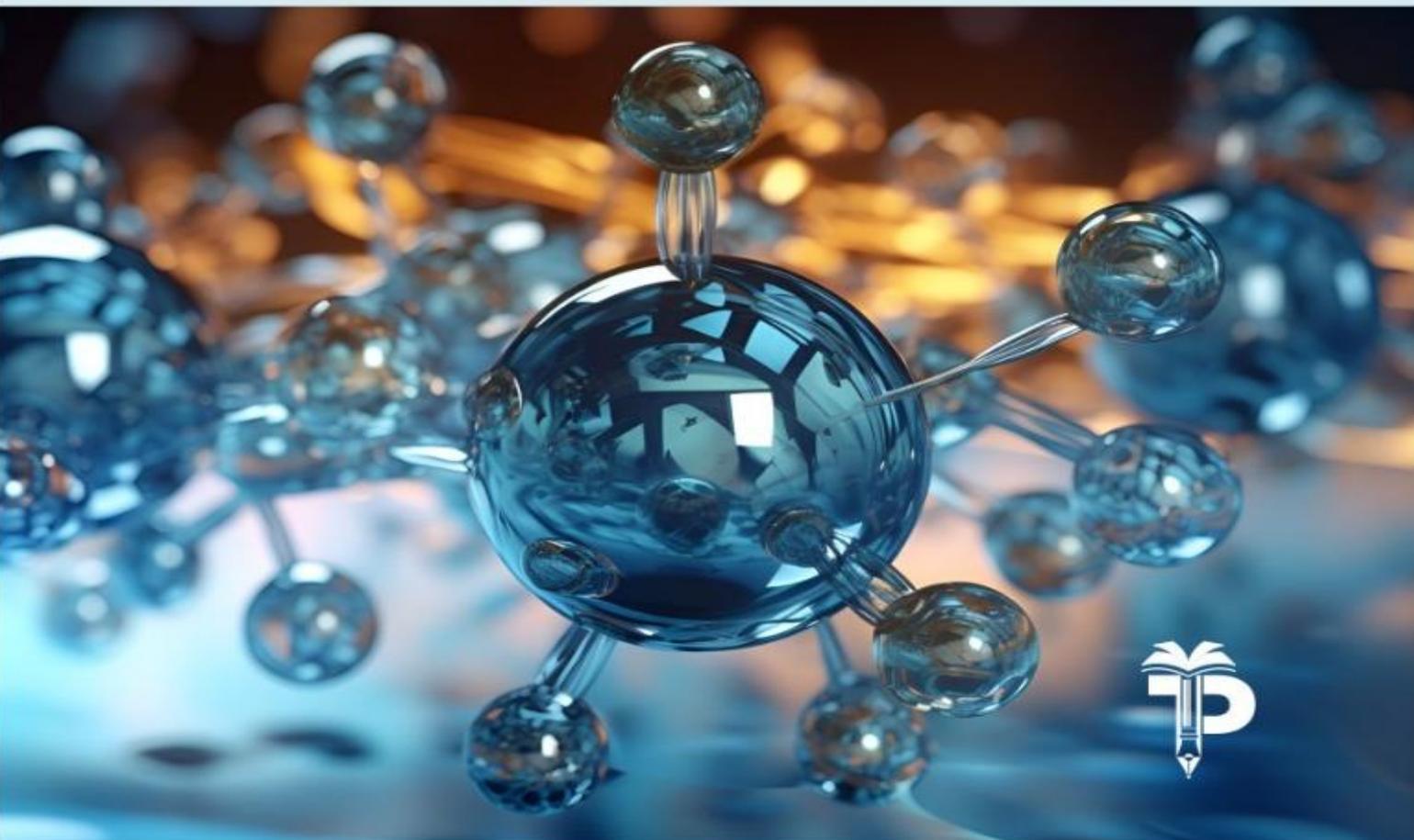




# **INNOVATIONS, ADVANCES IN MATERIAL SCIENCE FOR SUSTAINABLE GOALS (IAMSSG 2025)**

**(Sponsored by ANRF, DST-RAJASTHAN)**



*Organized by*  
**Department of Physics, JECRC University, Jaipur (29–31 October, 2025)**

*In Association with*  
**MRSI, IAPT, and SMRS**

# Conference Proceedings

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### *Editors*

Prof. Pranav Saxena  
Dr. Abhishek Sharma  
Dr. Hariom Pawar



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## Message from the Vice Chairperson



It fills me with immense pride and joy to witness the organization of the International Conference on “Innovations, Advances in Material Science for Sustainable Goals (IAMSSG-2025)” by the Department of Physics, JECRC University. I extend my warm congratulations to the organizing committee, the distinguished speakers, and all participants whose collective efforts have made this academic gathering possible.

At JECRC University, we have always believed in nurturing a culture where innovation, research, and learning move hand in hand. It is heartening to see our faculty and students taking forward this vision by engaging in research that not only advances scientific knowledge but also addresses the pressing challenges of sustainability and global well-being.

Conferences like IAMSSG-2025 serve as a vibrant platform for young minds to interact with experts, exchange innovative ideas, and gain inspiration to explore beyond conventional boundaries. Such initiatives strengthen our academic ecosystem and reflect JECRC University’s steadfast commitment to excellence and impactful research.

I wish the conference grand success and hope it inspires every participant to continue pursuing knowledge with curiosity, passion, and purpose.

**Arpit Agarwal**  
**Vice Chairperson**  
JECRC University, Jaipur

## Message from the President



It is a matter of great pride and joy to witness the organization of the International Conference on “Innovations, Advances in Material Science for Sustainable Goals (IAMSSG-2025)” by the Department of Physics, JECRC University. I extend my warm greetings and best wishes to all distinguished speakers, delegates, researchers, and participants who have gathered here to share their knowledge and experiences.

At JECRC University, we firmly believe that meaningful research and innovation are the driving forces of progress. This conference beautifully reflects our institutional ethos—of encouraging inquiry, promoting collaboration, and creating an ecosystem where ideas transform into impactful outcomes. The theme of IAMSSG-2025 aligns perfectly with the global pursuit of sustainability and mirrors our commitment to contribute to science that serves humanity and the planet.

It is heartening to see the Department of Physics taking such an inspiring initiative to bring together academia, research organizations, and industry experts on a common platform. Such endeavors not only enrich academic discourse but also strengthen our vision of becoming a center of excellence that blends learning with purpose.

I congratulate the organizing committee for their commendable efforts and extend my heartfelt appreciation to all contributors who have made this conference possible. I am confident that IAMSSG-2025 will stimulate new ideas, foster lasting collaborations, and pave the way for innovations that support sustainable development goals.

With warm regards and best wishes for the grand success of the conference.

**Prof. Victor Gambhir**  
**President**  
JECRC University, Jaipur

## Message from the Registrar



It gives me great pleasure to extend my warm greetings to all participants and organizers of the International Conference on “Innovations, Advances in Material Science for Sustainable Goals (IAMSSG-2025)” organized by the Department of Physics, JECRC University.

This conference reflects our University’s strong commitment to promoting research, innovation, and academic collaboration. The focus on sustainable development through advances in material science truly aligns with JECRC’s mission to foster knowledge that benefits society and the environment.

I appreciate the dedicated efforts of the organizing committee and wish all delegates and participants fruitful discussions, meaningful interactions, and great success in this academic endeavor.

**S L Agarwal**

**Registrar**

JECRC University, Jaipur

## Message from the Dean, School of Sciences



It gives me immense pleasure to extend my heartfelt greetings to all participants of the International Conference on “Innovations and Advances in Material Science for Sustainable Goals” (IAMSSG-2025). This conference provides an excellent platform for researchers, academicians, and industry professionals from diverse domains to exchange ideas, share their latest research findings, and explore innovative approaches toward achieving sustainability through material science.

In today’s rapidly evolving world, material science plays a crucial role in addressing global challenges related to energy, environment, and technology. The interdisciplinary nature of this field continues to open new avenues for innovation, aligning perfectly with the United Nations’ Sustainable Development Goals (SDGs). I am confident that the deliberations and interactions during this conference will foster meaningful collaborations and inspire novel solutions that contribute to a sustainable future.

I congratulate the organizing committee for their dedicated efforts in bringing together such a distinguished gathering and for compiling this abstract book, which reflects the diversity and depth of ongoing research in the field. I extend my best wishes for the grand success of IAMSSG-2025 and hope that all participants will have a fruitful and enriching experience.

**Widhi Dubey**  
**Dean, School of Sciences**  
JECRC University, Jaipur

## Message from the Convener & Head, Department of Physics



It is my privilege and delight to welcome you all to the First International Conference on “Innovations, Advances in Material Science for Sustainable Goals (IAMSSG-2025)”, to be held from October 29–31, 2025 at JECRC University, Jaipur.

In organizing IAMSSG-2025, our objective has been to create a vibrant interdisciplinary platform where scholars, researchers, and industry professionals converge to share insights, exchange pioneering ideas, and forge collaborations in the realm of sustainable materials. The conference themes spanning functional nanomaterials, hybrid composites, biomaterials, materials modelling, green chemistry, energy materials, and more reflect the diverse challenges and opportunities before us in advancing sustainable goals through materials science.

We are honored to have eminent experts and distinguished speakers joining us from across the country and beyond, and we look forward to spirited discussions, rigorous debates, and creative synergies. The review and publication opportunities with leading SCI/SCOPUS-indexed journals further enhance the value and reach of this event.

I extend my sincere gratitude to the JECRC University leadership, the Department of Physics, the organizing committee, sponsors (including RSC, ACS, IAPT), and all persons who have worked tirelessly behind the scenes to bring this conference to fruition.

To all participants, whether presenting, listening, or networking I encourage you to engage with open minds, challenge boundaries, and seek new connections. May IAMSSG-2025 stimulate fresh ideas, spark lifelong collaborations, and contribute meaningfully to sustainable innovations that serve our planet and people.

Wishing the conference a grand success, and may it leave every attendee inspired and enriched.

**Prof. Pranav Saxena**  
**Convener & Head, Department of Physics**  
JECRC University, Jaipur

## **About the JECRC University**

JECRC University is a leading private institution located in Jaipur, Rajasthan, established in 2012. Recognized by the University Grants Commission (UGC) and holding the prestigious 12(B) status, the university is eligible to receive central government grants for research and development, underscoring its commitment to academic excellence and innovation.

The university offers a wide range of undergraduate, postgraduate, and doctoral programs in fields such as engineering, management, sciences, law, humanities, and design. With a strong emphasis on practical learning, JECRC University promotes hands-on projects, internships, and industry collaborations to equip students with real-world skills. JECRC University has a robust research ecosystem with dedicated centers focusing on emerging technologies like artificial intelligence, data science, robotics, and renewable energy.

The university boasts state-of-the-art infrastructure, including modern laboratories, well-equipped libraries, and digital learning resources to support academic growth. The university's vibrant campus life encourages student participation through cultural events, sports, and various clubs, ensuring holistic development. Its strong ties with industry leaders facilitate excellent placement opportunities for students. We have multiple seminar hall and conference rooms with maximum capacity of 600 and minimum capacity of 90.

## **About the Department of Physics, JECRC University**

The Department of Physics at JECRC University, School of Sciences, is dedicated to excellence in both teaching and research. With faculty members specializing in diverse fields such as Material Science, Solar Astronomy, Plasma Physics, Hydrogen Energy, Thin Films, Nuclear Physics, and Microwave Electronics, the department offers students a rich academic experience supported by quality research and publications in SCOPUS/SCI-indexed journals.

The department runs a M.Sc. (Physics) program and contributes to multiple other disciplines, including Forensic Sciences, B.Sc. (Law), and B.Tech programs, where students are introduced to cutting-edge technologies like Nanotechnology, Spintronics, Quantum Computing, and Photonics. The newly established R&D Material Science Laboratory provides a platform for experiential learning, innovation, and global competence in line with NEP 2020. Students also gain exposure through projects and internships with reputed organizations such as ISRO, DAE, Solar Observatories, and the Ministry of Earth Sciences, along with opportunities under the IAESTE Student Exchange Program.

The department fosters an inspiring academic environment with invited talks from eminent scientists at institutions like NASA, PRL, BARC, and IITs, motivating students to pursue higher studies and qualify in competitive exams such as JAM, JEST, and NET. With its strong academic foundation, research ecosystem, and global collaborations, the Department of Physics at JECRC University is committed to nurturing future-ready researchers and innovators.



**1<sup>st</sup>International Conference on  
“Innovations, Advances in Material Science for Sustainable Goals” - IAMSSG 2025  
Material Science Research Lab, Department of Physics  
JECRC University, Jaipur; October 29 - 31, 2025**

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# **Speaker's Abstract**

# **AI is not sustainable, what we need is ABI (Artificial Biological Intelligence)**

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## **Abstract**

Modern computing systems, despite their remarkable speed and capabilities, remain fundamentally limited by their architecture, resulting in high power consumption. In stark contrast, the human brain achieves extraordinary cognitive feats and massive parallel processing with only about 20 W of power. This efficiency has inspired global efforts to develop artificial neural networks and neuromorphic computing platforms that emulate the brain's intelligence using advanced algorithms on high-speed computational hardware. However, even the most sophisticated computers struggle to solve complex, real-world problems in real time—tasks that biological brains routinely manage with ease.

A key distinction lies in the biological synaptic junction, which seamlessly integrates processing and memory functions in parallel, a feature closely associated with neuroplasticity—the brain's ability to adapt and reorganize in response to experience. While the mechanisms linking neuroplasticity to memory and processing are still being explored, recent research increasingly focuses on replicating various forms of neuroplasticity using artificial synaptic devices. Neuromorphic computing, by mimicking neural processes, promises a paradigm shift: enabling low-power, efficient, and adaptive systems that overcome the limitations of traditional CMOS and Boolean logic architectures.

The presentation will review relevant literature in the field, highlight ongoing challenges and summarize key findings. Recent results from our laboratory will also be presented.

# **Another Route to produce Hydrogen Thermochemical Hydrogen Production**

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## **Abstract**

Japanese government set the target about hydrogen production of 3 million and 20 million ton/year, respectively in 2030 and 2050. In order to realize carbon neutrality, this hydrogen must be produced from not fossil fuel but renewable energy and carbon free energies. Of course, renewable energy should be the most important candidate to be realized, however the typical properties of the renewable energy is “fluctuation”. On the other hand, 50 kWh electricity is needed to produce 1 kg hydrogen, therefore, 20 million ton ( $2 \times 10^{10}$  kg)  $\times$  50 kWh / 8000 h (ca 90% machine operation rate) means that 125 GW electrolyzer and corresponding “stable” electricity are necessary for the green hydrogen production. Moreover, from the electrochemical efficiency (50kWh/kg), we can estimate the hydrogen production costs equivalent to electricity supply costs. In Japan, target total costs of hydrogen production is set to be 2 USD/kg (1 USD/kg in USA). The expected electricity price should be less than 0.04 USD/kWh. So, if the green hydrogen is produced by electrolyzer, we have to reduce electricity price and improve quality of renewable electricity from unstable to stable.

In this situation, we would like to propose another route to produce green hydrogen, that is thermochemical hydrogen production. In general, technologies of thermochemical hydrogen production are categorized into 3 groups with different temperature range. The first is more than 1000 C (high temp.

system), the second is more or less 900 C(middle temp.), and the third is less than 500 C(low temp.). The high temperature system is quite simple but the green production requires only concentrated solar heat with quite low machine operation rate. The middle temperature system is quite complicated, so nuclear heat can be only the heat source thanks to high machine operation rate. Although the low temperature system is also complicated, not only various heat sources but also concentrated solar heat with thermal storage materials can promises high operation rates. Therefore, we focus on the low temperature system, which is so called Na redox system. This system is composed of three reactions, that is hydrogen generation by solid-liquid reaction, metal separation by thermolysis, and oxygen generation by hydrolysis. This novel thermochemical cycle was inspired by research and development of hydrogen storage materials. By further developing this reaction and linking it to large-scale production, we are able to expect to have the effect of mass production.

## **Fullerene-Enabled Resistive Switching for Next-Generation Memoryics**

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### **Abstract**

Fullerene molecules such as C<sub>84</sub> exhibit intriguing electronic and magnetic characteristics; however, their multiferroic behavior and potential for memory applications remain underexplored. In this study, few-layer C<sub>84</sub> films were deposited onto Si(111)-7×7 substrates using thermal evaporation in an ultra-high vacuum (UHV) system. The electronic properties of the C<sub>84</sub>/Si(111) interface were characterized by UHV-STM, revealing a bandgap of approximately 3.7 eV. Multiferroic behavior was confirmed via magnetic force microscopy (MFM) and piezoresponse force microscopy (PFM). The observed ferromagnetism is attributed to localized spin-exchange interactions, while ferroelectricity is linked to spin-orbit coupling effects. Density functional theory (DFT) calculations using the VASP package further demonstrated that external electric fields induce intermediate electronic states near the Fermi level. Spectroscopic techniques including Raman, X-ray photoelectron spectroscopy (XPS), and photoluminescence were employed to investigate the structural features of the interface, revealing the presence of sp<sup>2</sup>/sp<sup>3</sup> hybridization, dangling bonds, and defect-related states.

Device-level characterization of Au/C<sub>84</sub>/Si(111) structures exhibited bipolar resistive switching behavior, as confirmed by conductive atomic force microscopy (C-AFM). The switching mechanism involves defect-mediated charge transport and field-induced bond reconfiguration, particularly between sp<sup>2</sup> and sp<sup>3</sup> configurations. These findings highlight the potential of C<sub>84</sub> fullerenes as active materials in future non-volatile memory devices, such as ReRAM and FeRAM.

