cathode materials based on mixed ionic and electronic conductivity are the next generation of electrodes which operate at low or intermediate temperatures (500–800°C) and have every single qualities needed to be a good cathode for SOFC [3,4]. In this work, we have investigated the Samarium-based perovskite cathode ($\text{Sm}_{1-x}\text{Sr}_x\text{Fe}_{0.8}\text{Co}_{0.2}$). The perovskite cathode material has been characterized by using suitable techniques by considering different compositions to enhance the triple phase boundary length (TPB) and superior ORR activity at lower temperature. The formation of crystal structure of cathode material has been confirmed by X-Ray Diffraction whereas the porosity, particle size and elemental distribution Scanning Electron Microscopy and Energy-Dispersive Spectroscopy. Astonishingly the result shows the lower thermal expansion indicating good thermal compatibility. These findings suggest that chosen perovskite can be considered as a promising candidate for futuristic cathode material for low-temperature SOFC applications.

Keywords: Cathode, Mixed ionic and electronic conductivity (MIEC), Solid Oxide Fuel Cell (SOFC).**REFERENCES**

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P0016 • Kamana Kumari Mishra

ICEAM2026-POSTER-0016 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Understanding the Role of NiCoO_x Mass Loading in Enhancing Oxygen Evolution Kinetics for AEM Water ElectrolysisKamana K. Mishra¹, Karthik Kannan², Manisha Sharma¹, Swarnima Singh¹, Jay N. Mishra¹, Yong- Song Chen², Prabhakar Singh^{*,1}¹*Department of Physics, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India*²*Department of Mechanical Engineering, Advanced Institute of Manufacturing with High-Tech Innovations, National Chung Cheng University, Chiayi, 621301, Taiwan*

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Abstract

With the rising concern over CO₂ emissions and their severe environmental impact, transitioning from fossil fuels to clean energy from renewable sources has become imperative. Hydrogen production via electrocatalytic and photoelectrocatalytic water splitting offers a sustainable pathway for clean energy conversion and environmental remediation. Among various approaches, Anion Exchange Membrane (AEM) water electrolysis has emerged as a promising and cost-effective technology, particularly due to its compatibility with non-precious metal oxide catalysts. In water electrolysis, the Oxygen Evolution Reaction (OER) at the anode poses challenges due to its sluggish kinetics and high overpotential requirements, limiting large-scale hydrogen production. A valid approach for accelerating the OER process is developing advanced electrocatalysts with enhanced kinetics and reduced overpotentials.

This study investigates the influence of varying NiCoO_x mass loadings on the anode's catalytic performance and stability in Anion Exchange Membrane (AEM) water electrolyzers. The NiCoO_x catalyst was synthesized in a 1:1 ratio using the hydrothermal method. Following successful synthesis, catalyst ink was prepared and coated onto a nickel foam gas diffusion layer (GDL) with loadings of 2 mg/cm², 4 mg/cm², and 6 mg/cm². The performance of NiCoO_x as an anode catalyst was tested in an AEM water electrolyzer across a temperature range of 25–70 °C using a 1 M KOH electrolyte. At 70 °C and 1.8 V, current densities of 260, 220, and 260 mA cm⁻² were recorded for 2, 4, and 6 mg cm⁻² loadings, respectively. The electrochemical measurements were further conducted to identify the optimal catalyst loading for achieving the best performance. The 2 mg cm⁻² catalyst loading demonstrated the most favourable OER performance, achieving a low overpotential of 320 mV at 10 mA cm⁻² and a Tafel slope of 112.35 mV dec⁻¹, supported by its highest Electrochemical active surface area (ECSA) and lowest charge-transfer resistance from EIS analysis. The pre- and post- electrochemical XPS analysis of different mass loading also supported these results. The durability test of 2 mg/cm² loading over ~70 h showed no significant change in OER activity, confirming the robustness, long-term durability, and excellent stability under the harsh operational conditions.

Keywords: CO₂ emissions; Hydrothermal process; Oxygen Evolution Reaction; water electrolyzer; overpotential

P0021 • Neeta Kumari

ICEAM2026-POSTER-0021 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Effect of Annealing temperature on phase formation and electrocatalytic performance of CoCrFeNiMn HEAs for overall water splitting

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Abstract

The development of efficient, stable, and cost-effective electrocatalysts is essential for sustainable hydrogen production through water electrolysis. In this work, FeCoCrMnNi high-entropy alloy (HEA) was synthesized by mechanical alloying and investigated as a noble-metal-free bifunctional electrocatalyst for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in 1 M KOH. The structural evolution during mechanical alloying was examined by X-ray diffraction (XRD), while the morphology and elemental distribution were investigated using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS). Complete alloying was achieved after 40 h of mechanical alloying, resulting in a multiphase structure comprising FCC, BCC, and sigma phases, with crystallite sizes of 7.84 and 15.51 nm for the FCC and BCC phases, respectively. The synthesized HEA exhibited a homogeneous distribution of Fe, Co, Cr, Mn, and Ni, with an average particle size of approximately 1.4 μm . The effect of annealing on phase evolution was also investigated at 300, 500, 700 and 900 $^{\circ}\text{C}$, revealing a significant transformation in the FCC/BCC phase fractions, crystallite growth, and reduction in lattice strain with increasing annealing temperature. Further, to investigate the ionic state of the synthesized samples, XPS analysis will also be provided. We also investigated the electrocatalytic performance of synthesized HEAs. The as-synthesized FeCoCrMnNi HEA exhibited HER and OER overpotentials of 232 and 346.6 mV, respectively, at a current density of 10 mA cm^{-2} . Also, the 500 $^{\circ}\text{C}$ annealed sample showed an OER overpotential of 268 mV, however the 900 $^{\circ}\text{C}$ annealed sample exhibited the better OER performance, with an overpotential of 203 mV and a Tafel slope of 109 mV dec^{-1} . The 500 $^{\circ}\text{C}$ annealed sample also demonstrated HER performance with overpotential of 251 mV, whereas the 900 $^{\circ}\text{C}$ annealed sample showed an HER overpotential of 253 mV. Chronopotentiometric measurements further demonstrated the operational stability of the HEA electrodes, with the 900 $^{\circ}\text{C}$ annealed sample maintaining OER activity for up to 110 h and the as-synthesized and 500 $^{\circ}\text{C}$ annealed samples showing prolonged HER activity. Overall, the results demonstrate that mechanically alloyed FeCoCrMnNi HEA is a promising bifunctional, noble-metal-free electrocatalyst for alkaline water electrolysis, while annealing provides an effective route for tailoring its phase constitution and electrochemical performance.