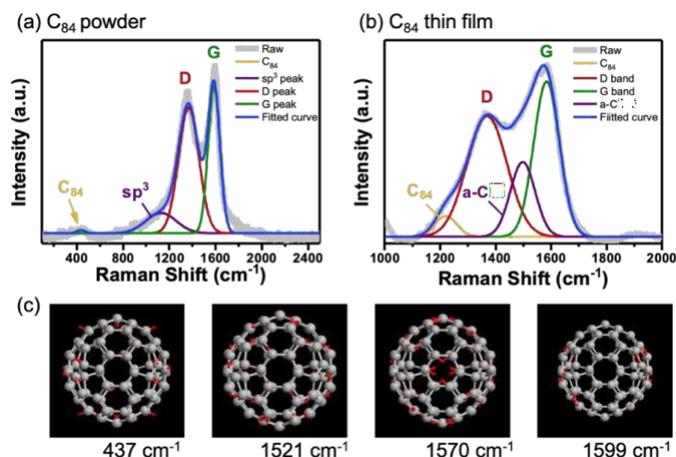


Figure 1. Raman spectra of (a) C<sub>84</sub> powder, (b) few-layer C<sub>84</sub> on Si(111)-7×7, and (c) simulated modes of isolated C<sub>84</sub>.

## Designing Advanced Materials for Unlocking Sustainable Chemical Conversions and Energy Catalytic Processes

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### Abstract

In the past century, industrial growth has significantly impacted the environment, particularly in the energy generation for transportation and electricity. While converting raw materials into chemical products has improved lives, it has also released pollutants into ecosystems. These technologies contribute to climate change and environmental contamination. We need innovative solutions focused on advanced catalysts and energy materials to tackle these issues. This lecture will discuss advancements in catalytic materials designed for environmentally friendly energy generation processes and the conversion of biomass-derived platform molecules into chemical derivatives. It will present our achievements in developing catalytic materials that leverage thermo-catalytic conversion technologies to produce chemicals from biomass and energy fuel chemicals, as well as the photocatalytic valorisation of biomass platform molecules into valuable downstream chemicals. Furthermore, the lecture will share the design and application of photocatalytic materials for CO<sub>2</sub> reduction into chemical derivatives. Finally, we will discuss hydrogen energy production from water splitting and the fossil-derived concept of biogas (CH<sub>4</sub>), using examples of catalytic materials explored from our studies. In particular, the lecture will cover examples of catalytic material designs based on nanosized metal-supported carbon and hetero-mixed oxides as heterogeneous thermo-catalysts and electrocatalysts, as well as layered metal oxide/halides heterostructured photocatalysts, elucidating their structure-activity relationships to achieve efficient catalytic chemical conversions and energy processes.

# **The Role of Hydrogen in Sustainable Transportation**

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## **Abstract**

The purpose of this presentation is to present an overview of current and planned efforts in achieving sustainable transportation goals in a hydrogen economy where hydrogen and electricity as energy carriers are produced using primary energy sources such as solar and wind energies. The presentation will cover past and on-going efforts and will present a vision for the intermediate- and long-term futures.

# **Advances in Sustainable Materials for Next Generation Biocomposites**

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## **Abstract**

The need for sustenance and innovation in biomedical materials warrant immediate attention to finding solutions to associated trauma of bacterial infection, especially after post-surgery. Thus, the perspective of biomedical engineers in originating antibacterial materials and eliciting enhanced resistance to bacterial adhesion is addressed in the current presentation. Herein, attachment of *S. Aureus* gram positive bacteria on various substrates, i.e. metallic (316L stainless steel and Ti-6Al-4V), polymeric (ultra-high molecular weight polyethylene, UHMWPE), and ceramic (hydroxyapatite, HA) is assessed. The adhesion strength of bacterium is evaluated using atomic force spectroscopy by gluing *S. Aureus* on its tip-less cantilever. Lowest adhesion strength of bacterium observed on UHMWPE surface contrasts with conventional results of lowest colony forming units (with most %dead bacteria on HA surface. Poisson's regress has elicited lower long-range and short-range adhesion forces in UHMWPE compared to that of HA and others. Computational modelling has been utilized to visualize the adhesion of bacterial surface proteins with biomaterial surfaces. Multi length scale damage assessment with antibacterial ZnO and Ag reinforcement have rendered elicited reduced wear. Extension to utilization of 58S Bioglass as bioresorbable material to encourage bone-regrowth, the transient response (up to 1000 ms), and role of antioxidant CeO<sub>2</sub> and antibacterial Ag are also elucidated. Further, a step towards 3-D printing is directed for eventual bio-printing and scale up for sustenance. In addition, the design of newer bioresorbable materials also appears to be potential direction for customized and advanced bone-replacement applications.

# Vertical Graphene Nanowalls: a Novel Route to Sustainable Carbon-Based Spintronics Platform

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## Abstract

Graphene and its vertical nanostructure derivatives, such as Vertical Graphene Nanowalls (VGN), have emerged as promising low-dimensional carbon-based materials with unique electrical, magnetic, and spin transport properties. Their tunable electronic structure, high mobility, and low spin-orbit coupling make them highly attractive for next-generation spintronics applications. This talk highlights an in-depth experimental investigation of magneto transport in ferromagnetic vertical graphene nanowalls across a wide temperature range (300 K to 10 K). Between 300 K and 200 K, the longitudinal resistivity exhibits Arrhenius-type behavior with decreasing activation energy, transitioning from thermal band conduction to weak localization. In this regime, the anomalous Hall Effect (AHE) and negative magneto resistance (MR) are observed, both of which are well-explained using modified Hikami–Larkin–Nagaoka (HLN) models, incorporating Rashba spin-orbit coupling and Berry curvature-induced spin-dependent scattering. Below 200 K, the system transitions into a strongly localized 3D Mott variable range hopping regime, characterized by a complete suppression of AHE, persistence of negative MR, and dominance of spin-independent (NSS model) and spin-dependent (Osaka model) hopping mechanisms. Despite localization, ferromagnetic hysteresis in magnetization persists down to 10 K. These results provide strong evidence of spin-orbit and magnetic correlation effects in carbon-based nanostructures, highlighting their potential in energy-efficient and sustainable spintronics device platforms. Such insights are critical for realizing sustainable spintronics devices based on earth-abundant, carbon-based materials without relying on heavy magnetic dopants.

## **Scientific advances in gas sensing for environmental, industrial, and indoor air-quality monitoring**

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## Abstract

This work discusses the scientific advances in gas sensing pertinent to environmental, industrial, and indoor air quality monitoring. The research emphasizes the rational design of nanostructured semiconducting metal oxides, binary and ternary heterojunctions, and defect-engineered nanomaterials, thereby enabling sensors with enhanced sensitivity, selectivity, and long-term stability under real-world conditions. Through pioneering strategies, such as interface band alignment tuning, oxygen vacancy modulation, light-activated sensing, and humidity-resilient material constructions, the research addresses significant challenges in detecting trace levels of hazardous gases, including oxidizing gases (e.g., CO<sub>2</sub>, NO<sub>2</sub>) and reducing gases (CO, H<sub>2</sub>S, CH<sub>4</sub>, and VOCs). Ultimately, the objective is to achieve low-cost, low-power, and room-temperature operational sensors suitable for the near future in wearable applications and Internet of Things-based air quality monitoring.

# **Magnetotransport studies on Topological Quantum Materials including XMR in rare earth mono pnictides**

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## **Abstract**

Topological Quantum Materials is a class of materials with distinct band structures from common metals and insulators. The electronic structures of these materials are topologically nontrivial due to which various interesting properties emerge such as topologically protected states, anomalous transport properties, high charge carrier mobilities, spin-momentum locking, quantum Hall effect, anomalous quantum hall effect. These exotic properties in topological quantum materials are unaffected by deformations, e.g., stretching, compressing, or twisting of the material, or by adding disorder. Study of transport properties at low temperatures and in magnetic fields can probe the unusual electrical properties of topological materials, providing the unique information about electronic band structures. Topological states can be confirmed by analyzing the quantum phenomena like weak antilocalization, SdH oscillations and Quantum Hall effect. A relatively new category among these materials known as extremely large magnetoresistance (XMR) materials have been reported to show huge MR  $\sim 10^5\%$ - $10^7\%$  at low temperatures and high magnetic fields including in rare earth monpnictides. These properties are promising for technological applications involving electronic devices, spintronics, magnetic field sensors and data storage devices, as well as important to understand the mechanism of XMR in wide range of materials for actual application performance. In this talk some of the relevant results will be discussed.

# **Engineered Nanocomposites for Applications in Flexible and Wearable electronics**

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## **Abstract**

Nanomaterials hold tremendous potential in shaping the next generation of flexible and wearable electronic systems due to their exceptional electrical, mechanical, and chemical properties. When combined with flexible polymers, these composites exhibit high conductivity, mechanical flexibility, and stretchability that can conform to complex surfaces, endure repeated mechanical deformations, and maintain long-term stability. This talk will focus on the design and development of such nanomaterial composites for a wide range of high performance devices including pressure sensors, strain sensors, gas sensors, biosensors, and self-powered energy harvesters. Particular emphasis will be placed on their practical, real-time applications such as detection of physiological signals including pulse rate and muscle movement as well as physical and chemical stimuli, which are critical in healthcare and human-machine interface technologies. Furthermore, the presentation will highlight recent advances in integrating functional nanomaterials such as piezoelectric, triboelectric components, with flexible polymers through novel nanoscale architectures. These innovations have led to optimized material interfaces, enhanced charge generation, and improved output performance, thereby enabling the development of self-powered electronic systems, including sensors and low-power devices.

# Development of Polymer Hybrid Nanomaterials for Highly Selective and Sensitive Gas Sensors

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## Abstract

The demand for reliable and efficient gas detection technologies has driven extensive research into materials that offer high sensitivity, selectivity, and stability under ambient conditions. In this work, we report the development of polymer hybrid nanomaterials based on polyaniline (PANI) and polypyrrole (PPy) engineered for advanced gas sensing applications. By integrating functional nanostructures such as metal oxides, carbon-based nanomaterials, and conducting polymers within tailored polymer matrices, the resulting hybrids exhibit synergistic properties that enhance charge transport, surface reactivity, and molecular adsorption. These nanocomposites demonstrated rapid response and recovery times, excellent repeatability, and high selectivity toward target gases such as ammonia (NH<sub>3</sub>), nitrogen dioxide (NO<sub>2</sub>), and volatile organic compounds (VOCs) at low concentrations. The study highlights the potential of PANI and PPy hybrid nanomaterials as efficient active layers for next-generation gas sensors, combining the advantages of polymer flexibility, facile processability, and nanomaterial-enhanced sensitivity.

## Functional Materials: Gas Sensors Applications

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## Abstract

Functional materials find promising applications in sensors as chemical and biosensors, energy storage devices as supercapacitors, energy conversion devices as solar cells, nanoscale electronic devices, laser technology, and catalysis. Last few years many researchers are working on to find different approaches to synthesize smart and techno materials containing polymers, metal oxide semiconductors and many more at the nanometer scale to capture the benefit of their enriched properties like surface to volume ratio, sensing, electrical, optical, superior chemical reactivity etc. as compare to their bulk scale equivalents. The functional materials as metal oxides (CeO<sub>2</sub>, TiO<sub>2</sub>, WO<sub>3</sub>, SnO<sub>2</sub>, ZnO, CuO, Fe<sub>2</sub>O<sub>3</sub> etc.) and conducting polymers polypyrrole (PPy) polyaniline (PANI), etc. are synthesized by different physical as well as chemical techniques as thermal evaporation, simple chemical method, hydrothermal, sol-gel, chemical bath deposition, electrodeposition and electrospinning. The structural, surface morphological, compositional, wettability as well as optoelectronic transport properties of functional nanomaterials are studied and characterized by advanced microscopy techniques. (XRD, RAMAN, FTIR, FESEM, HRTEM, EDS, AFM, XPS, CA etc.) The functional materials of polymers and metal oxides used as a sensing material for detection of NO<sub>2</sub>, NH<sub>3</sub>, H<sub>2</sub>S, SO<sub>2</sub> toxic gases. A novel flexible, high-sensitive, selective, and room temperature operable polyaniline-based hybrid (PANI/WO<sub>3</sub> PANI/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) ammonia (NH<sub>3</sub>) gas sensors were developed onto a flexible polyethylene terephthalate (PET) substrate by in situ polymerization method. The metal oxides nanostructured (nanoparticles, nanoflowers, nanorods, nanowires etc) sensor shows maximal response to various oxidizing and reducing gases along with high selectivity, rapid response/recovery time, notable reproducibility and stability also.

# **In search of Novel Superionic Solid Electrolytes for All Solid-State Battery Applications**

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## **Abstract**

Superionic solid Electrolytes are promising and essentially important for next generation batteries offering improved properties and high energy density as compared to liquid electrolytes. The key challenges are to develop and achieve a good high ionic conductivity, thermally and mechanically stable solid electrolyte in crystalline, glassy or amorphous phase for electrochemical device applications. Structure plays an important role of ion transport mechanism in the matrix. As less work has been reported on the new solid electrolytes with high ionic conductivity. So, the main focus in this paper is to explore the possibility and to develop the new structure of solid electrolytes (especially oxides) with high ionic conductivity to fulfill the ideal criteria of solid electrolytes.

# **Size Selected Pd and Pd-C Nanoparticles for Hydrogen Gas Sensing**

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## **Abstract**

Size selected Pd and Pd-C core-shell nanoparticles are grown by the integrated gas phase synthesis method. The core size and shell thickness in core-shell nanoparticles are independently controlled. The effect of different parameters such as spark frequency, carrier gas flow rate and sintering temperature on the growth of nanoparticles has been studied.

Hydrogen gas sensing response of Pd-C core-shell nanoparticles having a fixed core size and different shell thickness has been investigated and the effect of carbon shell around size selected Pd nanoparticles on hydrogen sensing has been studied. It is observed that Pd-C nanoparticle sensor shows higher sensitivity and faster response/ recovery in comparison to that of Pd nanoparticle samples and these parameters further improve with increase in shell thickness. Further, it has been observed that Pd-C nanoparticles exhibit H<sub>2</sub> sensitivity at room temperature in contrast to Pd nanoparticles which respond only at higher temperatures.

# **Design and synthesis of 2D-based heterojunction materials for enhanced solar photocatalytic hydrogen evolution**

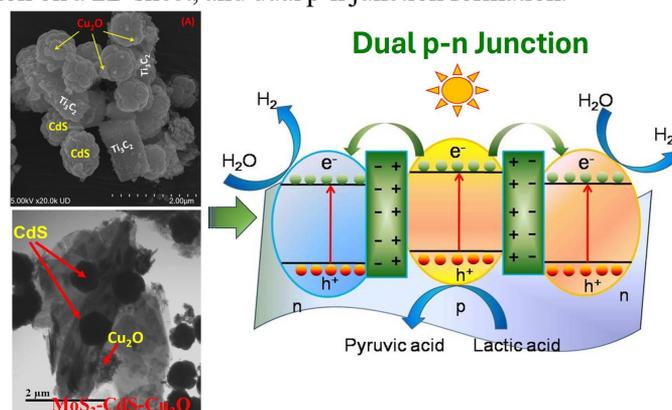
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## **Abstract**

Due to its high energy density, H<sub>2</sub> has recently been projected as a scalable green fuel for carbon-free clean energy. However, so far, current industrial hydrogen generation is based on the grey or blue process. Presently, the electrochemical process for water splitting is at the forefront of commercial

exploration, but requires a lot of electrical energy, which creates doubt about its greenness in practice. On the other hand, getting green H<sub>2</sub> via photocatalytic water splitting is the cheapest and simplest way, but suffers from sluggish reaction kinetics. An extended solar light absorption window, long-term stability, and improved interfacial charge transfer are the keys to scalable and superior solar photocatalytic performance. In recent years, heterojunction-based photocatalysts have become attractive due to the improved catalytic efficiency through delayed electron-hole recombination. In this context, various p-n junctions are studied to improve the charge separation. Very recently, dual p-n junction-based photocatalysts<sup>1</sup> are gaining importance for long-term stability and improved efficiency. However, designing and fabricating such materials is tricky to achieve a proper p-n junction interface. In this context, 2D materials provide a better scope in fabricating the proper catalyst due to the high surface area having a sheet-like structure for the deposition of other semiconductors. Transition metal chalcogenides [1] & MXenes [2] are important new 2D materials that exhibit improved surface properties after exfoliation to 2D structures. Both few-layered MoS<sub>2</sub> and Ti<sub>3</sub>C<sub>2</sub> (MXene) 2D materials were explored for the synthesis of tertiary heterostructures by depositing cauliflower-shaped CdS and nanosized Cu<sub>2</sub>O on a 2D sheet by hydrothermal and precipitation techniques. MoS<sub>2</sub> is a potential semiconductor, whereas doped TiO<sub>2</sub> formed on the surface of Ti<sub>3</sub>C<sub>2</sub> during hydrothermal treatment serves as a potential photocatalyst. The defect formation on TiO<sub>2</sub> & MoS<sub>2</sub> is indicated in HRTEM. XPS spectra of Ti2p and O1s confirm the formation of defect-enriched TiO<sub>2</sub> with sufficient oxygen vacancy on the surface of Ti<sub>3</sub>C<sub>2</sub> during hydrothermal treatment, which can serve as a potential photocatalyst. ESR analysis also corroborates the presence of oxygen vacancy in the material. Interestingly, defects on the 2D structure played a major role in tuning the band gap and influencing catalytic properties. TEM and SEM prove the proper distribution of CdS and Cu<sub>2</sub>O on the nanosheets with desired interface formation. MXene-based heterojunction absorbs light both in the visible and NIR range, thus creating a prospective photocatalyst with wide range solar light utilization. Observed extended light absorption is mostly due to the presence of oxygen vacancy in the material. Direct photocatalytic water splitting was monitored using both the binary and tertiary composite under visible/NIR light in a table-top setup. Lactic acid is found to be most efficient with the obtained rate of 11.5mmol/g/h and 16.26mmol/g/h on MoS<sub>2</sub>-CdS-Cu<sub>2</sub>O and (TiO<sub>x</sub>)Ti<sub>3</sub>C<sub>2</sub>-CdS-Cu<sub>2</sub>O, with good repeatability and long-term stability. Mott-Schottky analysis confirms the p-type nature of Cu<sub>2</sub>O, thus facilitating the p-n junction formation and efficient interfacial charge separation. Substantial increased hydrogen evolution on tertiary materials is discussed based on the proposed mechanism of dual p-n junction based on XPS and Mott-Schottky analysis. Better efficiency of the MXene-based tertiary junction is explained through the high conductivity of Ti<sub>3</sub>C<sub>2</sub> and defect-induced extended light absorption up to NIR and its upconversion. Increased efficiency and stability of the developed catalyst are explained on the basis of the synergistic effect of defect-enriched TiO<sub>x</sub> formation, extended light absorption with up conversion, high conductivity, enhanced interfacial charge separation on a 2D sheet, and dual p-n junction formation.



# **Economical and Sustainable Development of Nanostructured materials engineering for Lubrications, Photovoltaic, Gas Sensors, and Energy Storage Applications**

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## **Abstract**

Nanostructured materials engineering and technology has progressed rapidly in the direction of 2D layers and materials development for the need of the industry developments. Nanostructured materials engineering and technology are pervasive in many applications, optoelectronics, optical coatings (anti-reflection coatings), magnetic films (data storage), environmental (smart window), energy (solar cells, batteries), gas sensors, and super hard coatings, etc. Energy is essential for economic development and growth. Especially with the development of nanotechnology, electrochemical, and material science, interest in research and production of both efficient and lower-cost materials is increasing progressively. With the rapid growth of development and the drive to expand the economy, society demands more lubrication and electricity. Solar energy is the most prolific method of energy capture in nature. However, the economic drive to make solar cells more cost effective and efficient has driven developments in many different deposition technologies, including dipping, plating, thick film deposition and thin film deposition. The use of nanostructured thin films for efficient use of solar cells in production of n & p-type semiconductor materials is one of the most important sources of energy and new-generation energy. The Nano lubrication and energy storage can be most practically realized by electrochemical storage technologies using reversible conversion of chemical to electrical energy. In this sector, Lithium-ion battery (LIBs) is the good alternative energy storage device option compared to the other energy storage systems. Furthermore, it is lightweight, non-toxic, has high power and energy density and longer cycle lifetime compared to other energy storage devices. We have developed thin films of TiO<sub>2</sub>, LiS, LiSe, LiSeS, and MnO<sub>2</sub> electrode materials by employing simple, green and cost-effective methods and exploring them into energy storage devices. It shows the reversible specific capacity of more than 206 mAh g<sup>-1</sup> at a current density of 33 mA g<sup>-1</sup> and it is comparatively higher than the earlier literature reports. Pure and doped SnO<sub>2</sub> nanoparticles thin films have been synthesized using remnant water collected from soaked Bengal gram beans extract. The synthesis method described in this work is facile and versatile, providing opportunities to control the morphology of various other semiconducting metal oxides, with particular promise for application in gas sensors. The pure and doped biosynthesized SnO<sub>2</sub> nanoparticles were coated onto the glass substrate using doctor blade method to form thin films. These thin films were investigated for their gas sensing properties and were found to be highly sensitive to different gases. The pure SnO<sub>2</sub> sample showed a response of 34% for 600ppm NH<sub>3</sub> at room temperature (~30 °C). With cobalt doping, this response got enhanced to 43% for 100ppm NH<sub>3</sub> gas at room temperature. The gold and nickel doped SnO<sub>2</sub> thin films were found to be sensitive to NO<sub>2</sub> gas at 200 °C operating temperature. The gold doped SnO<sub>2</sub> exhibited a response of 30% while Ni-doped SnO<sub>2</sub> showed 40% response. The Cu doped SnO<sub>2</sub> thin films were found to be highly sensitive to H<sub>2</sub>S gas at 200 °C operating temperature. It gave a response of 38.33% for 100ppm H<sub>2</sub>S gas. Considering the indicated trends and energy requirements, it has been important to transfer this technology in detail regarding the surface technologies related to the nanostructured materials engineering and technology instead of bulk materials.

# **Polyelectrolyte membranes for strategic devising of electrochemical energy systems**

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## **Abstract**

Rapid changes in global energy trends and sustainable energy policies has catalysed the demands for scientific and technological innovations to avail net-zero carbon footprint energy harvesting technologies. Ever since 1970s, the electrochemical energy devices (EEDs) seems to be reliable and most promising alternative to intermittent renewables. In EEDs like fuel cell, redox flow batteries and electrolyzers, the polyelectrolyte membranes (PEMs) plays a crucial role and allows selective passage of ions (preferably,  $H^+$  and  $OH^-$ ) to complete the electrochemical circuit and generation/store electricity. To introduce, the PEMs are advanced functional thin films bearing fixed charged groups viz positive ( $-N^+R_4$ ) in anion conducting PEMs and, negative ( $-SO_3^-$ ) in cation conducting PEMs which allows counter-ions to pass through it and exclude any co-ion migration.

In recent years, the challenges underlies developing strategic designing of stable and cost-effective membrane materials. Thus, the objective of this work focuses on the introduction of some efficient PEM designs for its strategic devising in electrochemical energy storage and conversion systems like vanadium redox flow batteries, redox flow batteries and fuel cells, respectively. It is expected that the polyelectrolyte membrane materials are potential alternative to elite fluorinated PEMs for respective energy applications.

# **Altering the transparency and color of flexible solar cells using 3-D printed structures**

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## **Abstract**

Halide perovskite solar cells (PSCs) have emerged as a promising candidate for efficient and cost-effective photovoltaic technology. Colored semitransparent flexible solar cells with advanced and simplified fabrication methods are crucial for building-integrated Photovoltaics (BIPV) implementation. Here, we present the fabrication of perovskite-based solar cells, which can be used for existing windows, as a retro-fitting process. The fabrication approach is based on the coating of halide perovskite, followed by depositing a transparent electrode, to attain a tunable color to the cell with high transparency. The wide range visible transparency is achieved with altering the perovskite composition or bandgap using 3D printed micro patterned optical cavities. We have tailored the perovskite concentration, and electrode compositions, including the layer's thickness to control the light transmittance and power conversion efficiency. Different color shades (between RGB spectrums) can be achieved without adding any extra colorants. These structures are more convenient and suitable for large-area deposition than conventional sputtered TCO deposition. These solar cells are geared towards advancing the development of sustainable energy systems and advanced upcoming photovoltaic such as Agrivoltaic and Space photovoltaic.

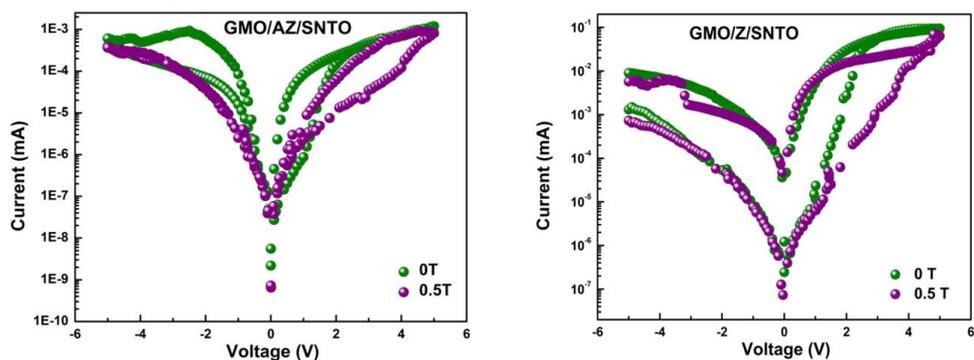
# Manganite-Based Thin films: Bridging Material Science and Sustainable Device Applications

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## Abstract

Driven by the escalating demand for energy-efficient, high-density memory and computing technologies, this work explores perovskite manganite thin films (for example, gadolinium manganite  $\text{GdMnO}_3$  and Ga-doped lanthanum calcium manganite  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3:\text{Ga}$ ) as sustainable alternatives to conventional silicon-based electronics. Using pulsed laser deposition (PLD), we fabricate epitaxial heterostructures (for example,  $\text{GdMnO}_3$  on Nb-doped  $\text{SrTiO}_3$  and LCMGO on silicon) with precisely tailored structures and electronic properties. In these heterostructures, we demonstrate ultralow-power resistive switching characterized by high ON/OFF current ratios ( $\sim 10^3$ ) and robust endurance (over 50 cycles), enabling energy-efficient resistive random-access memory (RRAM) and neuromorphic computing devices. Through strain engineering and defect control, we optimize oxygen vacancy distributions to achieve tunable switching voltages and enhanced device reliability. In addition, LCMGO/Si heterostructures exhibit strong infrared (IR) photoresponsivity ( $>4.85$  A/W) at room temperature, highlighting their potential for efficient IR photodetectors in low-power sensing applications. These multifunctional material platforms integrate memory, logic, and sensing capabilities while operating at low voltages ( $<2$  V) and reducing energy consumption by about 40% compared to state-of-the-art technologies. This work integrates fundamental materials science with scalable fabrication processes to develop sustainable electronics, focusing on practical outcomes such as low-power devices compatible with existing silicon-based manufacturing processes



## Advances in photocatalytic materials for Environmental Remediation

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## Abstract

The rapid industrial development led to the increased pollutant concentration in the ecosystem which is threat to ecological systems and biotic component's. The persistent organic pollutant and heavy metals are of main concern and have gained the interest of the scientific community across the globe. In recent years, adsorption and photocatalysis have emerges as the best solution for the elimination of these

diverse classes of pollutants due to their non-toxic and energy efficient process. This process degrades persistent and toxic organic compounds into the non-harmful compounds using sun light.

In this process, a wide range of the advanced functional materials—such as MXenes, metal sulfides, carbon-based nanostructures, metal-organic frameworks (MOFs), and metal oxides have been extensively studied due to their versatile physicochemical properties that assist the photocatalysis decontamination. The pure photocatalytic materials possess the low efficacy due to little absorption in the visible region and faster charge carrier recombination. The efficiency can be enhanced by means of doping, surface modification and combination of two or more materials to get the advanced materials having enhanced properties. These modifications have been shown to significantly augment both the surface characteristics and absorption in the visible region which in turn elevate the photocatalytic activity towards a wide variety of environmental contaminants. These multifunctional materials with desired characteristics provide the sustainable solution for comprehensive water purification and environmental remediation applications.

## **Ion beams in Materials engineering & modifications and advanced materials for environmental remediation.**

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### **Abstract**

In this talk, I would discuss various Accelerator and characterization facilities at IUAC, New Delhi. Ion-matter interaction and energy loss mechanism will be discussed for the benefit of the students and potential users. Further, a functional composite of ZnO tetrapods and Polyethylene Glycol (PEG) polymer for its potential in organic dye degradation has been synthesized. Thus, it provides a solution towards the SDG #7 for 'pure and clean water. Zinc oxide tetrapods (ZNT) based films were synthesized with different concentration of ZNT dissolved in Polyethylene Glycol (PEG) solution through chemical routes. Synthesized solution was probe sonicated and spin coated on SI, Glass and CaF<sub>2</sub> substrates followed by characteristic analysis using SEM with EDX, Raman and FTIR. SEM and He-ion microscope images show the composite formation of ZNT with PEG with their legs intact, thus forming a 3D catalysis electrode. FTIR shows the functional groups bond energies for the synthesized samples. Further, photodegradation test were performed to test the stability of the synthesized samples for the degradation of organic dyes, as both the materials are UV sensitive. The sample would be treated with energetic ions for the enhancement in the properties further. The polymer composite samples/electrodes are known to exhibit enhanced photocatalytic performance and stability and found to be promising alternative for wastewater treatment and thus, environmental remediation.

# **Binder-free light-weight nanostructured anode with designed interface delivering high performance in electrical energy storage/Li-ion batteries**

*Prof. Dr. Sudeshna Chattopadhyay*

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## **Abstract**

The progress of rechargeable metal-ion batteries (such as lithium-ion batteries (LIBs), aluminium ion batteries (AIBs)) with higher energy storage capacity, energy density, and power density is critical to meet the growing power demands of modern technologies. At the same time, light-weight, micro-devices are attracting attention due to their growing demand in flexible and portable electronics, such as wearable health monitors, implanted medical devices, smart cards, and IoT sensors etc., emphasizing the need for miniaturization of energy storage/batteries. In view of that the study of a high-performance light-weight, binder-free nanostructured thin-film anode for rechargeable LIBs will be discussed in this talk. The talk will provide an insight into manifestation of interfacial effect in designing of advanced high-performance light-weight electrode for next-generation energy-storage devices.

# **Nanostructured Thin Films for Enhanced Energy Performance: The Role of Artificial Nanodefects**

*Prof. Paolo Mele*

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## **Abstract**

Global challenges such as energy shortages and environmental degradation necessitate the development of advanced materials for sustainable energy technologies. Superconducting and thermoelectric materials play a pivotal role, offering efficient solutions for energy transport and conversion, respectively. This presentation focuses on recent advances in nanostructured thin films incorporating artificial nanodefects to significantly enhance the performance of these materials in energy applications.

Superconducting materials, particularly  $\text{YBa}_2\text{Cu}_3\text{O}_x$  (YBCO), benefit from the introduction of nanosized defects to improve critical current ( $J_c$ ) and global pinning force ( $F_p$ ). By incorporating one-dimensional (1D)  $\text{BaSnO}_3$  (BSO) nanorods through pulsed laser deposition (PLD), YBCO films achieved  $F_{p\text{MAX}} = 28.3 \text{ GN/m}^3$  at 77K and 3T, with isotropic  $J_c = 0.3 \text{ MA/cm}^2$ —double the performance of conventional  $\text{Nb}_3\text{Sn}$  superconductors [1]. Three-dimensional (3D)  $\text{Y}_2\text{O}_3$  nanoparticles were also integrated into YBCO films, resulting in an  $F_{p\text{MAX}}$  of  $14.3 \text{ GN/m}^3$  at 77K and 3T [2]. The combination of 1D and 3D APCs, realized through alternating layers of BSO nanorods and  $\text{Y}_2\text{O}_3$  nanoparticles, produced films with enhanced pinning, achieving  $F_{p\text{MAX}} = 17.6 \text{ GN/m}^3$  at 77K and 2.2T [3]. These results underscore the critical role of nanoengineering in optimizing vortex pinning and improving superconducting performance for applications such as current transport and magnet winding.

In the field of thermoelectrics, thin films with nanostructured defects exhibit significant improvements in thermal properties. The introduction of artificial defects such as hydroquinone nanolayers in Al-doped ZnO (AZO) films, prepared by atomic layer deposition (ALD), resulted in thermal conductivity  $\kappa = 3.56 \text{ W/m}\times\text{K}$  at 300 K [4]. Similarly, AZO films with polymethylmethacrylate (PMMA) particles, prepared via multi-target PLD (MAPLE), showed  $\kappa = 5.9 \text{ W/m}\times\text{K}$  at 300 K and a figure of merit  $ZT = 0.07$  at 600

K [5]. Further nanostructuring of AZO films via Mist-CVD led to the formation of nanopores, yielding  $\kappa = 0.60 \text{ W/m}\times\text{K}$  and  $ZT = 0.06$  at 300 K [6]. The dispersion of  $\text{Al}_2\text{O}_3$  nanoparticles in AZO films, prepared by surface-modified target PLD, resulted in  $\kappa = 3.98 \text{ W/m}\times\text{K}$  and  $ZT = 0.0007$  at 600 K [7]. Collectively, these efforts achieved a 1/10 to 1/100 reduction in thermal conductivity and a 3-5 times enhancement in ZT, demonstrating the potential of nanodefects to improve thermoelectric performance. In conclusion, these findings emphasize the importance of artificial nanosized defects in enhancing the performance of superconducting and thermoelectric thin films. These advances position nanostructured materials as key candidates for future large-scale energy applications, paving the way for more efficient and sustainable technologies.

## **Quantum Technology for Sustainable Healthcare, Environment and Agriculture**

*Prof. Shaibal Mukherjee*

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### **Abstract**

With the advent of new quantum technologies and the sustained development of society, the requirement for reliable and cost-effective mechanisms for monitoring of toxic gases in the environment, heavy elements in the water bodies in rural, urban and industrial environments become more critical as both these are indirectly and directly related to sustainable agricultural practices. On the other side in the healthcare diagnostics, uric acid and creatinine, which are major products of the catabolism of the purine nucleosides, adenosine, guanosine, creatine and creatine phosphate, are produced in various human tissues including muscles, kidneys, liver, intestines, and the endothelium. Abnormalities of uric acid and creatinine are responsible for chronic kidney disease (CKD), obesity, gout, cardiovascular and neurological disorders in human. Traditional analytical techniques are expensive, time-consuming and cumbersome. Therefore, it is desired to overcome the drawbacks and limitations associated with existing solutions and develop a mean of point-of-care diagnosis systems.

This lecture will provide a journey of translation from innovative lab-based R&D work to market-based products and solutions with a self-reliant mission, providing portable AI and IoT solutions for real-time environmental monitoring, early disease detection in plants, soil fertility assessment, and water quality assessment. The lecture would emphasize on the successful implementation of the engineering of the wafer-scale and electronic-grade Van der Waals semiconductor based portable and point-of-care (POC) sensor system that detects molecules with exceptional selectivity, even in the presence of potential interfering analytes.