Keywords: HEA, annealing, electrocatalyst, HER, OER

P0025 • SUNITA GHOSH

ICEAM2026-POSTER-0025 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Design and optimization of NiCoAl-Layered double hydroxide as an Electrocatalyst for Electrochemical Water Splitting for oxygen evolution reaction (OER) in alkaline medium for green hydrogen production

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Abstract

The global energy crisis has increased the need for clean and sustainable energy technologies. Renewable energy sources are crucial in this shift. Specifically, hydrogen production through electrochemical water splitting has become a key area of research [1]. To replace noble-metal-based catalysts, it is important to develop efficient, low-cost, and abundant bifunctional electrocatalysts that can facilitate both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) with low overpotentials and high stability [2]. In this study, NiCoAl- Layered double hydroxide (LDH) with different concentration of aluminum were created using a urea-assisted hydrothermal method, with metal nitrates as precursors [3]. Electrochemical measurements demonstrated that the NiFe₂O₄ nanosheets exhibited superior bifunctional activity, achieving an OER overpotential of 330 mV at 10 mA cm⁻². Favorable kinetics were indicated by low Tafel slopes of 106 mV dec⁻¹ for OER. Electrochemical impedance spectroscopy further corroborated these findings by confirming a notable reduction in charge transfer resistance for the NiCoAl-LDH. Furthermore, the NiCoAl-LDH demonstrated excellent long-term stability over 1000 electrochemical cycles. These comprehensive results presenting NiCoAl-LDH as a promising bifunctional electrocatalyst for efficient overall water splitting.

Keywords: Hydrogen Evolution Reaction, Oxygen Evolution Reaction, Bifunctional Electrocatalyst, Overpotential, Layered double hydroxide.

P0027 • PATEL KARAN DINESHBHAI

ICEAM2026-POSTER-0027 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

FIRST-PRINCIPLES INVESTIGATION ON BeCN₂ MONOLAYER FOR ELECTROCATALYTIC HYDROGEN GENERATION

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Abstract

Achieving a sustainable energy future and mitigating reliance on conventional energy sources necessitate the development of carbon-neutral methods that can generate eco-friendly hydrogen. Water electrocatalysis provides an environmentally friendly way to produce green hydrogen using the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Density functional theory (DFT) simulations are used in this study to thoroughly investigate the structural stability, electronic properties, and electrocatalytic performance of a two-dimensional (2D) BeCN₂ monolayer. Initially, we optimize the structural features of the monolayer, then conduct an in-depth evolution of its energetic, dynamic, and thermal stability. The favorable cohesive energy, the lack of imaginary frequencies in the phonon spectrum, and consistent performance during ab initio molecular dynamics simulation collectively verify the stability of the proposed 2D BeCN₂ structure. We then analyze its electronic properties through band-structure assessments, electron localization function, and charge-density distribution, offering insights into the bonding environment and the electronic interactions among Be, C, and N atoms. The catalytic effectiveness of BeCN₂ for hydrogen generation is explored by evaluating various inequivalent hydrogen adsorption configurations. By using comparative adsorption energy calculations, we identify the most favorable surface site, while the corresponding Gibbs free energy (ΔG_{H^*}) for hydrogen adsorption serves as the main indicator for assessing HER performance. We also investigate the thermodynamic nature of the OER employing the computational hydrogen electrode approach, considering the sequential adsorption of O, OH, and OOH intermediates. The determined reaction energetics point to good catalytic activity for hydrogen and oxygen evolution together with a low theoretical HER/OER overpotential. The combined aspects of structural integrity, appropriate electronic characteristics, and advantageous HER/OER thermodynamics position BeCN₂ as an attractive lightweight, noble-metal-free 2D electrocatalyst for upcoming renewable energy conversion technologies.

Keywords: Density functional theory (DFT); Hydrogen evolution reaction (HER); Oxygen evolution reaction (OER);

P0030 • Akanksha Patel

ICEAM2026-POSTER-0030 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

ENERGY INTEGRATION IN AMMONIA CRACKING FOR HYDROGEN PRODUCTION BY PRODUCT STREAM UTILIZATIONAkanksha Patel¹, Amit Kumar Gomey¹, Rakesh Kumar², MS Balathanigaimani², Arvind Singh^{2*}¹*Department of Chemical & Biochemical Engineering, Rajiv Gandhi Institute of Petroleum Technology, Jais Campus, Amethi, 229304, India*

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Abstract

Ammonia is increasingly recognized as a practical hydrogen carrier due to its high volumetric hydrogen density and ease of storage. However, ammonia cracking is an endothermic process that requires significant external heat input, which reduces overall efficiency. This work investigates the use of a hot product stream for preheating the ammonia feed in a cracking unit, thereby reducing external utility demand. A process model was developed in Aspen Plus for a base case of 100 kmol.h⁻¹ ammonia feed at 25°C, cracked at 450°C over an RGibbs reactor. Energy and mass balances indicate that the reaction produces 150 kmol.h⁻¹ H₂ and 50 kmol.h⁻¹ N₂. Without heat recovery, the external heat requirement is 1.17 MW. Incorporating a product-to-feed heat exchanger (HX1) reduces this duty by ~739 kW, lowering utility consumption by 63% and further reduced to 74% by waste heat recovery of cooler to pre-heater. Sizing calculations ($U = 100 \text{ W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$, $\Delta T_{\min} = 10\text{-}20 \text{ K}$) indicate HX1 requires $\approx 7.4 \text{ m}^2$ of heat transfer area ($\approx 14.7 \text{ m}^2$ at $U = 50 \text{ W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$). Sensitivity analyses show the heat recovery scales with feed rate, conversion, and reactor outlet temperature, and that preheating the feed to 150 °C reduces the external duty by $\approx 18.8\%$ for the base case. The results demonstrate that straightforward energy integration significantly improves efficiency and sustainability of ammonia cracking systems, offering a promising route for decentralized hydrogen generation.