# **Track - I**

## **Physics of Materials and Technology**

# Structural, Morphological and Optical Properties of La<sub>2</sub>CrMnO<sub>6</sub> Double Perovskite

*Suresh Kumawat<sup>1</sup>, Sahil Singh<sup>1</sup>, Akshita Jain<sup>1</sup>, Mamta Jha<sup>1</sup>, Suchitra Yadav<sup>1,\*</sup>*

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## Abstract

This Study involved the synthesis of La<sub>2</sub>CrMnO<sub>6</sub> sample via Sol-Gel Auto combustion Method. In this study structural, morphological & optical properties have been examined. The X-ray diffraction analysis indicates the formation of single phase La<sub>2</sub>CrMnO<sub>6</sub> with orthorhombic crystal structure. Scanning electron microscope demonstrates the morphological structure which has characterized by irregular forms. In contrast we use the EDX technique by which we verify the existence of elemental composition in the sample. The Band gap analyses of the sintered samples were carried out by UV-VIS using Tauc plot. The XPS data confirms the electronic structure of the La<sub>2</sub>CrMnO<sub>6</sub>. This material is potential candidate for industrial scale applications as solid oxide fuel cell, lead free solar cell, photovoltaics, superconductors, spintronics and magneto electric devices.

# Structural, Morphological and Optical Properties of Fe-Doped BaSnO<sub>3</sub>

*Sahil Singh<sup>1</sup>, Suresh Kumawat<sup>1</sup>, Akshita Jain<sup>1</sup>, Mamta Jha<sup>1</sup> and Suchitra Yadav<sup>1,\*</sup>*

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## Abstract

BaSnO<sub>3</sub> has attracted attention as a transparent conducting oxide with high room temperature carrier mobility. This study reveals that the preparation of Fe- Doped BaSnO<sub>3</sub> samples via solid-state reaction method. In this study the structural, morphological & optical aspects of Fe-doped BaSnO<sub>3</sub> with different concentration (BaFe<sub>x</sub>Sn<sub>1-x</sub>O<sub>3</sub>, where x=0.00,0.01,0.03,0.05,0.07) have been examined. The XRD indicated the formation of single phase pure and Fe doped BaSnO<sub>3</sub> with cubic perovskite structure. SEM -EDX technique is used for morphological study & to verify the necessary composition in the sample. The UV-spectroscopy has been used for the calculate the Band Gap, Urbach Energy and refractive index of the sample. The XPS analysis data confirms the electronic structure of Fe-doped BaSnO<sub>3</sub> sample.

# Oxygen Ion-Induced Enhancement of Transparent Conductive ZnO/Ag/ZnO Multilayer Films for Advanced Optoelectronic Applications

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## Abstract

ZnO/Ag/ZnO multilayer thin films were deposited using radio frequency magnetron sputtering and subsequently irradiated with 100 MeV O<sup>7+</sup> ions at fluences ranging from 1E11 to 5E12 ions/cm<sup>2</sup>. The structural, morphological, and electrical properties of the pristine and irradiated films were investigated using X-ray diffraction (XRD), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and Hall measurements. XRD analysis confirmed the crystalline and stoichiometric nature of ZnO, while AFM revealed a smooth surface with an RMS roughness of approximately 2.41 nm, which is comparable to that of ITO films. XPS analysis indicated that the metallic intermediate layer remained stable during ion irradiation. Hall measurements showed an increase in carrier concentration from  $5.16 \times 10^{21} \text{ cm}^{-3}$  for pristine ZAZ films to  $1.01 \times 10^{22} \text{ cm}^{-3}$  at the highest fluence, while the Hall mobility decreased from 10.56 to 3.92 cm<sup>2</sup>/V-s. The electrical resistivity and sheet resistance increased with increasing fluence, indicating the presence of a continuous Ag layer. These findings demonstrate that oxygen ion irradiation can modify the electrical properties of ZnO/Ag/ZnO multilayers, making them promising candidates for various optoelectronic applications. This comprehensive analysis offers valuable insights into the current state and future prospects of modifying metal-dielectric multilayer structures. It serves as an invaluable resource for researchers and engineers within the optoelectronics community.

## Synthesis of Ni Doped $\delta$ -MnO<sub>2</sub> (TMO) For Electrode Material of Supercapacitor

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## Abstract

Transition metal oxides are promising electrode materials for supercapacitors because of their multiple oxidation states and high theoretical capacitance. In this work, Ni-doped  $\delta$ -MnO<sub>2</sub> nanostructures were prepared using Hydrothermal method and examined for their suitability in electrochemical energy storage. X-ray diffraction (XRD) confirmed the incorporation of Ni into the  $\delta$ -MnO<sub>2</sub> lattice, with slight peak shifts suggesting lattice modification. Scanning electron microscopy (SEM) demonstrates well-defined nanoflake structures, and a reduction in their size with Ni doping, which can help in faster ion transport. Energy-dispersive X ray spectroscopy (EDX) and elemental mapping further confirmed uniform Ni distribution within the host matrix. The combined effect of Ni doping and controlled nanostructure is expected to enhance conductivity, active surface area, and cycling stability. These results

suggest that Ni-doped  $\delta$ -MnO<sub>2</sub> has strong potential as an electrode material for supercapacitor applications.

## Green Synthesis of Novel Carbon Nanostructures Using Garlic Peels for NO<sub>2</sub> Gas Sensing Application

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### Abstract

Carbon nanostructures synthesized from waste garlic peels through a sustainable carbonization approach, highlighting an eco-friendly route for developing advanced novel materials for gas sensing applications. The material exhibits flaxes and sponge-like structures with interconnected pores, as confirmed by a scanning electron microscope. The X-ray diffraction pattern of the carbon nanostructures exhibits broad diffraction peaks at  $2\theta \approx 20.1^\circ$  and  $42.2^\circ$ , corresponding to the (002) and (100) planes, respectively, of carbon nanostructures. The direct band gap of the synthesized carbon nanostructures was calculated to be 4.28 eV based on Tauc plot analysis. The NO<sub>2</sub> gas sensing properties of the synthesized carbon nanostructures were analyzed, and the sensor exhibited a high sensitivity of 117% with response time and recovery time of 200 and 1000 seconds, respectively, for a 50 ppm NO<sub>2</sub> concentration.

# Dual-Functional NiCo/MOF@CoMo-LDH Catalyst for Energy-Efficient Hydrogen Generation and Glycerol Valorization

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## Abstract

Hydrogen is an efficient and clean source of energy, but still, its production by water electrolysis remains energy-demanding and slow, particularly for the OER. To further improve efficiency and practicability, scientists are exploring alternative reactions, one of which is the glycerol oxidation reaction (GOR), which consumes less energy and can also yield beneficial chemicals. In this research, a new electrocatalyst composed of cobalt–molybdenum layered double hydroxide supported on Nickel cobalt MOF (NiCo/MOF@CoMo/LDH) was synthesized and deposited on nickel foam. This material is optimized to function effectively in the hydrogen production process, specifically in the hydrogen evolution reaction (HER) and glycerol oxidation (GOR). With a current density of 10 mA/cm<sup>2</sup>, the catalyst requires minimal voltages to catalyze HER—approximately 120 mV in an alkaline medium. For OER, the voltages required are 270, 288, and 300 mV, respectively. With the addition of glycerol, the catalyst facilitates GOR at much lower voltage (~1.22 V vs. RHE), thus making the entire process of water splitting more energy-efficient. In a two-electrode configuration, the voltage required for water splitting decreases from 1.75 to 1.83 V to merely 1.52 to 1.61 V when GOR substitutes for OER. This also prevents issues caused by chlorine and enhances the stability of the catalyst. The structure and surface of the catalyst were examined with utmost care using XRD, FESEM, HRTEM, and XPS, ensuring it possesses a good interface and active sites for instant reaction. Generally, this study presents a low-cost and feasible technique for producing hydrogen from seawater and generating valuable chemicals, such as formic acid, thereby providing a clean energy solution and a means for chemical production.

## Optimization of Dielectric Response for Zr-MOF / PVDF Nanocomposites

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## Abstract

In this study we are reporting synthesis & characterization of Zr-MOF in the amount of 1-5 wt% dispersed into PVDF nanocomposites. These nanocomposites have been synthesized by solution casting

method. The prepared polymer nanocomposites have been characterized using XRD, FTIR, SEM, DSC and Impedance analyzer. XRD spectra showing the enhanced crystallinity of the polymer nanocomposites, However SEM images confirms homogeneous dispersion of the MOF into the PVDF nanocomposites. The glass transition temperature improvement has been found via DSC. Dielectric response has been improved with the high contents of MOF into PVDF nanocomposites. The detailed results will be presented during the conference presentation.

## **Structural and Chemical Analysis of Flexible Barium Titanate/Polyethylene Oxide Nanocomposite Films**

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### **Abstract**

The escalating demand for advanced flexible electronics has spurred significant research into novel materials for high-performance energy storage. This study reports the successful synthesis of flexible nanocomposite thin films composed of high-permittivity barium titanate (BaTiO<sub>3</sub>) nanoparticles integrated into a polyethylene oxide (PEO) polymer matrix, using a simple solution casting technique.

The primary objective is to create a multifunctional material with tailored properties for next-generation supercapacitors and other electronic applications, by leveraging the synergistic interplay between the ceramic filler and the polymer host.

Strong interfacial bonding—confirmed by FTIR—and a modified crystalline structure—observed via XRD—suggest the formation of a unique material. The successful incorporation of high-permittivity BaTiO<sub>3</sub> into a more amorphous polymer matrix indicates that the resulting film will possess enhanced dielectric properties.

These tailored structural and chemical characteristics make the nanocomposite a highly promising candidate for dielectric layers in electronic components such as supercapacitors. Furthermore, the material's designed structure opens possibilities for its use in flexible sensors and actuators, where specific mechanical and dielectric responses are required.

# Self-supported and binder-free cobalt-doped nickel tellurite electrocatalyst for simultaneous hydrogen generation and glycerol oxidation

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## Abstract

The production of hydrogen using electrochemical water splitting has garnered increasing interest in recent times owing to current energy demands. Since, the oxygen evolution process (OER) needs high overpotentials to proceed at a sufficient rate and is thermodynamically less favourable. In this regard, incorporation of alcohol as anodic reactants, especially glycerol could enhance the oxidation process and lower the overpotential. Integrating the glycerol oxidation reaction (GOR) with the hydrogen evolution reaction (HER) provides a low-energy alternative to the conventional oxygen evolution reaction (OER), significantly reducing energy input. In this study, Co-doped NiTe (4CNT) is developed as a bifunctional electrocatalyst for HER, OER, and GOR. Structural characterization (XRD, XPS, HRTEM, FESEM, EDX) confirms successful Co incorporation into the NiTe lattice, improving electronic conductivity and catalytic performance. The 4CNT electrode delivers 100 mA cm<sup>-2</sup> at an overpotential of 235 mV for HER and 1.62 V vs. RHE for OER. For GOR, it achieves the same current density at only 1.34 V. For overall water splitting process in 1 M KOH, the required potential is 2.01 V, which drops to 1.80 V upon adding 0.1 M glycerol, highlighting improved efficiency. This work positions Co doped NiTe as a promising catalyst for sustainable hydrogen and formate co-production.

## Effect of Particle Size and Halide Composition on Structural and Optical Properties of CsPbX<sub>3</sub> Nanocrystals

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## Abstract

Halide perovskites (CsPbX<sub>3</sub>; X = Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>) are a class of semiconductor materials that have attracted significant attention due to their excellent optical and electronic properties, including tunable bandgap, high photoluminescence quantum yield (PLQY), and ease of synthesis[1,2]. Their nanocrystals (NCs) further enhance these features because of strong quantum confinement effects, which allow fine-tuning of emission color, bandgap energy, and carrier dynamics by simply adjusting their size and composition. Such unique characteristics make halide perovskite NCs highly promising for applications in light-emitting diodes (LEDs), lasers, photodetectors, and other optoelectronic devices.

The halide perovskite NCs' size and halide composition can significantly influence their optical properties. Both can affect the bandgap, PL intensity, PLQY, as well as charge carrier dynamics [3,4]. To study the effect of NC sizes, CsPbBr<sub>3</sub> of different sizes was synthesized, and the impact of particle size on the structural and optical properties was explored. Further, to study the effect of halide composition,

CsPbCl<sub>3</sub>, CsPbBr<sub>3</sub>, and CsPbI<sub>3</sub> were synthesized under identical conditions. The CsPbCl<sub>3</sub> shows a higher band gap, stability, and exhibits lower PLQY [5,6]. CsPbI<sub>3</sub>, while offering a narrower bandgap and higher PLQY, suffers from poor phase stability, leading to rapid degradation under ambient conditions. CsPbBr<sub>3</sub>, on the other hand, provides an optimal balance of bandgap, luminescence, and structural stability. Thus, this study deals with the combined effect of halide composition and particle size on the structural and optical properties of halide perovskite NCs, providing a comprehensive understanding of how these parameters can be optimized to achieve stable and efficient nanomaterials for future optoelectronic technologies.

## **Optimization of Gas sensing response of Ni intercalated ZnO thin films**

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### **Abstract**

In the present work, we fabricated nickel-doped zinc oxide (Ni:ZnO) thin films with different doping concentrations (1%, 3%, 5%, and 10%) on ITO Substrates by spin coating for gas sensor applications. The structural characterization of the films was carried out using X-ray diffraction (XRD), Surface morphology by Scanning Electron Microscopy (SEM), Optical band gap energy by Ultraviolet–Visible (UV-Vis) spectrophotometer. The sensitivity, response time and recovery time of gas sensing behaviour of films were systematically investigated. The sensitivity and response/recovery time of Ni-doped ZnO films improved significantly compared to the pristine ZnO thin films, which showed promising prospects for future gas detection applications.

## **Synthesis and Characterization of Ag/PMMA Nanocomposites for Charge Storage**

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### **Abstract**

In present study we are reporting outcomes of silver/polymethyl methacrylate (Ag/PMMA) nanocomposites synthesized via a solution casting method. X-ray diffraction confirmed the incorporation of crystalline Ag nanoparticles within the amorphous PMMA matrix, while scanning electron

microscopy revealed a relatively uniform nanoparticle dispersion. UV–Vis spectroscopy exhibited a distinct surface plasmon resonance peak, indicating well-formed Ag nanoparticles and FT-IR spectra suggested interfacial interactions between the polymer chains and embedded nanoparticles. Impedance spectroscopy, demonstrated enhanced dielectric response consistent with interfacial polarization and percolation effects. These results highlight the potential of Ag/PMMA nanocomposites for advanced applications in flexible electronics, optoelectronic devices, energy storage and electromagnetic interference (EMI) shielding.

## **Synthesis and Characterization of Sr-doped LaMnO<sub>3</sub> Perovskite Nanoparticles**

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### **Abstract**

Sr-doped LaMnO<sub>3</sub> (La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>) perovskite samples were successfully synthesized using the modified sol-gel method with varying Sr concentrations. The influence of Sr substitution on the structural, optical and electric properties was systematically investigated of the prepared samples. these sample were characterized using XRD, UV- Vis Spectroscopy, FESEM and FTIR. In order to know the structural phase purity of the prepared samples, X-ray diffraction was carried out. XRD analysis confirms the formation of pure crystalline phase with rhombohedral symmetry in R-3C space group. Optical band gap of the prepared samples was carried out using UV- Vis spectroscopy. The surface morphology of the samples was analyzed using FESEM. Whereas These results imply that Sr-doped LaMnO<sub>3</sub> has encouraging potential for use in photocatalysis, spintronic devices, and solid oxide fuel cells.

## **Theoretical Design and Exploration of Emergent Phenomena in Nanoscale Heterojunction Devices**

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### **Abstract**

Nanoscale devices constitute an important part of nanotechnology. In principle, such devices can be designed with unique functionalities based on emergent phenomena at the nanoscale. Here, we propose and demonstrate that first-principles quantum mechanical calculations can be exploited to explore various novel interfacial emergent phenomena in ultrathin nanoscale heterojunctions. These phenomena include the interfacial magnetoelectric effect, the formation of switchable two-dimensional electron gases (2DEGs), spin-polarized 2DEGs, phono-voltaics, and others in heterojunctions based on oxides, semiconductors, and metals. We present how *ab initio* quantum mechanics can be used to study these phenomena and thereby assist in the design of nanoscale devices. Such devices, based on emergent

interfacial phenomena, are of great interest and have significant implications for a wide range of technological applications.

## Multi-Functional Dy<sup>3+</sup>: Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub> Phosphors for White LEDs and Temperature Sensing

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### Abstract

Rare-earth-doped inorganic phosphors have gained a lot of attention recently because they hold great promise for use in things like optical temperature sensing and solid-state lighting. Among these materials, dysprosium ions (Dy<sup>3+</sup>) stand out due to their unique ability to emit blue, yellow, and white light through specific electronic transitions. In this study, we focused on creating Dy<sup>3+</sup>-activated Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub> phosphors using a traditional solid-state reaction method. Our goal was to explore their structure, light-emitting behavior, and ability to sense temperature, with potential applications in LEDs and temperature sensors. Specifically, we aimed to design a stable Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub> host material doped with Dy<sup>3+</sup> ions that could serve two purposes, one to produce visible light suitable for white LEDs and acting as a temperature sensor through optical ratiometry. To make these phosphors, we carefully mixed exact amounts of high-purity raw materials barium carbonate (BaCO<sub>3</sub>), vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>), and dysprosium oxide (Dy<sub>2</sub>O<sub>3</sub>) then ground them thoroughly and heated the mixture at high temperatures to obtain pure, crystalline samples ready for testing. Structural analysis confirmed the successful incorporation of Dy<sup>3+</sup> ions into the Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub> lattice without noticeable secondary phases. Photoluminescence (PL) studies showed strong excitation in the near-UV region, with intense emission bands observed at around 480 nm (blue, corresponding to the <sup>4</sup>F<sub>9/2</sub> → <sup>6</sup>H<sub>15/2</sub> transition) and 573 nm (yellow, corresponding to the <sup>4</sup>F<sub>9/2</sub> → <sup>6</sup>H<sub>13/2</sub> transition). The relative intensity of these emissions produced near-white light with good color coordinates, confirming the applicability of the phosphor for warm white LED fabrication. Temperature-dependent PL experiments demonstrated the sensitivity of the emission intensity ratio to thermal variations, highlighting the potential of Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub>: Dy<sup>3+</sup> as an efficient optical thermometer. The calculated relative sensitivity increased with temperature, making the material suitable for contactless temperature sensing in various high-temperature environments. The results suggest that Dy<sup>3+</sup>-doped Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub> phosphors, prepared via a simple solid-state method, exhibit excellent luminescent properties with dual functionalities: white light generation for LED applications and reliable ratiometry thermometry for non-invasive temperature monitoring. This dual performance positions Ba<sub>3</sub>V<sub>2</sub>O<sub>8</sub>:Dy<sup>3+</sup> as a promising candidate for integration into next-generation optoelectronic devices.

# High-Sensitivity SPR Biosensor Employing Cu/Si/2D-WS<sub>2</sub>/BP Heterostructure for Malaria Detection

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## Abstract

Malaria causes nearly one million deaths globally each year, with about 90% of these fatalities occurring among African children. As a major health burden in tropical and subtropical regions, malaria necessitates rapid and reliable diagnostic approaches for effective management and control. In this work, we present the design and numerical analysis of a high-performance Kretschmann-configured surface plasmon resonance (SPR) biosensor. The proposed structure incorporates copper as the plasmonic layer, silicon as the dielectric medium, and two-dimensional (2D) materials- tungsten disulphide (WS<sub>2</sub>) and black phosphorus (BP)- to enhance optical response for medical diagnostics, specifically targeting malaria-infected red blood cells at different developmental stages within erythrocytes. The sensor performance was extensively evaluated in terms of sensitivity using the finite element method (FEM) in COMSOL Multiphysics, with results validated through the transfer matrix method (TMM) in MATLAB. Optimization of the thickness and layer configuration yielded maximum sensitivity values of 408.16°/RIU, 329.25°/RIU, and 298.46°/RIU for the ring, trophozoite, and schizont stages of malaria, respectively. Furthermore, the proposed structure demonstrates a high-quality factor of 65.30 for the ring stage and achieves a detection accuracy of 0.16<sup>-1</sup>. These findings highlight the potential of the Cu/Si/2D-WS<sub>2</sub>/BP- based SPR sensor as a promising platform for early and precise malaria diagnosis, leveraging enhanced plasmonic responses to detect minimal refractive index variations associated with malaria infection.

## Optoelectronic Properties of NanoStructured ZnS Thin Films Grown by Soft Chemical Technique for Glucose Sensor

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## Abstract

Zinc sulphide thin film were deposited on the glass substrate at 85<sup>0</sup>C temperature by solution growth technique (SGT). The deposition parameters were standardized. The uniform deposition of the thin films were achieved by using aqueous solutions of zinc chloride, thiourea, ammonia along with complexing agent triethanol amine in alkaline medium. The effect of different deposition time and annealing on the properties of ZnS thin films were investigated by SEM, EDAX, XRD, FTIR and UV-vis. The X-ray diffraction revealed that sample technique showed nano peaks of the crystal structure. Scanning electron microscopy (SEM) micrograph exhibit 250 nm length and 78 nm width. The direct band gap energy is obtained to be about 3.10, 3.67, 3.84, 3.75, 3.75, 3.71 and 3.63 eV at pH 9.45, 9.75, 10.5, 10.76, 10.8, 11.5, 11.5. The band gaps of ZnS thin films were found in increasing order from 3.74 eV to 3.95 eV after adsorption of glucose at 1 to 6 hours.

# Non-Toxic Chalcopyrite-ZnGeP<sub>2</sub> based Segmented Cladding Photonic Crystal Fiber for MIR Supercontinuum Generation

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## Abstract

The proposed research work deal with the numerical designing of Photonic Crystal Fiber (PCF) exhibiting square core and segmented cladding having eight bunches of air holes (four bunches having two arrays of air holes each placed at 0° to 360° at a gap of 90° and four bunches having one array of air holes each placed at 45° to 315° at a gap of 90°). The PCF is composed of ZnGeP<sub>2</sub> which is Arsenic-free chalcopyrite material having nonlinear refractive index at range of  $\sim 10^{-18}$  m<sup>2</sup>/W. The designed PCF is theoretically constructed and numerically simulated by Finite Element (FEM) based COMSOL Multiphysics Software for the electric field modal analysis. Following the modal analysis in a spectral range of 1-7 μm, calculations for dispersion characteristics are done in which 2.6 μm is derived as Zero Dispersion Wavelength (ZDW) which accompanied us towards the selection of pump wavelength as 2.75 μm. The selected pump wavelength falls in anomalous dispersion regime. At discussed ZDW, the PCF offers a smaller effective mode area as 4.29 μm<sup>2</sup> and maximized nonlinearity as 5632.783 W<sup>-1</sup>km<sup>-1</sup>. The final observation discusses about the Supercontinuum (SC) measurements at different peak powers, different fiber lengths and different pulse widths. The final conclusion drawn is that a wide band SC spanning from 1.2 μm to 13 μm (covering full transparency of ZnGeP<sub>2</sub>) is extracted at just 8 kW of peak power, 50 fs of pulse width and at just 3.5 mm of fiber length. The proposed PCF may be a better counterpart for nonlinear applications for its wide SC generation with non-toxic nature.

## Substrate-Dependent Performance Evaluation of Microstrip Patch Antennas: A Case Study on FR4 and RT Duroid

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## Abstract

This research undertakes a detailed comparative study of microstrip patch antennas designed on two widely used substrates—FR4 and RT Duroid—with the objective of evaluating their performance for 5G and IoT applications in the 24–32 GHz frequency range. The analysis focused on key parameters including return loss, bandwidth, gain, and impedance matching, using HFSS simulation software.

The FR4-based antenna ( $\epsilon_r = 4.4$ ,  $h = 1.6$  mm) demonstrated multiple resonances across the operating band. Significant results were observed at 27.25 GHz, 28.40 GHz, and 29.60 GHz, where return loss values reached as low as -29.40 dB. The design achieved high gain performance, with peak gain up to 10.47 dBi at 29.6 GHz. Moreover, the FR4 substrate supported broader bandwidth, making it suitable for broadband communication systems, though higher dielectric losses slightly reduced overall efficiency.

On the other hand, the RT Duroid substrate, with its low dielectric loss tangent and superior high-frequency stability, provided consistently improved impedance matching. Simulations revealed return loss values better than  $-25$  dB across key resonance points and gain values peaking at 8.96 dBi at 32.56 GHz. However, compared to FR4, the bandwidth of RT Duroid-based designs was narrower, indicating a trade-off between spectral coverage and efficiency.

The comparative results underline the material-dependent nature of antenna performance. While FR4 offers the advantages of cost-effectiveness and wider bandwidth, it is limited by higher dielectric losses. RT Duroid, though more expensive, delivers superior gain stability and impedance characteristics, albeit with restricted bandwidth. These findings suggest that substrate selection should be guided by specific design priorities—FR4 being favorable for broadband and low-cost applications, and RT Duroid for high-efficiency, narrowband, and precision-driven systems in advanced 5G/mmWave communications.

## **Improving Gas Separation Performance of UiO-66 incorporated PVDF Mixed Matrix Membranes**

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### **Abstract**

UiO-66, a metal-organic framework (MOF) known for its exceptional thermal and chemical stability, holds great promise for enhancing gas separation performance in membranes. This work explores the fabrication and performance analysis of mixed matrix membranes (MMMs) comprising UiO-66 nanoparticles incorporated into a polyvinylidene fluoride (PVDF) polymer matrix. The aim is to leverage the selective gas separation properties of UiO-66 to improve the gas separation performance of the base PVDF membrane. The UiO-66 nanoparticles were synthesised using solvothermal method and characterised using techniques such as XRD, FTIR, TGA and FESEM. The MMMs were prepared via a knife-casting method, varying the UiO-66 loading to optimize the membrane structure and performance. Gas permeation experiments were conducted using a custom-built gas permeation system to evaluate the separation performance of the MMMs for various gas pairs (e.g., H<sub>2</sub>/CO<sub>2</sub>, H<sub>2</sub>/N<sub>2</sub>). The influence of UiO-66 loading on gas permeability and selectivity was investigated. The results demonstrate that the incorporation of 10% concentration of UiO-66 into the PVDF matrix significantly enhances the gas separation performance compared to the neat PVDF membrane, particularly for H<sub>2</sub> permeability increased by 108%. The selectivity values for H<sub>2</sub>/CO<sub>2</sub> and H<sub>2</sub>/N<sub>2</sub> increased by 53% and 58%, respectively. This study highlights the potential of UiO-66/PVDF MMMs for efficient gas separation applications.

# PCF technology-based gas sensor with improved sensitivity in terahertz regime

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## Abstract

This study presents the design and theoretical analysis of square-core photonic crystal fiber (PCF) sensors designed for detecting three gaseous analytes:  $\text{CH}_4$  ( $n=1.562$ ),  $\text{CO}_2$  ( $n=1.5022$ ), and  $\text{H}_2\text{O}$  ( $n=1.518$ ). Key performance parameters were analyzed over a broad terahertz (THz) range from 0.8 to 2.5 THz, using Zeonex as the background material for gas sensors. The sensing properties, including relative sensitivity, confinement loss, effective mode area, and numerical aperture (NA), were investigated through simulations performed using the finite element method in COMSOL Multiphysics. The proposed PCF structure achieved high relative sensitivity, reaching 97.52% for  $\text{CH}_4$ , 96.89% for  $\text{CO}_2$ , and 99.07% for  $\text{H}_2\text{O}$  at an operating frequency of 2.5 THz. The confinement loss was exceptionally low, with values of  $1.08 \times 10^{-12}$  dB/m for  $\text{CH}_4$ ,  $8.61 \times 10^{-11}$  dB/m for  $\text{CO}_2$  and  $5.07 \times 10^{-12}$  dB/m for  $\text{H}_2\text{O}$ . Additionally, the power fraction has been recorded as 97.19% for  $\text{CH}_4$ , 92.93% for  $\text{CO}_2$ , and 95.93% for  $\text{H}_2\text{O}$ . At 2.5 THz, the PCF exhibited a large effective mode area (EMA) of  $1.49 \times 10^{-7}$   $\mu\text{m}^2$  for  $\text{CH}_4$ ,  $1.64 \times 10^{-7}$   $\mu\text{m}^2$  for  $\text{CO}_2$  and  $1.54 \times 10^{-7}$   $\mu\text{m}^2$  for  $\text{H}_2\text{O}$ . The corresponding numerical aperture values were 0.17 for  $\text{CH}_4$ , 0.16 for  $\text{CO}_2$ , and 0.17 for  $\text{H}_2\text{O}$ . The simple square-core design ensures ease of fabrication using current manufacturing techniques, making the proposed PCF highly practical for sensing applications.

## A Preliminary Study of optically stimulated luminescence (OSL) and thermoluminescence (TL) of LiCaAlF<sub>6</sub>: Eu Phosphor

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## Abstract

The demand for OSL (optically stimulated luminescence) based dosimeters in the field of medical dosimetry is increasing worldwide. Therefore, it is indispensable to develop highly sensitive efficient OSL dosimetry material. LiCaAlF<sub>6</sub> is emerged as a potential OSL material due to its wide band gap, good storage efficiency, non-toxicity and high thermal stability. In this work, we have attempted to prepare the LiCaAlF<sub>6</sub> phosphor doped with Eu using melting method in argon gas atmosphere and investigated its CW-OSL and TL properties. The photoluminescence (PL) studies confirm the incorporation of Eu in LiCaAlF<sub>6</sub> host by showing strong emission at 590 nm with excitation from 340nm. The CW-OSL decay curve was recorded on Risø TL/OSL reader after irradiation with a beta dose of 500 mGy. The OSL sensitivity of beta irradiated LiCaAlF<sub>6</sub>: Eu phosphor is found to be ~30 times higher than

undoped LiCaAlF<sub>6</sub> and ~ 3 times higher to that of commercially available OSL phosphor Al<sub>2</sub>O<sub>3</sub>:C(BARC). The enhanced sensitivity may be attributed to the creation of additional defect centers introduced by Eu doping, which act as efficient charge trapping sites. TL glow curve structure has shown a broad TL peak positioned around 169°C which is mainly composed of overlapping peaks. Further, TL and CW-OSL correlation has been studied by preheating of samples at different temperatures. This helps in understanding the contribution of different TL traps on respective OSL intensity.

## **Optimization of Dielectric Response for Zr-MOF / PVDF Nanocomposites**

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### **Abstract**

In this study we are reporting synthesis & characterization of Zr-MOF in the amount of 1-5 wt% dispersed into PVDF nanocomposites. These nanocomposites have been synthesized by solution casting method. The prepared polymer nanocomposites have been characterized using XRD, FTIR, SEM, DSC and Impedance analyzer. XRD spectra showing the enhanced crystallinity of the polymer nanocomposites, However SEM images confirms homogeneous dispersion of the MOF into the PVDF nanocomposites. The glass transition temperature improvement has been found via DSC. Dielectric response has been improved with the high contents of MOF into PVDF nanocomposites. The detailed results will be presented during the conference presentation.

## **Electrical and optical study of Dy<sup>3+</sup> doped SrBi<sub>2</sub>Nb<sub>2</sub>O<sub>9</sub> aurivillius ceramic for advanced electronic applications**

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### **Abstract**

A series of ferroelectric ceramics with the composition SrBi<sub>2-x</sub>Dy<sub>x</sub>Nb<sub>2</sub>O<sub>9</sub> (SBN), where dysprosium (Dy<sup>3+</sup>) serves as the dopant, was synthesized using the conventional solid-state reaction method. X-ray diffraction (XRD) analysis confirmed the successful formation of a single-phase orthorhombic structure, attributed to the space group A21am. The incorporation of Dy<sup>3+</sup> ions led to noticeable modifications in the lattice constants and unit cell volume, which were systematically analyzed as the doping concentration increased. Scanning electron microscopy (SEM) revealed that the synthesized samples exhibited a plate-like grain morphology with random orientation. Optical characteristics of the Dy<sup>3+</sup>-

substituted SBN ceramics were extensively investigated through photoluminescence Spectra (PL). Dielectric measurements demonstrated a well-defined ferroelectric–paraelectric phase transition, accompanied by low dielectric loss across the samples. These findings highlight the influence of Dy<sup>3+</sup> substitution on the structural, optical, and dielectric behavior of SBN ceramics. The combined results suggest that Dy-doped SBN materials possess desirable properties for potential use in high-frequency electronic devices and energy storage systems, making them promising candidates for advanced functional applications.

## **Engineering Zn-Doped $\delta$ -MnO<sub>2</sub> via Potentiostatic Electrochemical Deposition for Supercapacitor Applications**

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### **Abstract**

Zn-doped  $\delta$ -MnO<sub>2</sub> has emerged as a promising electrode material for high-performance supercapacitors due to its enhanced electrochemical properties. In this work, Zn-doped  $\delta$ -MnO<sub>2</sub> was synthesized via a simple potentiostatic electrochemical deposition method and annealed at four distinct temperatures, producing samples labeled ZM4, ZM5, ZM6, and ZM7. X-ray diffraction confirmed successful Zn integration, while Field Emission Scanning Electron Microscopy (FESEM) revealed a strong dependence of morphology on annealing temperature: ZM4 (400 °C) formed a nanowire structure, whereas ZM5–ZM7 (500 °C–700 °C) developed nanosheet morphologies. Morphology played a major role in electrochemical performance, with specific capacitances of 796, 776, 654, and 499 F/g for ZM4, ZM5, ZM6, and ZM7, respectively, in 0.1 M NaOH electrolyte. Among these, ZM4 exhibited superior energy and power densities of 3 Wh/kg and 2.9 kW/kg, respectively. These findings demonstrate that controlled Zn doping and annealing can tailor  $\delta$ -MnO<sub>2</sub> morphology, offering an effective pathway toward high-performance supercapacitor electrodes.

## **Preparation Techniques and Structural, Optical, and Electrical Properties of TiO<sub>2</sub>-Based Thin Films for Optoelectronic Applications: A Review**

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### **Abstract**

Titanium dioxide (TiO<sub>2</sub>)-based thin films have garnered a lot of research interest because of their remarkable structural stability, adjustable optical transparency, and advantageous electronic

characteristics, and are therefore promising materials for a variety of optoelectronic applications. Recent developments in TiO<sub>2</sub> thin film preparation methods and property optimization are thoroughly compiled in this review. The process parameters, film uniformity, crystallinity, and cost-effectiveness of several deposition techniques—such as sol-gel processing, sputtering, chemical vapor deposition, atomic layer deposition, and electron beam evaporation—are compared. The phase transition between anatase, rutile, and brookite structures is discussed in relation to the effects of deposition conditions and post-deposition treatments, especially thermal annealing. The optical and electrical properties of the films are associated with the structural features, including grain size, morphology, and crystallographic orientation. With a focus on customizing light absorption for enhanced device performance, the optical behavior—including band gap modulation, refractive index variation, and transmittance—is examined. Similarly, it is discussed how intrinsic defects, dopants, and annealing temperature affect electrical conductivity and carrier concentration. The review also emphasizes the significance of compositional engineering to improve visible-light response and charge transport through metal and non-metal doping. The structure-property-function relationships of TiO<sub>2</sub>-based thin films are highlighted in the discussion of their potential in optoelectronic devices like photodetectors, solar cells, and transparent conducting layers. The paper ends with a review of current issues, such as reproducibility and interface engineering, and future directions for multifunctional, high-efficiency TiO<sub>2</sub>-based thin film systems for next-generation optoelectronic technologies.