Keywords: Ammonia cracking¹; Hydrogen production²; Heat integration³; Aspen Plus⁴; Process simulation⁵

P0032 • Rekha Devi

ICEAM2026-POSTER-0032 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Efficient Hydrogen Storage in Ti_2CS_2 MXene : DFT StudyRekha Devi¹, Saurabh Srivastava², Santu Baidya¹¹ *Department of Physics and Materials Science, Jaypee University of Information Technology, Solan, Himachal Pradesh, India*² *Department of Mathematics, Jaypee University of Information Technology, Solan, Himachal Pradesh, India*

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Abstract

Solid-state hydrogen storage attracts more attention for storing hydrogen than other storage methods due to its higher safety and lower storage pressure. MXene with a high surface area gain attention for hydrogen and energy storage applications. In this study, we investigate the hydrogen storage capacity of a two dimensional Ti_2CS_2 MXene using first-principles density functional theory calculations. Our findings reveal that this system have potential to adsorb maximum 12 H_2 molecules, corresponding to a gravimetric capacity of 4.14 wt%. This is higher than that of other materials such as $\text{Ti}_3\text{C}_2\text{T}_x$ ($\text{T}_x = \text{F/O/OH}$), graphyne, and metal-organic frameworks (MOFs). Ti_2CS_2 MXene adsorption energy decreases and gravimetric energy increases as the number of H_2 increases. Furthermore, for practical applications, 8 H_2 molecules show better adsorption energy of about 0.5 eV and moderate desorption temperature, with a gravimetric capacity 2.8 wt% for Ti_2CS_2 MXene. Our findings demonstrated that the Ti_2CS_2 monolayer can be a promising candidate for efficient hydrogen storage applications.

Keywords: MXene; Hydrogen Storage; DFT; Hydrogen Adsorption; Hydrogen Desorption

P0070 • Kaustubh Bhaskar Nerkar

ICEAM2026-POSTER-0070 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

The Metallic and Bimetallic Cluster-Decorated C_{24} Nanocage for Hydrogen Storage Using Density Functional Theory

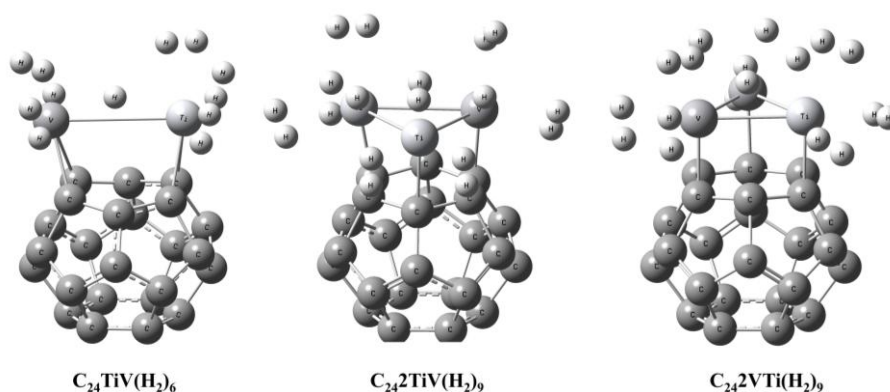
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Abstract

The increasing energy demand and excessive use of fossil fuels have caused serious problems such as global warming, pollution, and energy supply issues. Hydrogen is a promising clean energy carrier, but conventional storage systems have several limitations. Hence, solid-state hydrogen storage materials are needed. Nanocages are promising materials for this purpose, but pristine nanocages show weak interaction with H_2 molecules. In this work, we investigated Ti and V metallic and Ti-V bimetallic clusters decorated C_{24} nanocages for hydrogen storage using DFT calculations. The calculations were performed using Gaussian 09 software with the wb97XD functional and 6-311++G(d,p) basis set. Ti, Ti_2 , Ti_3 , V, V_2 , V_3 , TiV , Ti_2V , and V_2Ti clusters were considered for decoration on C_{24} nanocage. $C_{24}V_3$ gets distorted during optimization, and the remaining eight systems were further considered for hydrogen storage. The negative formation and cohesive energies confirm the thermodynamic stability of the complexes, while the binding energies show strong interaction between the metal clusters and C_{24} nanocage. For dimers, $C_{24}TiV$ shows stronger H_2 adsorption and a higher desorption temperature than $C_{24}Ti_2$ and $C_{24}V_2$, while its H_2 uptake is in between their H_2 uptake capacity. For trimers, the bimetallic clusters show different behavior depending on the metal arrangement. The $C_{24}V_2Ti$ shows better adsorption and desorption characteristics than $C_{24}Ti_2V$, even though its H_2 uptake is lower than $C_{24}Ti_3$. In conclusion, bimetallic decoration shows better control over H_2 adsorption, uptake, and desorption properties. The $C_{24}TiV$ and $C_{24}V_2Ti$ are better candidates for hydrogen storage.