## **The Quest for Electrospun Manganese Cobaltite Nanofibers as Flexible Supercapacitor Electrode**

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### **Abstract**

Many long-term investigations are associated to their primary objective of finding new nanostructures for versatile applications. Supercapacitors are an innovative energy storage device with a high power density and extraordinary cycling stability. Supercapacitors' energy density, power density, cycling stability and safety may all be directly impacted by their electrochemical performance, which is mostly dependent on electrolytes. The accurate synthesis of 1D nanomaterials, particularly nanofibers, is hence essential to the pursuit of furthering research in efficient energy storage. Effective electrochemical performance is the goal of transitional metal oxide electrodes, as long as their precise structural composition is achieved. As a reliable supercapacitor electrode material, we present here the attainable synthesis of Manganese Cobaltite using the Electrospinning Method on a flexible stainless-steel substrate. To utilize the detailed electrochemical assets of the material, the annealing temperature was attuned to varying values. Contact Angle Measurement was utilized to confirm the electrode's hydrophilic nature. Using XPS, the material's electrochemically contributing chemical states were confirmed. To comprehend the synergistic effects of electrochemical behaviour of the as-prepared Manganese Cobaltite films, they were analyzed with regard to a variable class of electrolytes. The best performance of the electrode is found in aq. KOH electrolyte

at scanning rate of 5 mV/s, which provides an incredible 1094.4 F/g specific capacitance. The material's specific energy, at 1 volt working potential, significantly increased to 27.3 Wh/kg, revealing 3.8 kW/kg specific power. To serve supercapacitor applications, this work assembles the appropriate parameter tunability and analytical insights in demonstrating dependable, flexible and efficiently stable electrode material.

## **Structural, Electronic, and Magnetic Properties of Silver-Doped ZnO Nanostructures for Spintronic Applications**

*Dr. Chiv Charan Sharma*

### **Abstract**

Silver-doped zinc oxide (AgZnO) nanostructures were successfully synthesized and systematically characterized to investigate their structural, chemical, and magnetic properties. X-ray diffraction (XRD) analysis confirmed the formation of a hexagonal wurtzite structure of ZnO with no secondary phases, indicating the successful incorporation of Ag into the ZnO lattice. The diffraction peak shifts and crystallite size variations suggested lattice distortion due to Ag substitution or interstitial incorporation. X-ray photoelectron spectroscopy (XPS) revealed the presence of Ag in the +1-oxidation state, confirming its successful doping and indicating strong interaction with the ZnO matrix. The binding energy shifts also suggested modulation of the electronic environment around Zn and O atoms. Magnetic measurements using vibrating sample magnetometry (VSM) at room temperature exhibited weak ferromagnetic behavior in AgZnO samples, contrasting the diamagnetic nature of pure ZnO. The observed magnetism is attributed to the formation of bound magnetic polarons facilitated by oxygen vacancies and Ag-induced defect states. These results suggest that Ag doping not only modifies the structural and electronic properties of ZnO but also induces room-temperature ferromagnetism, making AgZnO a promising candidate for spintronic and multifunctional applications.

## **Nano-Catalytic Approaches for Optimizing the Sorption Behavior of Metal Hydrides: A Comprehensive Review**

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### **Abstract**

Over the past few decades, numerous materials have been investigated for hydrogen storage. Among these, metal hydrides have attracted considerable attention due to their high volumetric hydrogen density, making them promising candidates for practical hydrogen storage applications. However, their widespread adoption is limited by challenges such as sluggish hydrogen sorption kinetics, high activation energies, and limited reversibility. To address these issues, various strategies have been explored, among which the incorporation of catalysts has emerged as one of the most effective approaches. Catalysts play a crucial role in enhancing surface kinetics and significantly improving the overall hydrogen absorption and desorption behavior of metal hydrides. Recent advancements in nano-catalysis have shown

promising results in addressing these challenges. This review focuses on the role of nanocatalysts in improving the hydrogenation/dehydrogenation behavior of various metal hydrides, the mechanisms involved, and recent advances in the field. Various nanostructured catalysts, including transition metals, metal oxides, and carbon-based materials, are examined, highlighting their mechanisms of interaction with metal hydrides. The impact of catalyst dispersion, surface chemistry and particle size on hydrogen sorption properties is discussed, along with recent experimental and computational insights. Finally, future research directions and challenges in optimizing nano-catalysts for hydrogen storage applications are outlined. The findings presented in this review underscore the crucial role of nanomaterials in advancing metal hydrides toward practical hydrogen storage solutions.

## **Magnetotransport Signature and Semimetal-to-Semiconductor Crossover in Elemental Bismuth Single Crystals**

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### **Abstract**

Elemental bismuth, a semimetal characterized by strong spin-orbit coupling and nontrivial topological ordering, has emerged as a model system for exploring quantum phenomena in condensed matter physics. In this study, we present a comprehensive investigation of the structural and low-temperature transport properties of high-quality bismuth single crystals. Rietveld refinement of powder X-ray diffraction data confirms the rhombohedral crystal structure with space group R-3m. Temperature-dependent resistivity, magnetoresistance, and Hall measurements were performed at cryogenic temperatures to elucidate the carrier dynamics. A semimetal-to-semiconductor crossover was observed at low temperatures, attributed to lattice contraction and consequent modification of the electronic band structure. A pronounced, non-saturating magnetoresistance approaching 100% at 3.9 K was recorded, which diminishes with increasing temperature. Hall measurements reveal a sign reversal of the Hall resistance near 1000 G, indicating multicarrier transport and a magnetic-field-induced shift of the Fermi level. These results establish the coexistence of semimetallic and semiconducting characteristics in elemental bismuth, underscoring its potential as a tunable platform for investigating topological electronic phases. The demonstrated magnetotransport tunability positions bismuth as a promising material for next-generation low-power quantum and spintronic applications.

# Quantitative Magnetotransport Analysis of $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$ Topological Insulators Using a Semiclassical Two-Band Model

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## Abstract

The ternary compounds  $\text{Bi}_2\text{Te}_3$ ,  $\text{BiSbTe}_3$ , and  $\text{Sb}_2\text{Te}_3$  are well-known topological insulators exhibiting robust, gapless surface states protected by time-reversal symmetry. Understanding the interplay between bulk and surface conduction in these materials is essential for realizing their quantum transport potential. In this work, we systematically investigate the electronic and Magneto transport properties of  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$  ( $0 \leq x \leq 2$ ,  $\Delta x = 1$ ) single crystals, synthesized as model systems for studying tunable topological behaviour. Structural characterization via X-ray diffraction confirms the rhombohedral crystal structure (space group  $R\bar{3}m$ ), with lattice parameters and unit cell volume decreasing monotonically with increasing Sb concentration, consistent with the substitution of smaller Sb atoms for Bi. Temperature-dependent resistivity measurements (2-300 K) reveal metallic behaviour across all compositions, while low-temperature (4-55 K) data conform to Fermi liquid behaviour, indicating dominant electron-electron scattering. Magnetoresistance (MR) measurements up to 9 T exhibit linear, non-saturating MR with pronounced quantum oscillations in  $\text{BiSbTe}_3$  at 2 and 10 K. Quantitative analysis of MR and Hall data using a semiclassical two-band model yields carrier densities on the order of  $10^{19} \text{ cm}^{-3}$  and mobilities of  $\sim 10^4 \text{ cm}^2/\text{V}\cdot\text{s}$ , consistent with reported values for topological insulators. The successful application of the two-band model, typically used for semimetals, demonstrates its capability to capture essential transport characteristics in topological systems, offering valuable insights into carrier compensation and scattering mechanisms. These findings provide a quantitative framework for understanding magneto transport phenomena in Bi-Sb-Te-based topological materials.

# Effect of Chromium Doping on the Structure and Phase Stability of BiSbTe<sub>3</sub> Single Crystals

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## Abstract

The discovery and exploration of Bi/Sb-based topological insulators (Bi<sub>x</sub>Sb<sub>1-x</sub>)<sub>2</sub>Te<sub>3</sub> have been instrumental in unlocking the path to the experimental realization of the Quantum Anomalous Hall Effect (QAHE) and the advanced developments in low-power spintronic applications. However, synthesizing magnetically doped single crystals without secondary phases remains challenging due to the limited solubility of transition metals. In this work, we investigate the effect of chromium doping (2.5 and 5 at.%) on the structural and morphological properties of BiSbTe<sub>3</sub> (BST) single crystals grown by the Modified Bridgman method. X-ray diffraction (XRD) and Rietveld refinement confirm the rhombohedral (R-3m) structure, with lattice parameters decreasing as Cr content increases, indicating substitution at Bi/Sb sites. At 5 at.% doping, however, an abrupt increase in the *c* parameter accompanies the formation of Cr<sub>2</sub>Te<sub>3</sub> as a secondary phase. The effect of various synthesis parameters was systematically investigated to address this issue. With variations in synthesis parameters, the formation of Cr<sub>2</sub>Te<sub>3</sub> was observed to undergo a significant reduction, from 30% to approximately 0% at selected regions of the synthesized lump under optimized conditions. Scanning electron microscopy revealed the layered morphology, while energy dispersive spectroscopy (EDS) indicated compositional uniformity except in the upper region of the ingot. Our results suggest a solubility limit of <5 at.% for chromium in the BST lattice and highlight optimized growth conditions for obtaining phase-pure, Cr-doped BST single crystals.

## Carbon based Nanomaterials, Optimization, and Characterization and Applications

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## Abstract

Carbon has played a pivotal role in the advancement of human civilization owing to its exceptional bonding versatility and ability to form diverse structures. Over the past three decades, significant progress has been made in the synthesis and application of carbon-based nanomaterials, which exhibit unique morphologies and remarkable physicochemical properties. These materials have found extensive

use in multidisciplinary domains, including energy storage and conversion, environmental remediation, and biomedical engineering.

This review highlights four of the most notable carbon-based nanomaterials carbon nanotubes, buckminsterfullerene (fullerenes), activated carbon, and graphene oxide. It provides a comprehensive discussion of their synthesis methods, structural characteristics, and wide-ranging applications. Furthermore, the challenges and limitations associated with their large-scale production and integration into practical systems are critically examined. The study aims to present an in-depth understanding of these materials, offering insights that will foster future advancements and broaden their technological applications.

## **Electrochemical and Structural Properties of PVdF-HFP:PEG blended solid polymer electrolytes with varying Na salt concentration**

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### **Abstract**

In this study, poly (vinylidene fluoride-co-hexafluoropropylene) (PVdF-HFP) and polyethylene glycol (PEG) were blended to form a polymer matrix, and different concentrations of sodium chloride (NaCl) were incorporated to investigate their effect on structural and electrochemical properties. The solid polymer electrolytes (SPEs) were synthesized using the solution casting technique and characterized using various techniques. Electrochemical impedance spectroscopy (EIS) was performed to evaluate the ionic conductivity and dielectric behavior of the SPEs over a wide frequency range. The results indicate that increasing NaCl concentration initially enhances ion dissociation, leading to improved ionic conductivity. However, beyond an optimal concentration, the formation of ion aggregates reduces charge carrier mobility, resulting in decreased conductivity. Fourier transform infrared spectroscopy (FTIR) was used to examine polymer-salt interactions and the degree of ion dissociation. The flexible nature of PEG aids in ionic transport, while PVdF-HFP provides mechanical stability and structural integrity. This study highlights the crucial role of NaCl concentration in tailoring the electrochemical performance of PVdF-HFP:PEG-based SPEs. The findings contribute to the development of high-performance solid-state electrolytes for applications in batteries, supercapacitors, and other energy storage devices.

# Competence of Electrodeposited Nickel doped Cobalt oxide Thin Film Electrode by Chronopotentiometry Route for Supercapacitor Applications

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## Abstract

Worldwide researchers are after extensive efforts to upgrade current energy conversion technology namely an alternative, a quest for environmentally acceptable energy sources and meet the tenacious demands of crucial energy requirements. The best option in this case is a Supercapacitor, an energy storage device that can store large energy when it is available and release it when needed. Chronopotentiometry method was employed to electrodeposit a nanocrystalline and extremely porous Cobalt oxide electrode and Nickel doped Cobalt oxide electrode onto stainless steel substrates. The electrodes then were annealed for six hours at 500°C to generate metal oxide. X-ray diffraction analyses SEM characterizations confirmed the structural and morphological features respectively, whereas, contact angle measurement determined the wettability. Cyclic voltammetry and galvanostatic charge-discharge methods were used to investigate the electrochemical characteristics of the thin films. Chronopotentiometry mode determined the optimal values of specific capacitance (284 Fg<sup>-1</sup>), specific energy (4.33 Whkg<sup>-1</sup>), specific power of 3.0 (kWkg<sup>-1</sup>) in 1M aqueous Na<sub>2</sub>SO<sub>4</sub> electrolyte at a current density of 1 mAcm<sup>-2</sup> for Cobalt oxide thin film. Similarly, for 2% Ni-doped Cobalt oxide thin film, the values elevated to specific capacitance (727 Fg<sup>-1</sup>), specific energy 10.5 (kWkg<sup>-1</sup>), specific Power of 13.62 (kWkg<sup>-1</sup>) in 1M aqueous Na<sub>2</sub>SO<sub>4</sub> electrolyte at a current density of 1 mAcm<sup>-2</sup>. Thus, the as-synthesized Nickel doped Cobalt oxide electrode holds reliable potential to be executed in supercapacitor applications.

## Development of Optimised Calcite Thin Film on Silicon Nanowires for Hydrophilic Applications

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<sup>1</sup>Department of Physics, Manipal University Jaipur, Jaipur-303007, Rajasthan, India

## Abstract

Calcite-based calcium carbonate (CaCO<sub>3</sub>) thin films hold immense importance due to their unique combination of physical, chemical, and biological properties. Calcium carbonate (CaCO<sub>3</sub>), particularly in its calcite phase, has attracted significant attention due to its excellent biocompatibility, optical transparency, and chemical stability, making it highly suitable for sensors, photonic devices, coatings, and bio-interface applications. The controlled fabrication of calcite thin films on semiconductor substrates, such as silicon, is crucial for integrating these materials into practical optoelectronic and

biomedical devices. In the present study, we developed nanostructured calcite thin films on silicon nanowire (SiNW) substrates using a sequential dipping method. The deposited films were characterised using XRD, FTIR, FESEM, UV–Vis, AFM, and contact angle measurements to understand their structural, chemical, and surface properties. The results confirm that nanostructured calcite thin films can be successfully grown on silicon nanowires, exhibiting a highly hydrophilic surface with a contact angle above 30°. These findings were analysed with respect to process parameters and their influence on the resulting microstructure. The crystallite size, lattice strain, and dislocation density were determined from XRD data, while FESEM and EDX provided insight into the surface morphology and elemental composition. Furthermore, AFM and contact angle studies revealed that the surface microstructure could be tuned to obtain a lower contact angle, making the films suitable for hydrophilic or functional coating applications.

## **Advanced Simulation and Performance Optimization of Eco-Friendly Bilayer Perovskite Solar Cells Using SCAPS-1D**

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### **Abstract**

This study is a comprehensive simulation conducted to develop and enhance the efficiency of a bilayer Perovskite Solar Cell (PSC) through SCAPS-1D software. The primary aim of this work is to optimize the bilayer PSC using two non-toxic, efficient, eco-friendly and stable absorber materials, i.e., (i) calcium zirconium sulphide ( $\text{CaZrS}_3$ ), a chalcogenide material, and (ii) formamidinium tin iodide ( $\text{FASnI}_3$ ), a tin-based material. The single-layer PSCs with configurations FTO/ $\text{TiO}_2$ / $\text{CaZrS}_3$ /Spiro-OMeTAD and FTO/ $\text{TiO}_2$ / $\text{FASnI}_3$ /Spiro-OMeTAD are first analysed separately using SCAPS-1D software. Subsequently, the two absorber layers  $\text{CaZrS}_3$  and  $\text{FASnI}_3$  are integrated to design a bilayer structure which is further optimized. The simulation results indicate that the bilayer perovskite solar cell achieved a Power Conversion Efficiency (PCE) of 33.38% and a Fill Factor (FF) of 89.49% surpassing the performance of both single layer perovskite solar cells and it also indicates improved charge transport dynamics, minimized recombination losses, and enhanced overall photovoltaic performance due to the synergistic effect of the two absorber layers within the bilayer design. This work highlights the significance of incorporating bilayer structures and strategic material selection in advancing perovskite solar cell technology.

# Role of Biodegradable Nanoparticles for Detection and Bioremediation of Environmental Pollutants

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## Abstract

Environmental pollution caused by heavy metals, pesticides, plastics, dyes, and industrial effluents poses serious risks to ecosystems and human health. Conventional remediation techniques are often costly and generate secondary waste, creating demand for safer and sustainable alternatives. Biodegradable nanoparticles (BDNPs) have emerged as an innovative solution for pollution detection and remediation. Made from natural or synthetic polymers such as chitosan, polylactic acid, and alginate, BDNPs degrade into non-toxic products, reducing long-term environmental impact. In detection, BDNPs are employed as biosensors for highly sensitive monitoring of pollutants including pesticides, dyes, and heavy metals. In remediation, they enhance pollutant removal via adsorption, biodegradation, and catalytic mechanisms, often supporting enzymes or microbes to improve efficiency. Green synthesis approaches using plant extracts and microbes further add to their eco-friendly potential. Despite these advantages, challenges such as large-scale production, economic feasibility, and long-term ecological safety remain. This review highlights the principles, applications, limitations, and future prospects of BDNPs in sustainable environmental management.

## Competence of Electrodeposited Nickel doped Cobalt oxide Thin Film Electrode by Chronopotentiometry Route for Supercapacitor Applications

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## Abstract

Worldwide researchers are after extensive efforts to upgrade current energy conversion technology namely an alternative, a quest for environmentally acceptable energy sources and meet the tenacious demands of crucial energy requirements. The best option in this case is a Supercapacitor, an energy storage device that can store large energy when it is available and release it when needed. Chronopotentiometry method was employed to electrodeposit a nanocrystalline and extremely porous Cobalt oxide electrode and Nickel doped Cobalt oxide electrode onto stainless steel substrates. The

electrodes then were annealed for six hours at 500°C to generate metal oxide. X-ray diffraction analyses SEM characterizations confirmed the structural and morphological features respectively, whereas, contact angle measurement determined the wettability. Cyclic voltammetry and galvanostatic charge-discharge methods were used to investigate the electrochemical characteristics of the thin films. Chronopotentiometry mode determined the optimal values of specific capacitance (284 Fg<sup>-1</sup>), specific energy (4.33 Whkg<sup>-1</sup>), specific power of 3.0 (kWkg<sup>-1</sup>) in 1M aqueous Na<sub>2</sub>SO<sub>4</sub> electrolyte at a current density of 1 mAcm<sup>-2</sup> for Cobalt oxide thin film. Similarly, for 2% Ni-doped Cobalt oxide thin film, the values elevated to specific capacitance (727 Fg<sup>-1</sup>), specific energy 10.5 (kWkg<sup>-1</sup>), specific Power of 13.62 (kWkg<sup>-1</sup>) in 1M aqueous Na<sub>2</sub>SO<sub>4</sub> electrolyte at a current density of 1 mAcm<sup>-2</sup>. Thus, the as-synthesized Nickel doped Cobalt oxide electrode holds reliable potential to be executed in supercapacitor applications.

## **Metal/Metal Oxide doped SnO<sub>2</sub> Nanoparticles for Gas Sensor: A Review**

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### **Abstract**

Tin dioxide (SnO<sub>2</sub>) is an n-type semiconductor with a wide band gap (~3.6 eV), widely used in gas sensing and photocatalytic applications. Its performance depends strongly on morphology and surface modification. Doping with zinc oxide (ZnO) or Zn ions enhances sensitivity, selectivity, and response by creating oxygen vacancies and improving charge transfer. ZnO–SnO<sub>2</sub> nanostructures show nanosheet or porous morphologies with high surface area, leading to excellent detection of gases like ethanol and glycol at lower operating temperatures. Moreover, ZnO incorporation improves photocatalytic activity through efficient charge separation, making ZnO–SnO<sub>2</sub> composites promising multifunctional materials for sensing and environmental applications.

## **Nanostructured Ni<sub>1-x</sub>Mg<sub>x</sub>Fe<sub>2</sub>O<sub>4</sub> Nanocomposite for Advanced Sensing Technology**

*Prerna Gurjar<sup>1</sup> Suraj Samal<sup>1</sup>, Priyank Dhakad<sup>1</sup>, Abhishek Sharma<sup>1</sup>, Hariom Pawar<sup>1\*</sup>*

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### **Abstract**

Nanostructured materials have emerged as transformative components in advanced sensing technology, fundamentally revolutionizing detection capabilities across diverse application domains. The Magnesium-doped nickel ferrite nanocomposites (Ni<sub>1-x</sub>Mg<sub>x</sub>Fe<sub>2</sub>O<sub>4</sub> with x = 0, 0.5, 1) were synthesized and systematically characterized to explore their suitability for advanced gas sensing applications. X-ray diffraction (XRD) confirmed the formation of single-phase cubic spinel structures with crystallite sizes of 20–35 nm, demonstrating successful nanocomposite synthesis. Optical characterization via UV-visible spectroscopy revealed a compositional dependence of the band gap energy, ranging from 3.1 to 3.8 eV, indicating semiconductor behavior favorable for sensing applications. Dielectric properties measured using an LCR meter across frequencies from 40 Hz to 5 MHz displayed significant variation in dielectric constant correlated to Mg content, suggesting tunable electrical characteristics. These combined structural, optical, and dielectric features contribute to the enhanced sensitivity and selectivity of these

nanocomposites for detecting reducing gases at very low concentrations. The materials exhibit stable operation at low optical temperatures, positioning them as promising candidates for next-generation chemiresistive gas sensors in environmental monitoring and industrial safety.

## Overview of the Gas-Sensing Properties of Magnetic $\text{CoFe}_2\text{O}_4$ Nanoferrites

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### Abstract

Magnetic spinel  $\text{CoFe}_2\text{O}_4$  nanoferrite offers various applications in biomedical, water treatment, and industrial electronic devices, which has sparked a lot of attention. The synthesis, properties, and uses of spinel ferrites in various fields, especially doped spinel ferrites are the main topics of this review. Spinel ferrites nanoparticles doped with the elements have a wide range of applications due to their remarkable electrical and magnetic properties, including magnetic fields, microwave absorbers, and biomedicine. Furthermore, the physical properties of spinel ferrites can be modified by substituting metallic atoms, resulting in improved performance. The most recent and noteworthy applications of magnetic ferrite nanoparticles are reviewed and discussed in this review. This review goes over the synthesis, doping and applications of  $\text{CoFe}_2\text{O}_4$  nanoferrites, as well as views on how to choose the appropriate doped metal ferrites based on the intended application.

## Ni Doping-Induced Optical Property Modulation in $\text{Ni}_{1-x}\text{Mg}_x\text{Fe}_2\text{O}_4$ Nanocomposites for Smart Sensing Devices

*Priyank Dhakad<sup>1</sup>, Suraj Samal<sup>1</sup>, Prerna Gurjar<sup>1</sup>, Abhishek Sharma<sup>1</sup>, Hariom Pawar<sup>1\*</sup>*

<sup>1</sup>Material Science Research Lab, Department of Physics, JECRC University, Jaipur, Rajasthan, 303905, India  
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### Abstract

Nanostructured materials have emerged as pivotal constituents in modern sensing technologies, offering transformative improvements in detection sensitivity and selectivity across a broad spectrum of applications. In this study, magnesium-doped nickel ferrite nanocomposites ( $\text{Ni}_{1-x}\text{Mg}_x\text{Fe}_2\text{O}_4$ ;  $x = 0, 0.5, 1$ ) were synthesized and comprehensively characterized to evaluate their potential for advanced gas-sensing applications. X-ray diffraction (XRD) analysis confirmed the formation of single-phase cubic spinel structures with crystallite sizes in the range of 20–35 nm, validating the successful synthesis of the nanocomposites. Optical properties, investigated using UV–visible spectroscopy, revealed a systematic compositional dependence of the optical band gap, varying from 3.1 to 3.8 eV, consistent with semiconductor characteristics suitable for gas-sensing functionality. Density Functional Theory (DFT) simulations further corroborated the experimental band gap trends and supported the observed crystal geometry. The synergistic structural, optical, and dielectric attributes of these materials contribute to their enhanced gas sensitivity and selectivity, particularly toward reducing gases at trace concentrations. Furthermore, their stable operation at low temperatures underscores their potential as efficient candidates for next-generation chemiresistive gas sensors aimed at environmental monitoring and industrial safety applications.

# **Track - II**

## **Chemistry of Materials and Technology**

# A Facile co-precipitation synthesis of $Mg_2P_2O_7$ towards the energy storage application

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## Abstract

Recent advances in energy storage devices have revealed considerable progress within the energy sector and electrical components, fundamentally changing power storage methods and showcasing these innovations. Metal pyrophosphates, particularly Mg-based pyrophosphates, are unique and exceptional due to their low cost, layered structure, and strong electrochemical characteristics. The  $Mg_2P_2O_7$  was produced using a simple co-precipitation process and calcined at 650 C in air. Further, the  $Mg_2P_2O_7$  was characterized by X-Ray Diffraction (XRD), Fourier Transfer infrared Spectroscopy (FT-IR), and Scanning Electron Microscopy (SEM) techniques. The monoclinic structure and purity of  $Mg_2P_2O_7$  were validated using X-ray diffraction and FT-IR techniques. Morphological study was carried out using a SEM, which confirmed the porous nature of the materials. The electrochemical behaviour of  $Mg_2P_2O_7$  particles as supercapacitors was examined employing cyclic voltammetry and chronopotentiometric techniques. The electrode demonstrates a specific capacitance of 465 F/g at a current density of 6 A/g, as determined by galvanostatic charge-discharge measurements. This performance is attributed to the favourable interactions between the transition magnesium metal and pyrophosphate within a potential window of 0 to 0.8 V in a 3 M KOH electrolyte solution. The findings suggest that  $Mg_2P_2O_7$  materials, synthesized via the hydrothermal method, possess potential applications as electrode materials in supercapacitors.

# Structural and Electrochemical Properties of Hexagonal CuFeO<sub>2</sub> Nanoparticles for Next-Generation Supercapacitors

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## Abstract

The increasing demand for advanced energy storage systems has made supercapacitors promising devices because of their high power density, quick charge–discharge ability, and long cycle life. Transition metal oxides, with their multiple oxidation states, rich redox activity, and structural stability, have become attractive electrode materials for these devices. However, their practical use is often hindered by issues like poor electrical conductivity and limited rate capability, emphasizing the need to explore new oxide materials with improved electrochemical performance. In this work, CuFeO<sub>2</sub> nanoparticles were successfully synthesized using a simple hydrothermal method. X-ray diffraction analysis confirmed the rhombohedral structure with an R-3m space group, while FESEM showed a well-defined hexagonal shape. The elemental composition of Cu, Fe, and O was further validated by EDX analysis. Electrochemical tests demonstrated the excellent energy storage performance of the CuFeO<sub>2</sub> electrode, reaching a maximum specific capacitance of 800 F g<sup>-1</sup> at a current density of 2 A g<sup>-1</sup>. Additionally, the electrode achieved an impressive energy density of approximately 54.4 Wh kg<sup>-1</sup> with a corresponding power density of 700 W kg<sup>-1</sup>. These results highlight the potential of CuFeO<sub>2</sub> as an effective electrode material for high-performance supercapacitor applications.

## Structural, optical, electrical and magnetic measurements of Na-doped ZnO nanoparticles synthesized via co-precipitation method

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## Abstract

A simple co-precipitation method was used to synthesize Na-doped ZnO nanoparticles with 0, 1, 3, and 5 wt % of Na to Zn precursor salts. The structural, optical, electronic and magnetic properties of Na-doped ZnO nanoparticles were studied via XRD, XPS, PL, FTIR, FESEM, UV spectroscopy and VSM. The X-Ray diffraction pattern shows the hexagonal wurtzite crystal structure, with crystalline size for (101) peak in the range of 47 nm to 34 nm. The X-ray photoelectron spectroscopy (XPS) revealed the increase in oxygen vacancies (V<sub>o</sub>) with Na-doping. The 5% Na-doped ZnO nanoparticles have maximum number of oxygen vacancies. UV spectroscopy was used to determine energy band gap (E<sub>g</sub>) and Urbach Energy.

The obtained data shows decrease in bandgap with increasing Na-doping concentration. The Photoluminescence (PL) spectra indicates the increase in oxygen vacancies with Na-doping in agreement to the XPS results. The surface morphology and average particle size has been studied using SEM images, which depicts hexagonal and spheroid like structure, with average particle size in the range of 40 nm to 100 nm. FTIR spectroscopy data proved the formation of functional groups and the presence of chemical bonding at ZnO interface. Further, Na-doped ZnO shows good room temperature ferromagnetism (RTFM) with increasing in doping concentration.

## Visible light activated Sb<sub>2</sub>O<sub>3</sub>/SnS<sub>2</sub> nanocomposite for pollutant degradation

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### Abstract

Binary Sb<sub>2</sub>O<sub>3</sub>/SnS<sub>2</sub> at various percentages of SnS<sub>2</sub> (2 & 4 wt%) were synthesized by hydrothermal method. Photocatalysts were analyzed for their optical properties, morphological characteristics, crystalline structures, dynamics of charge recombination, chemical compositions, surface charge. Photocatalytic performance of constructed materials was examined on Rhodamine B (RhB) and antibiotic ciprofloxacin (CP) in the illumination of visible light. Sb<sub>2</sub>O<sub>3</sub>/SnS<sub>2</sub> (2 wt%) exhibited highest photocatalytic decontamination efficiency i.e., 77.14% in 140 min for RhB 71.25% in 180 min for CP at highest rate constant of 0.0068 min<sup>-1</sup> for RhB & 0.0057 min<sup>-1</sup> for CP. This is owing to the formation of heterojunctions in Sb<sub>2</sub>O<sub>3</sub>/SnS<sub>2</sub> which facilitate effective separation of charges and increase light harvesting, thus boost efficiency. •OH and •O<sup>2-</sup> were recognized as active species in both the removal of CP and RhB. The catalyst was stable and little loss in efficiency was observed even after the five runs.

## Synthesis of Metal Oxide Nanoparticles and Evaluation of Their Biological Potential Using Different Parts of *Acacia tortilis* plant collected from Dhosi Hill, Haryana

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### Abstract

*Acacia tortilis* is a medicinal plant belongs to Fabaceae family and widely distributed in arid and semi-arid regions of North, East and Southern Africa, the Middle East and the Arabian Peninsula is frequently used in traditional medicine to treat conditions like burns, hepatitis, diabetes, and asthma. A range of phytochemicals with various biological functions, including antibacterial, antifungal, antiparasitic, antioxidant, antiproliferative, anti-diabetic, and anti-inflammatory activities, were found through phytochemical investigations. The disruption of cellular membranes and ultrastructural alterations driven

on by *A. tortilis* phytochemicals are the cause of the antimicrobial and antiparasitic properties. However, the anti-inflammatory, anti-cancer, and anti-diabetic effects are caused by physiological and molecular mechanisms include apoptosis induction, inhibiting cell proliferation, and inflammatory mediators. Present study was performed with leaves, bark and fruits of *Acacia tortilis*, collected from Dhosi hill, Haryana; to find out various pharmacological aspects of plant. Extractive value in water was calculated for selected parts of *Acacia tortilis*. Bark recorded with highest extractive value 0.2325 mg/g.dw, brown in color and in powder form. For leaves, value was reported as 0.1595 mg/g.dw with brown color and powder form of extract while fruit extract was found to be radish brown in color, sticky in nature and with 0.132 mg/g.dw extractive value. Disc Diffusion Assay was performed and Inhibition zone (IZ) was calculated to evaluate the antibacterial and antifungal activity of selected extracts against selected bacteria and fungi, at different concentrations i.e. 20 µg/ml, 40 µg/ml and 60 µg/ml. Results reported that antibacterial and antifungal activities increased with rise in concentration. Bark extracts were found to be most potent antibacterial agent as highly active against all the selected bacteria; *E.coli* (IZ=14mm, AI= 0.32), *S. aureus* (IZ=13mm, AI= 0.28), *B. subtilis* (IZ=13mm, AI= 0.45), *P. aeruginosa* (IZ=9mm, AI= 0.30). *P. aeruginosa* was the most resistant bacteria among all four. Antifungal potential was also highest for bark extracts against all the selected fungi; *A. alternata* (IZ=10mm, AI= 0.526), *F. oxysporum* (IZ=9mm, AI= 0.33), *A. niger* (IZ=11mm, AI= 0.55), *P. chrysogenum* (IZ=13mm, AI= 0.81). *A. alternata* was the most resistant bacteria among all four. DPPH Assay was performed to evaluate the antioxidant activity of the selected extracts at different concentrations, i.e. 20 µg/ml, 40 µg/ml, 60 µg/ml, 80 µg/ml and 100 µg/ml. Bark extracts found to have highest antioxidant activity with least IC50 value i.e 421.74±2.16 µg/ml followed by leaves and bark with higher IC50 values. Glucose DNSA method was performed to evaluate the antidiabetic potential of the selected extracts at different concentrations, i.e. 20 µg/ml, 40 µg/ml, 60 µg/ml, 80 µg/ml and 100 µg/ml. Fruit extracts found to have highest antidiabetic potential with least IC50 value, i.e. 528.69±3.02 µg/ml followed by leaves and bark. BSA was performed to evaluate the anti-inflammatory potential of the selected extracts at different concentrations, i.e. 20 µg/ml, 40 µg/ml, 60 µg/ml, 80 µg/ml and 100 µg/ml. Bark extracts found to have highest anti-inflammatory potential with least IC50 value, i.e. 967.64±6.30 µg/ml followed by leaves and fruit with higher IC50 values. Conclusively, all the selected plant parts exhibited good activities but bark extract was found to be the most potent part of *A. tortilis* for pharmacological purposes.