Keywords: Hydrogen storage, Density Functional Theory, Bimetallic cluster, C_{24} nanocage, Metal decoration

P0090 • Pramod Mani

ICEAM2026-POSTER-0090 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Techno-Economic and Reliability-Oriented Optimization of a Solar PV–Wind–Battery–Diesel Hybrid Energy System for Industrial Applications

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Abstract

Reliable and sustainable electricity supply is essential for industrial facilities, where power interruptions can cause production losses, while conventional diesel-based generation results in high operating costs, fuel consumption, and carbon emissions. This study develops a reliability-oriented multi-criteria optimization framework for a solar photovoltaic (PV)–wind–battery–diesel hybrid renewable energy system (HRES) designed for continuous industrial electricity supply. An annual 8760-h industrial load profile is integrated with site-specific solar and wind resources and techno-economic models of PV, wind turbine, diesel generator, lithium-ion battery storage, and bidirectional power conversion. HOMER Pro is employed for chronological energy-balance simulation and optimization, while candidate configurations are evaluated using net present cost (NPC), levelized cost of energy (LCOE), renewable penetration, excess electricity, unmet load, capacity shortage, fuel consumption, and emissions. The optimized configuration comprises 315 kW PV, 10 kW wind generation, 300 kWh battery storage, a 76-kW diesel generator, and a 64.6 kW converter. The system produces 516.9 MWh annually, with PV contributing 96.5%, while achieving zero unmet electrical load and zero capacity shortage. Compared with the diesel-only reference system, NPC, LCOE, and annual operating cost are reduced by approximately 83.2%, 83.2%, and 91.6%, respectively. Annual diesel consumption and CO₂ emissions decline by approximately 97.2%. The results demonstrate that reliability-constrained renewable hybridization can simultaneously improve economic performance, supply adequacy, and environmental sustainability for industrial energy applications.

Keywords: Hybrid Renewable Energy System (HRES); Industrial Energy Management; HOMER Pro; Multi-Criteria Optimization; Energy Storage

P0098 • Yatendra Singh

ICEAM2026-POSTER-0098 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Defect-Engineered MoS₂ as a Sc-Anchored Platform for Strain-Tunable Molecular Hydrogen AdsorptionYatendra Singh¹, Anurag Srivastava*¹, Andrey Chibisov²¹Advanced Materials Research Group, Department of Engineering Sciences,

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Abstract

The combination of defect engineering and transition-metal decoration provides an effective strategy for enhancing the hydrogen-storage performance of two-dimensional materials. Here, first-principles density functional theory (DFT) calculations were performed to investigate molecular hydrogen adsorption on Sc-decorated sulphur-vacancy MoS₂. Among the investigated vacancy configurations, the single sulphur vacancy is the most favourable anchoring site for Sc, exhibiting a strong binding energy of –5.58 eV, exceeding the cohesive energy of bulk Sc and thereby suppresses metal clustering. The optimized Sc@1V_s–MoS₂ system accommodates up to five H₂ molecules with average adsorption energies ranging from –0.326 to –0.233 eV/H₂, within the desirable range for reversible hydrogen storage. Preserved H–H bond lengths and electronic structure analysis support molecular, non-dissociative molecular adsorption mediated by localized Sc–H₂ interactions. The desorption temperature decreases from 417 K for a single H₂ molecule to 298 K at saturated loading, indicating favourable hydrogen release under near-ambient conditions. AIMD calculation indicates the thermal stability of the structures. Pressure–temperature analysis reveals that increasing H₂ pressure favours adsorption, whereas increasing temperature promotes H₂ release. Furthermore, –4% biaxial compressive strain enhances adsorption strength by 26.18% respect to strain free hydrogen adsorbed system, demonstrating effective strain tunability. These findings establish sulphur-vacancy-stabilized Sc-decorated MoS₂ as a stable, strain-tunable platform for reversible molecular hydrogen storage.

Keywords: MoS₂, Sulphur vacancy, Sc decoration, hydrogen adsorption, density functional theory, strain engineering, gravimetric capacity, desorption temperature

P0126 • Abhinav Anand Sinha

ICEAM2026-POSTER-0126 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

EXPERIMENTAL INVESTIGATION OF RENEWABLE HYDROGEN PRODUCTION AND SEASONAL STORAGE USING SOLAR PV

Abhinav Anand Sinha, Satya Sekhar Bhogilla, Vivek Kumar, Sanjay Sharma

*Department of Mechanical Engineering, Indian Institute of Technology, Jammu, Jammu & Kashmir, India*Corresponding Author Email: satya.bhogilla@iitjammu.ac.in**Abstract**

The growing demand for clean and sustainable energy has increased the importance of green hydrogen production and its safe, efficient, and long-term storage. Hydrogen is considered a promising alternative to conventional fossil fuels because its utilization can significantly reduce harmful emissions associated with carbon-based energy sources. In this study, an experimental investigation of solar photovoltaic (PV)-based green hydrogen production and its solid-state storage is presented. The electricity generated by the PV panels is supplied to the grid, while grid electricity is subsequently used to operate an anion exchange membrane (AEM) electrolyzer for hydrogen production. The AEM electrolyzer uses water as the feedstock and produces hydrogen through an electrochemical process. To evaluate the seasonal variation in solar energy availability, experimental PV data corresponding to four representative dates, comprising two equinoxes and two solstices, are considered. The continuously produced hydrogen is initially collected in a buffer cylinder, which facilitates controlled hydrogen supply to the storage system. Subsequently, hydrogen is stored in a metal hydride (MH) tank, providing a safer alternative to conventional high-pressure gaseous hydrogen storage. In the MH storage system, hydrogen interacts with the metal hydride material, resulting in the dissociation of molecular hydrogen and its absorption within the metal hydride lattice. The hydrogen absorption process is exothermic; therefore, continuous water circulation around the storage tank is employed to remove the generated heat and maintain favorable operating conditions for hydrogen absorption. The experimental results demonstrate the feasibility of solar PV-based hydrogen production followed by solid-state storage, highlighting its potential for seasonal and long-duration renewable energy storage.

Keywords: Electrolyzer; Green hydrogen; Hydrogen production; Hydrogen storage; Metal hydride storage;

P0137 • SHWETA VERMA

ICEAM2026-POSTER-0137 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Vacancy and Strain Engineering Activates Basal-Plane of MoTe₂ for Hydrogen Evolution: A First-Principles Study

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Abstract

Two-dimensional transition-metal dichalcogenides (TMDs) are earth-abundant candidates which can replace platinum for the hydrogen evolution reaction (HER), among TMDs MoTe₂ is a viable HER catalyst due to its excellent mobility, conductivity, chemical stability and robustness during electrochemical reactions. Monolayer MoTe₂ can improve the charge transfer for HER due to its atomic thickness. However, basal plane of MoTe₂ is catalytically inert. Various strategies like defect engineering, strain engineering, doping, etc. are being adopted to activate the basal plane and increase the HER catalytic activity. These strategies have been proven to serve the same. In this study, we compare two polymorphs of MoTe₂ – the 2H (semiconducting) and the 1T' (metallic) monolayer – under identical computational parameters using density-functional theory (DFT), and assess how defect and strain engineering combinedly activate their basal planes for HER. Band-structure and density-of-states calculations confirm that 2H is semiconducting with a wide electronic gap, whereas 1T' is semi metallic with strongly hybridized Mo-d/Te-p orbitals that provides the conductivity essential for charge transfer to adsorbed hydrogen. For both phases we evaluate the Gibbs free energy for hydrogen adsorption (ΔG_H) on different adsorption sites. ΔG_H is strongly positive on the pristine basal planes of both phases which shows their inertness. Tellurium vacancies in 1T', drives ΔG_H toward the ideal thermoneutral value significantly as compared to 2H phase. Strain engineering on defected 1T' monolayer further pushes ΔG_H towards optimal value. The catalytic trends are explained through d-band center and Bader charge analysis, linking adsorption strength to the electronic structure of the active site. Our results establish defect engineering combined with strain engineering as a rational design approach for HER catalysts, and position 1T'-MoTe₂ as a tunable, noble metal-free alternative as HER electrocatalyst.

Keywords: Hydrogen evolution reaction (HER); Density Functional Theory (DFT); Vacancy engineering; Strain engineering; Transition-metal dichalcogenides

P0138 • Pooja tripathi

ICEAM2026-POSTER-0138 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

Orientation Optimization of Bifacial Photovoltaic Modules Using TraceProPooja Tripathi¹, Iqbal Ahmed Ghaffori¹, Satish Kumar Yadav², Jyotsna Singh¹, Rajendra Bahadur Singh¹¹*Department of Physics, University of Lucknow, Lucknow 226007*²*Institute of New and Renewable energy, University of Lucknow, Lucknow 226021***Abstract**

Bifacial photovoltaic (PV) modules can harvest solar irradiance from both, front and rear surfaces, making their orientation a critical parameter for maximizing energy yield in ground-mounted applications. Although a fixed tilt is commonly adopted for PV deployment, systematic optimization of bifacial module under outdoor conditions remains important because changes in tilt alter incident irradiance, rear-side irradiance, and consequently, electrical output. This study experimentally investigates two crystalline-silicon bifacial PV modules under outdoor ground-mounted conditions. One module is maintained at a fixed 22° tilt as the reference configuration, while the second module is operated under systematically varied tilt angles to determine the optimum orientation for enhanced energy yield. Solar irradiance, module voltage, current, power, surface temperature, ambient temperature, and wind velocity are recorded at 10-minute intervals. Instantaneous power, daily energy yield, conversion efficiency, performance ratio, and relative power gain, with respect to the 22° reference module, are evaluated to quantify the influence of tilt. The experimentally identified optimum configuration is subsequently investigated using TracePro three-dimensional optical modelling to analyse the orientation-dependent irradiance distribution over the front and rear surfaces of the bifacial module. The combined experimental and numerical approach enables identification of the tilt configuration providing enhanced irradiance capture and electrical energy yield. The proposed methodology provides a practical framework for optimizing bifacial PV module under realistic ground-mounted operating conditions and for validating outdoor performance through ray-tracing-based optical analysis.

Keywords: Bifacial PV module; Tilt angle; Experimental investigation; Thermal performance; Energy yield; Power gain; Performance ratio.

P0158 • Sunil Kumar

ICEAM2026-POSTER-0158 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

WATER MANAGEMENT IN PEM FUEL CELL THROUGH OPTIMIZATION OF POROUS TRANSPORT LAYER ARCHITECTURE AND PTFE LOADINGSunil Kumar¹, Ravita Lamba¹, Pranjali Sharma¹¹*Department of Hydro and Renewable Energy, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*

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Abstract

Proton exchange membrane (PEM) fuel cells are a promising electrochemical energy conversion technology due to their high-power density, low operating temperature, and zero emissions. Effective water management is essential for achieving high-performance and stable operation. At high current density, severe water accumulation obstructs gas-transport pores within the porous media, resulting in mass transport losses and degraded fuel cell performance. This porous media, referred to as the porous transport layer (PTL), consists of a gas diffusion layer (GDL) and a microporous layer (MPL) positioned between the flow channel and catalyst layer. The MPL plays an important role in regulating water removal and reactant gas diffusion. To address these issues, this study investigates the effects of PTL architecture and polytetrafluoroethylene (PTFE) loading on mitigating water accumulation and enhancing fuel cell performance. A 3-D PEM fuel cell model was developed in COMSOL Multiphysics to simulate liquid water transport and reactant gas distribution across the PTL. The novelty of this study lies in co-optimizing PTL geometry and PTFE hydrophobicity to create a capillary pressure gradient that directs water removal. The analysis examines various PTFE weight percentages and PTL architectures to establish the optimal balance among hydrophobicity, water removal, and gas accessibility. Simulated polarization curves and predicted peak power densities evaluate their coupled effects to isolate mass transport resistance. Results indicate that an optimized PTL induces a capillary pressure gradient across the porous interface, promoting directional water removal from active sites. Precise PTFE tuning prevents pore blockage while maintaining structural integrity and hydrophobic behavior. Consequently, the optimized PTL reduces mass transport resistance, improves oxygen transport, and sustains higher current density under fully saturated conditions. These findings highlight the practical application potential of combining PTL geometry modification, material composition, and hydrophobicity optimization to improve water management in next-generation, high-performance PEM fuel cells.

Keywords: Water management; Polytetrafluoroethylene optimization; Porous transport layer; Multiphysics simulation; Proton exchange membrane fuel cell.

P0159 • Akanksha Nanhet

ICEAM2026-POSTER-0159 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

A Holistic Review on Thermal Runaway Risk Assessment, Management, and Smart Monitoring in Li-ion Battery Systems

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Abstract

Driven by uncontrolled heat generation and improper thermal management in Li-ion batteries, thermal runaway (TR) remains a major safety concern in battery applications worldwide. This paper presents a comprehensive review of TR mechanisms focusing on heat generation, propagation of TR within a battery pack (BP) and subsequent failure incidents. This study systematically analyzes several techniques for TR suppression and mitigation for different BP structures and cell chemistry. From conventional cooling techniques to phase-change materials (PCMs), immersion cooling (IC), micro/mini-channels, thermoelectric coolers (TECs), heat pipes (HPs) and hybrid systems for TR mitigation are explored. Furthermore, this study suggested potential future research areas, emphasizing the incorporation of flame-retardant chemicals in composite PCMs for their safer use in large format batteries, compatibility for using IC, efficiency optimization of TEC, thermally efficient design structures for micro/mini-channels and development and testing of smart ML-driven early prediction systems. This review also highlights the advancements in early detection signs of TR by gas, temperature, voltage and pressure sensors followed by electrochemical impedance spectroscopy strategies. Intelligent monitoring using machine learning (ML) algorithms are discussed deeply with their framework for fault detection and different approaches used. Brief discussion of the adoption of ML based models in real-world applications for a more clarified basis of the safety evaluation is also involved in this review. Therefore, this study aims to contribute to a safer operation of battery applications, better heat management techniques under TR condition and high-performance energy storage systems for electric vehicles in the future.

P0161 • Amit Uniyal

ICEAM2026-POSTER-0161 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

OPTIMAL POWER BALANCE FOR HYBRID ENERGY STORAGE IN GRID INDEPENDENT DC MICROGRID USING ADAPTIVE FUZZY LOGIC ENERGY MANAGEMENT SYSTEM

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Abstract

With sustainability becoming an integral part of life, the energy sector sees a shift towards adopting renewable energy sources (RES) as decentralized energy generation units. These renewable-powered direct current (DC) microgrids face substantial operational stability and lifespan challenges due to solar intermittency and pulsed, high magnitude load steps. When supplied solely by battery storage, severe current gradients accelerate battery electrochemical aging and cause DC bus voltage fluctuations. To resolve these limitations, this paper presents a comprehensive simulation and control framework integrating a photovoltaic (PV) array with an active battery–supercapacitor hybrid energy storage system (HESS) coupled to a 400 V DC bus. An adaptive fuzzy logic-based energy management strategy (FLEMS) is proposed to overcome the rigid trade-offs of conventional fixed-parameter low-pass filters (LPF). The developed Mamdani fuzzy inference engine dynamically modulates the frequency-decoupling time-constant based on real-time net current demand, battery state-of-charge (SOC^{Bat}), and supercapacitor state-of-charge (SOC^{SC}). Concurrently, a closed-loop fuzzy logic based maximum power point tracking (FL-MPPT) algorithm guarantees optimal solar power harvesting across variable irradiance profiles. Comprehensive time-domain simulations under severe load transients demonstrate that the adaptive fuzzy controller reduces the battery current slew-rate RMS as compared to baseline LPF, effectively suppressing battery thermal shock and cyclic degradation. Furthermore, the fuzzy supervisory layer prevents supercapacitor over-depletion by maintaining supercapacitor $\text{SOC}^{\text{SC}} > 30\%$, eliminating the voltage collapse risk inherent in the filters with high time-constant, while maintaining tight 400 V DC bus voltage regulation. The proposed zero-dependency framework provides a robust, scalable energy management solution for resilient standalone DC microgrids.

Keywords: DC microgrid, Hybrid energy storage, Battery degradation mitigation, Adaptive fuzzy logic controller, Energy management system.

P0169 • Hariram N P

ICEAM2026-POSTER-0169 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

PUMPED HYDRO, HYDROGEN AND BATTERIES FOR HYBRID MICROGRIDS: A TECHNO-ECONOMIC ASSESSMENTHariram N P^{1,2}, Vidya Chandran³, Mekha K.B.⁴, Ajith Gopi⁵, *K Sudhakar^{4,6,7}¹*Faculty of Civil Engineering Technology, Universiti Malaysia Pahang Al Sultan Abdullah, Paya Besar 25150, Malaysia.*²*Integrated Centre for Green Development and Sustainability (ICFGS), ICFGS Foundation, Kazhimbram, Kerala 680568, India.*³*Department of Mechanical Engineering, SCMS School of Engineering and Technology, Karukutty, Kerala 683576, India*⁴*Faculty of Mechanical and Automotive Engineering Technology, Universiti Malaysia Pahang Al Sultan Abdullah, 26600, Malaysia.*⁵*Zonergia Pvt. Ltd., Technopark, Thiruvananthapuram, Kerala, 695581, India.*⁶*Centre for Sustainable Fluid Energy Research (Fluid Energy), Universiti Malaysia Pahang Al-Sultan Abdullah, Kuantan 26300, Pahang, Malaysia*⁷*Centre for Automotive Engineering (Automotive Centre), Universiti Malaysia Pahang Al-Sultan Abdullah, 26600, Malaysia.*

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Abstract

The increasing penetration of variable renewable energy sources in decentralized power systems has created a growing requirement for reliable, flexible, and economically viable energy-storage solutions. In India, renewable small-hydro resources combined with solar photovoltaic (PV) generation offer significant potential for developing resilient hybrid microgrids, particularly in regions with suitable dam and hydropower infrastructure. However, the intermittent nature of solar generation and variations in hydropower availability necessitate appropriate energy-storage technologies to maintain supply-demand balance, improve renewable-energy utilization, and enhance system reliability. This study presents a comparative analysis of an energy-storage system incorporating Pumped Hydro Energy Storage (PHES), Green Hydrogen Storage (GHS), and Battery Energy Storage Systems (BESS) for renewable small-hydro-solar hybrid microgrids in India. A hybrid microgrid configuration integrating small-hydro power generation and solar PV is considered as the renewable-energy backbone, with PHES, GHS, and BESS evaluated as alternative and complementary storage pathways. The assessment considers their ability to absorb excess renewable generation, provide energy during periods of low renewable availability, and improve overall system operational performance. The energy dimension evaluates renewable-energy utilization, storage efficiency, energy losses, dispatchability, storage duration, reliability, and the contribution of each storage vector to reducing renewable-energy curtailment. The economic assessment considers capital and operating expenditures, levelized cost of energy and storage, replacement requirements, lifecycle costs, and key financial indicators. The environmental dimension evaluates lifecycle greenhouse-gas emissions, avoided emissions associated with renewable-energy integration, and resource requirements throughout the system life cycle. The study further investigates the operational and economic trade-offs associated with short-, medium-, and long-duration energy storage. BESS provides rapid-response and high-efficiency storage suitable for short-duration balancing and transient load variations, whereas PHES offers large-scale and relatively long-duration storage with potential advantages where appropriate hydraulic infrastructure and elevation differences are available. GHS provides a complementary long-duration and seasonal storage pathway, enabling excess renewable electricity to be converted into hydrogen and subsequently utilized for electricity generation or other energy applications. The comparative framework therefore examines not only individual storage technologies but also the potential value of integrating storage systems within a single hybrid microgrid. The proposed approach provides a systematic basis for identifying technically suitable, economically competitive, and environmentally sustainable storage configurations for Indian renewable small-hydro-solar hybrid microgrids. The outcomes are intended to support technology selection, optimal energy-storage planning, and the development of resilient decentralized renewable-energy systems that can address India's evolving energy-storage requirements.

Keywords: Pumped Hydro Energy Storage (PHES), Green Hydrogen Storage (GHS), Battery Energy Storage Systems (BESS), Small Hydro-Solar Hybrid Microgrid, Techno-Economic-Environmental

P0179 • Jyoti Kahale

ICEAM2026-POSTER-0179 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

HYDROGEN GENERATION USING STABLE AND EFFICIENT ZEOLITIC IMIDAZOLE FRAMEWORK BASED ELECTROCATALYST

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The global surge in demand for clean and sustainable energy has increased considerably which has stimulated significant research in the field of Hydrogen production by electrochemical water splitting. Hydrogen Evolution Reaction (HER) although being favourable, due to its sluggish kinetics, requires an efficient electrocatalyst to reduce the energy barrier and improve hydrogen generation efficiency. This makes development of a low-cost, highly active and durable electrocatalyst desirable which remains as an important challenge. Metal-organic frameworks (MOFs) have emerged as promising materials for energy conversion applications because of their high surface area, tunable porosity, and well-defined metal centers. Among various MOFs, Zeolitic Imidazolate Framework-67 (ZIF-67) has attracted considerable attention due to its porous structure and accessible cobalt active sites. In the present study, ZIF-67 was synthesized and carbonized at varied temperature from 600°C to 900°C to obtain a porous conducting catalyst with cobalt active centers. The synthesized material was characterized using XRD and FTIR for structural and chemical characterization techniques to confirm the formation and properties of the ZIF-67 framework. The electrocatalytic activity of the prepared carbonized ZIF-67 was evaluated using electrochemical measurements in 0.5M H₂SO₄ electrolyte. Linear sweep voltammetry was employed to investigate HER activity where the overpotential at 10mA/cm² was found to be 318, 328, 374 and 196 mV for ZIF-67@600, ZIF-67@700, ZIF-67@800, ZIF-67@900 respectively. To understand the reaction kinetics Tafel slopes were found to be 238, 259, 194 and 651mV/dec for ZIF-67@600, ZIF-67@700, ZIF-67@800, ZIF-67@900 respectively. This study aims to establish the relationship between the structural characteristics of ZIF-67 and its HER performance. The porous architecture and cobalt-containing active centers of ZIF-67 provide a favourable platform for electrolyte interaction and electrochemical reactions. The findings are expected to contribute to the development of economical and efficient MOF-based electrocatalysts with trying to achieve values close to benchmark catalyst Platinum Carbon (Pt/C).

P0180 • Simran Verma

ICEAM2026-POSTER-0180 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

FROM DOTS TO BLOOMS: DIMENSIONAL EVOLUTION OF ZNO FOR SOLAR HYDROGEN GENERATION*Simran Verma¹, Narinder Kaur^{2*}*¹*Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida-62, Uttar Pradesh, India*²*Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida-62, Uttar Pradesh, India*

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Abstract

Hydrogen is regarded as a promising clean energy carrier owing to its high gravimetric energy density and potential to decarbonize energy-intensive sectors. Growing energy demand and the environmental consequences of fossil-fuel-dependent energy systems have intensified the need for sustainable hydrogen production routes. However, conventional hydrogen generation is still dominated by fossil-based processes, while renewable pathways face challenges including high energy requirements, limited conversion efficiency, sluggish reaction kinetics, and inefficient utilization of solar energy. Semiconductor-based photocatalytic and photoelectrochemical systems offer a promising approach by directly converting solar energy into chemical energy through water splitting. Their performance is strongly governed by electronic structure, charge-carrier dynamics, surface reactivity, and nanoscale architecture. Among various semiconductor materials, ZnO has attracted considerable attention because of its favourable band-edge positions, high electron mobility, chemical stability, abundance, and low cost. This work explores the dimensional evolution of ZnO from zero-dimensional quantum dots to one-dimensional nanorods and two-dimensional nanosheets for solar hydrogen generation. Dimensional variation enables modulation of surface characteristics, defect states, exposed facets, and carrier-transport pathways, thereby influencing photoinduced charge utilization and hydrogen-evolution activity. This dimensional perspective provides valuable insights for rationally designing ZnO-based architectures toward efficient solar hydrogen production.

Keywords: ZnO; Hydrogen Generation; Nanostructures; Photocatalysis; Water Splitting.

P0186 • Abubakar Sadiq Imam

ICEAM2026-POSTER-0186 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

PRODUCTION AND EVALUATION OF BIODIESEL FROM *DETARIUM SENEGALENSE* SEED OIL: FUEL CHARACTERIZATION, MOLECULAR CHARACTERIZATION, AND EMISSIONS BEHAVIOR

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Abstract

With the growing demand for renewable fuels for transportation, scientists are turning to non-food and underutilized oil sources for biodiesel production. The objective of this study was to investigate the production, characteristics, and performance of biodiesel in internal combustion engines (ICEs) from *Detarium senegalense* seed oil (DSSO). The oil was extracted from seed powder by Soxhlet extraction using 95% n-hexane and then transesterified to biodiesel via acid-catalyzed esterification and alkaline transesterification. The oil yield was $11.85 \pm 0.05\%$, the free fatty acid content was $1.86 \pm 0.02\%$, and the biodiesel (DSB100) yield was 90.34%. Density, viscosity, cetane number, flash point, cloud point, and pour point increased with increasing biodiesel concentration, while the heating value decreased. DSB100 exhibited a density of $858.24 \pm 0.11 \text{ kg m}^{-3}$, a viscosity of $5.12 \pm 0.02 \text{ mm}^2 \text{ s}^{-1}$, a cetane number of 57.53 ± 0.01 , and a heating value of $41.31 \pm 0.05 \text{ MJ kg}^{-1}$. The IR bands confirmed the presence of ester functional groups at 1744 and 1159 cm^{-1} , and the maximum absorption was observed at 210 nm in the UV-Vis spectrum, from which multiple chromatographic components were detected by GC-MS, the predominant one appearing at $t \sim 33 \text{ min}$. The braking power increased, and the braking thermal efficiency decreased with increasing load in the engine tests conducted at 1500 rpm . On the other hand, the braking thermal efficiency and the lowest specific fuel consumption were achieved by the DSB10 engine, while the highest braking power and exhaust gas temperature were achieved by the DSB100 engine. The general trend was an increase in CO_2 , NO_x , HC, and CO emissions with increasing load. Overall, DSSO was found to have potential as a non-food feedstock for the production of biodiesel for diesel engines.

Keywords: *Detarium senegalense*; Transesterification; Fuel characterization; Engine performance; Exhaust emissions

P0224 • Rashid khan

ICEAM2026-POSTER-0224 | Poster Presentation | Day 3, 10 Oct 2026, 11:20AM-11:50 AM, Tea Break & Poster Session

EXPLAINABLE MACHINE LEARNING FRAMEWORK FOR PREDICTING DIESEL ENGINE PERFORMANCE WITH KARANJA BIODIESEL BLENDSRashid Khan^{1*}, Brahma Nand Agrawal², Sudhir Kumar Singh¹, Gaurav Kumar¹¹ *Department of Mechanical Engineering, Galgotias University, Greater Noida, 201306, India*² *Department of Mechanical Engineering, Greater Noida Institute of Technology, Greater Noida, 201308, Uttar Pradesh, India*

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Abstract

Growing demand for clean energy is making biodiesel a popular alternative. Testing engines take too much time and money; therefore, we need accurate, easy-to-understand models to predict performance. This study uses XGBoost, LightGBM, and CatBoost to predict how a diesel engine runs on Karanja biodiesel. It also uses the SHAP (SHapley Additive exPlanations) to make these machine learning predictions easy to understand. Experimental investigations were conducted using diesel and Karanja biodiesel blends from K10D90 to K50D50. These tests used compression ratios of 15–18 and engine loads from 0 to 100%. The input variables included engine load, compression ratio, and fuel blend. The predicted targets were brake thermal efficiency (BThEff), specific fuel consumption (SFC), torque, and mechanical efficiency (Mecheff.). Experimental results revealed that increasing engine load and compression ratio improved engine performance, while the K20D80 blend exhibited the best overall performance with a maximum BThEff of approximately 29.0% and a minimum SFC of 0.30 kg/kWh at full-load operation. The XGBoost model outperformed the other machine learning frameworks in predictive accuracy. The XGBoost model achieved R^2 of 1.00, RMSE of 0.67, MAE of 0.53, and MAPE of 6.43% for BThEff and, R^2 of 0.97, RMSE of 0.33 kg/kWh, MAE of 0.18 kg/kWh, and MAPE of 16.00% for SFC. CatBoost model also produced reliable predictions with R^2 values of 0.97 for BThEff and 0.92 for SFC. The LightGBM model exhibited comparatively lower performance with R^2 values of 0.79 and 0.28, respectively. SHAP-based explainability consistently identified engine load as the most influential parameter for both BThEff and SFC predictions. Compression ratio was the second most important factor, followed by the fuel blend. SHAP dependence analysis confirmed that increasing engine load enhanced BThEff and reduced SFC. The strong agreement between experiments, machine learning, and SHAP interpretations validates the accuracy and transparency of the proposed framework.

Keywords: Karanja biodiesel; Machine learning; Explainable Artificial Intelligence; SHAP



Thank You

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