## **Lithiation mechanism of the Germanium-based composite electrode for All-solid-state lithium-ion batteries**

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### **Abstract**

Lithium-ion battery is a cornerstone for a sustainable energy future, powering everything from portable electronics to electric vehicles. For decades, there has been an increased worldwide interest in the

development of Li-ion batteries with improved capacity, longer cycle life, and safety. Significant improvement in safety through the employment of solid electrolytes has sparked a surge in research on all-solid-state lithium-ion batteries; however, the quest for compatible electrode material is still a great challenge. Germanium is a promising active material attributed to its high theoretical capacity (1640 mAh g<sup>-1</sup>), a result of the alloying reaction mechanism with lithium. Additionally, the low working potential and high Li-ion diffusivity favor the utilization of germanium anodes. In this work, germanium-based composite anodes have been investigated for all-solid-state lithium-ion batteries using LiBH<sub>4</sub> as a solid electrolyte and Li-foil as a counter electrode. The detailed electrochemical reaction mechanism has been established using cyclic voltammetry, galvanostatic charge-discharge, and XRD. During the first discharge, alloying of Li-Ge takes place, resulting in excellent discharge capacity of 1424 mAh g<sup>-1</sup> with high initial coulombic efficiency of 93% at a current rate of 0.1C. In subsequent cycles, the alloying-dealloying process occurred, and the cell retained a capacity of 335 mAh g<sup>-1</sup> up to 50 cycles. The ex-situ XRD of the cycled Ge-LiBH<sub>4</sub>-AB electrode conducted at various stages of lithiation/delithiation reveals the successful formation of the highly lithiated phase Li<sub>13</sub>Ge<sub>5</sub>. Thus, this work has the potential to revolutionize the energy storage industry, enabling the development of long-lasting, more efficient batteries for a wide range of applications.

## **Eco-Friendly Synthesis Of Zinc Oxide And Copper Oxide Nanoparticles Using Radish Leaf Extract And Their Effects On Seed Germination In Okra**

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### **Abstract**

The current research investigates the green synthesis of zinc oxide (ZnONPs) and copper oxide (CuONPs) nanoparticles employing radish (*Raphanus sativus*) leaf extract and assessing their impact on seed germination and early seedling growth of okra (*Abelmoschus esculentus*). The nanoparticles were synthesized through a cost-effective, environmentally friendly process and analyzed with FTIR, FESEM, EDS, zeta potential, and XRD methods, verifying their spherical shape, elemental purity, and crystalline nature. Different concentrations (25 ppm, 50 ppm, 100 ppm) of green-synthesized nanoparticles, their corresponding metallic salt precursors (zinc acetate and copper sulphate), and radish leaf extract were evaluated on okra seeds. Findings proved that although higher metal salt concentrations exhibited phytotoxicity and lower germination rates, green-synthesized ZnONPs and CuONPs significantly increased root and shoot length, fresh weight, and dry weight of seedlings. The highest germination (100%) was shown with CuONPs at the concentration of 50%. It indicates the possibilities of biosynthesized nanoparticles for green nano-agro-inputs as a new and safer platform compared to usual metal-based fertilizers for seedling growth augmentation.

# Visible-Light Active Fe<sup>2+</sup> doped ZnFe<sub>2</sub>O<sub>4</sub>/TiO<sub>2</sub> Nanostructures for Photocatalytic and Photoelectrochemical Hydrogen Evolution

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## Abstract

In response to the escalating global challenges of energy consumption, environmental degradation, and climate change, the conversion of abundant solar energy into clean and renewable hydrogen fuel has gained significant attention. Among the various solar energy conversion technologies, particulate photocatalytic water splitting represents a promising and cost-effective approach for sustainable hydrogen production. In this study, we report the synthesis and application of Fe<sup>2+</sup> doped ZnFe<sub>2</sub>O<sub>4</sub> (FZFO)/TiO<sub>2</sub> core-shell nanospheres as a visible-light-active photocatalyst for solar-driven water splitting. The FZFO core was synthesized using a microwave-assisted solvothermal technique (MAST), enabling the formation of nearly monodisperse spherical nanoparticles (~100 nm) within 60 minutes at a relatively low temperature of 200 °C [1], [2]. Subsequently, a TiO<sub>2</sub> shell was grown on the FZFO core via a microwave-assisted method within 30 minutes, resulting in core-shell nanospheres with an average particle size of ~120 nm. The structural and morphological characteristics of the synthesized materials were confirmed by X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM), indicating high crystallinity and uniform spherical morphology. Diffuse reflectance spectroscopy (DRS) revealed an optical band gap in the range of 1.5–1.7 eV, suggesting efficient absorption in the visible and near-infrared regions of the solar spectrum [3]. Further to check the photoactivity of the prepared material, we tested under UV lamp and as a result we were able to generate significant amount of hydrogen and the produced gas was quantified using Gas chromatograph (GC). The photoelectrochemical behaviour of the FZFO/TiO<sub>2</sub> core-shell nanoparticles was investigated using chronoamperometry, Linear sweep voltammetry (LSV) and Mott-Schottky analysis. The results revealed a strong photoelectrochemical response (~2 μA/cm<sup>2</sup>) under visible light illumination, highlighting the potential of these core-shell structures for application in photocatalytic systems. Overall, the synthesized FZFO/TiO<sub>2</sub> core-shell nanospheres exhibit broad solar absorption n, and enhanced charge separation, making them a promising candidate for efficient solar hydrogen production.

# Nanoporous Anodic Alumina as a Novel Heterojunction Photocatalyst for photocatalytic water splitting

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## **Abstract**

With the rapidly increasing global energy demand, hydrogen is gaining recognition as a clean, renewable, and sustainable energy carrier, particularly when generated through photocatalytic water splitting. Unlike conventional hydrogen production methods that rely on fossil fuels, photocatalytic processes harness solar energy, offering an environmentally friendly pathway for large-scale hydrogen generation. In this work, Nanoporous Anodic Alumina (NAA) was fabricated via a controlled electrochemical anodization process. The optimized conditions enabled the formation of well-ordered pores with diameters ranging from 130 to 400 nm and precise regulation of the oxide layer thickness, achieved at a growth rate of approximately  $2.5 \mu\text{m h}^{-1}$ . The high specific surface area and regular pore geometry of NAA provide a robust template for the deposition of photocatalytic materials, ensuring uniform distribution and intimate interfacial contact along the pore walls. Such features are critical for enhancing photon absorption and improving photocatalytic activity. However, pristine NAA exhibits inherent drawbacks, including wide bandgap-induced UV activity and severe charge carrier recombination, both of which significantly limit photocatalytic performance. To overcome these limitations, a heterojunction architecture was developed by coupling NAA with a visible-light-responsive semiconductor. Cobalt-doped zinc ferrite (CZFO), a spinel oxide with a narrow bandgap, was integrated onto the NAA framework through a hydrothermal approach. The process resulted in conformal decoration of CZFO nanoparticles selectively along the pore walls and surface of NAA, thereby facilitating efficient charge separation, suppressing recombination, and extending light absorption into the visible region. The photocatalytic activity of pristine NAA and the NAA–CZFO heterostructure was systematically evaluated under UV irradiation. While bare NAA exhibited a modest hydrogen evolution rate of  $\sim 75 \mu\text{mol g}^{-1} \text{h}^{-1}$ , the NAA–CZFO system demonstrated a significantly enhanced rate of  $\sim 200 \mu\text{mol g}^{-1} \text{h}^{-1}$ . This marked improvement highlights the potential of heterojunction engineering as an effective strategy to design high-performance photocatalysts for solar-driven hydrogen production.

# Multifunctional Fluorophore Based on Fluorene-Bithiophene Architecture for Latent Print Visualization and Stimuli-Responsive Eco-friendly Security Inks

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## Abstract

Latent finger and lip prints serve as critical forms of physical evidence in forensic analysis due to their uniqueness, permanence, and ease of deposition. However, the effective visualization of these prints on various surface types, particularly on complex substrates, remains limited by current development techniques. Simultaneously, the growing threat of counterfeit goods that challenge consumer safety, erodes brand trust, and causes substantial economic losses has driven demand for smart, multi-level security materials. The present study addresses these dual requirements through the design and synthesis of a new multi-functional fluorophore with conjugated fluorene–bithiophene (BTAF) structural framework intended for latent finger mark and lip print visualization and as a pigment in security ink applications. This  $\pi$ -extended molecule combines the rigidity and photostability of fluorene with the electron-rich nature of bithiophene, resulting in strong, red-shifted solid-state fluorescence and high quantum yield. The fluorophore demonstrated excellent performance in visualizing latent finger and lip prints across porous, semi-porous, non-porous, and complex substrates. The optical and microscopic images developed using BTAF enabled both qualitative and quantitative analysis of intricate details of the latent prints. The interaction of BTAF with glycine and myristic acid, the key constituents of fingerprint residue on glass substrate, was explored through computational and molecular dynamics simulations, and the findings were further validated by ATR-FTIR spectral analysis. Furthermore, BTAF was incorporated into a composite eco-friendly ink formulation that exhibits excellent flow properties suitable for continuous printing, strong adhesion across diverse substrates, and high printability compatible with offset printing systems, enabling application in multilevel anti-counterfeiting systems for enhanced security. The security feature exhibits a reversible, dual-mode response; shifting from magenta to yellow under daylight when heated above 31 °C while consistently displaying green fluorescence under 365 nm UV light. The facile synthesis, low toxicity, and dual functionality with stable performance of BTAF make it a promising material for integration in smart forensic tools and advanced security printing technologies.

# Functionalization Strategies of TMDs for Enhanced Electrochemical Performance in Energy Applications

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## Abstract

Transition metal dichalcogenides (TMDs) with the general formula  $MX_2$  form a versatile class of two-dimensional layered materials that are increasingly recognised for their potential as advanced energy applications. Their intrinsic properties, such as high surface area, adjustable electronic structure, and strong redox activity, make them ideal candidates to bridge the performance gap between energy-dense batteries and power-dense capacitors. This superior pseudocapacitive behaviour arises from their flexible architecture, efficient ion transport channels, and the ability to host multiple oxidation states. Our current study aims to gain a deeper understanding of the advanced functionalization techniques, such as metal ion doping, heteroatom substitution, chemical group modification, and defect engineering, all of which improve conductivity, ion adsorption, and active site availability. These enhancements lead to higher capacitance, power density, and cycle stability. Further, combining TMDs with graphene, carbon nanotubes, MXenes, and conductive polymers improves electron mobility and mechanical strength, while incorporating metal nanoparticles boosts catalytic activity and charge-discharge performance. Recent progress in phase control, atomic-scale engineering, and compositional adjustments illustrates TMDs' adaptability in creating multifunctional electrode structures. Hence, all these modifications lead to TMDs as a frontrunner for long-life, scalable, and high-performance electrodes for energy applications.

## Engineering La-Doped $BiVO_4$ Photoanodes: Toward High-Efficiency Solar Hydrogen Production

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## Abstract

A major obstacle to the efficient photoelectrochemical (PEC) splitting of water with bismuth vanadate ( $BiVO_4$ ) photoanodes is its limited charge separation and transport, despite its favorable  $\sim 2.4$  eV band gap for visible light absorption. Here, we report on a study that used lanthanum (La) doping to improve the structural and PEC properties of  $BiVO_4$ . We prepared a series of doped samples across a range of concentrations (1-10%) and performed a detailed characterization. X-ray diffraction (XRD) confirmed that the material maintained its monoclinic phase but showed a decrease in crystallite size, which was attributed to lattice strain from the doping. Among the various samples, the 3% La-doped  $BiVO_4$

exhibited the best performance. It achieved a photocurrent density of 0.8 mA/cm<sup>2</sup>, this significant improvement is linked to a reduction in charge transfer resistance and enhanced stability. The findings are further supported by first-principles density functional theory (DFT) calculations, which provide a fundamental understanding of the role of La doping in boosting the PEC efficiency of BiVO<sub>4</sub>.

## **Multifunctional Luminescent Phosphors for Secure Glass Applications**

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### **Abstract**

There has been a significant increase in attention to the use of glass-based materials. Counterfeiting in glass refers to the fraudulent production of glass items that are intentionally designed to imitate superior-quality or branded glass products. Glass, due to its inherent clarity and chemically inert nature, is offered by its composition. This research focuses on developing an anti-counterfeiting system for glass, involving the synthesis and characterization of both the host and the security marker. First, undoped alumino-borosilicate (ABS) glass was synthesized, with its structural integrity confirmed by XRD, SEM, and FTIR analyses, establishing it as a suitable transparent platform. Followed by the synthesis of an upconversion (UC) phosphor, Ho<sup>3+</sup>/Yb<sup>3+</sup> co-doped Na-Gd-Zn fluoride (NZG), was synthesized as the covert marker. The structural and morphological properties were analyzed using XRD and SEM. Optimal co-doping yielded bright, non-replicable green UC emission when excited by a 980 nm near-infrared laser, recorded using a photoluminescence spectrometer. This provides a highly specific and non-replicable primary security layer that can be incorporated into glass to prevent counterfeiting. We utilize stable, transparent ABS as a canvas to embed the synthesized, reliable UC phosphor, resulting in a completely hidden light signature that simplifies and secures authentication. Future work will focus on integrating the synthesized materials into coatings and inks for industrial applications.

## **Two-Dimensional Metal–Organic Frameworks for Next-Generation Chemi-Resistive Gas Sensors**

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### **Abstract**

Reliable gas sensing technologies are essential for environmental monitoring, industrial safety, and healthcare applications. Conventional chemi-resistive sensors, although widely used, often suffer from poor selectivity, limited sensitivity, and high operating temperatures. Two-dimensional metal–organic frameworks (2D MOFs) present a promising alternative due to their ultrahigh surface area, tunable porosity, and chemical versatility. This poster outlines a research framework for the development of 2D

MOF-based chemi-resistive sensors. The approach involves the synthesis of conductive 2D MOFs, and the systematic study of gas–framework interactions. Structural and electronic properties will be investigated through advanced characterization techniques, complemented by density functional theory (DFT) calculations to gain insights into adsorption energies and charge transfer mechanisms. The expected outcome is the realization of room-temperature sensors with improved sensitivity, rapid response–recovery dynamics, and tailored selectivity toward target analytes such as NO<sub>2</sub>, NH<sub>3</sub>, and volatile organic compounds (VOCs). By combining material design with theoretical insights, this work aims to establish a design roadmap for MOF-based chemi-resistive sensors and highlight their potential for next-generation, low-power, and sustainable gas-sensing technologies.

## **Exploring the Biological Potentials of Green-Synthesized Zinc Oxide and Iron Oxide Nanoparticles: A Comprehensive Review"**

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### **Abstract**

Nanotechnology involves production as well as usage of material with nanoscale dimension for various applications. Nanomaterials are bestowed with exceptional physicochemical properties in comparison to their bulk counterparts, including extremely small size with large surface area coupled with the ease of fictionalization and tagging with multiple groups as well as extremely high tensile strength. However, environmental pollution and hazardous effects of synthetic nanoparticles have raised widespread concerns over their usage in various sectors. Due to these unanswerable issues and concerns, the field of science and technology is currently dominated by green nanoparticles, with increased efficacy and decreased toxicity owing to their biodegradable nature. The current review talks about two metallic green nanoparticles, namely, Zinc oxide and iron oxide and summarizes the various studies showing their plant based biosynthesis as well as their applications like anticancer activity, antimicrobial activity, usage in wastewater treatment as well as usage in agriculture and plant biotechnology.

## **Forensic Electrochemical Detection of Promethazine as a Misused OTC Sedative Mimicking Club Drugs Using Graphene-Modified Electrodes**

*Nandini Chauhan*

### **Abstract**

Promethazine, a commonly available over-the-counter (OTC) antihistamine with sedative and hypnotic properties, has emerged as a substance of interest in forensic toxicology due to its potential misuse as an alternative to club drugs. Its easy accessibility in pharmacies and ability to induce sedation, relaxation, and drowsiness make it susceptible to recreational abuse, mimicking some effects of traditional club drugs. This study presents a sensitive voltametric method for detecting promethazine in various solvent systems using graphene-modified glassy carbon electrodes. The graphene modification enhances electron transfer rates and surface area, significantly improving detection sensitivity and selectivity. Optimised cyclic and differential pulse voltammetry techniques offer nanomolar-level detection limits, with rapid response times and minimal interference. The robust and portable nature of the sensor lends itself well to forensic on-site applications, enabling timely screening of promethazine in pharmaceutical formulations,

biological fluids, and seized drug samples. This addresses a growing forensic need to detect not only illicit substances but also increasingly misused OTC compounds. The technology supports law enforcement and forensic experts in monitoring promethazine misuse, mitigating public health risks, and providing reliable evidence in judicial processes. By combining advanced electrochemical sensing with forensic applicability, this research offers a crucial tool for combating novel drug abuse patterns involving OTC medications like promethazine.

## **A comprehensive study on structure, properties, synthesis and characterization of ferrites**

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### **Abstract**

The research on ferrites is fast moving owing to their exponentially growing usage in magnetic shielding, magnetic biosensors, magnetic recording devices, information storage, mobile communication, electronic devices, gyromagnetic device, medical devices, transformers, pollution control, catalysis, and pigments. This review comprises the present state of the art on hexagonal ferrites (HFs) and spinel ferrites (SFs). The article covers the background, properties, classification schemes, synthesis and characterization of ferrites. It focuses on a comparative understanding of four synthesis routes, magnetic properties and characterization of the ferrites. The article emphasizes X-ray diffraction, scanning electron microscopy, transmission electron microscopy, vibrating sample magnetometer, spectroscopy, thermal analysis and vector network analyser results. The present work is meant for the faster understanding of this research area.

## **Influence of MgO Nanoparticles Loading Epoxy Composite on Dielectric and Relaxation Behavior**

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### **Abstract**

Polymer nanocomposites have attracted attention for their improved electrical, thermal, and mechanical properties. On the other hand, the shortcomings of pure epoxy, including low thermal stability, brittleness, and low electrical conductivity hindered its use in advanced electrical applications. To mitigate these issues, magnesium oxide (MgO) nanoparticles were introduced into the epoxy matrix to improve the main material performance. The structural, dielectric, conductive, and relaxational properties of neat epoxy (NE) and MgO/epoxy nanocomposites containing 1 wt.%, 5 wt.%, and 10 wt.% of MgO were investigated in this article. XRD and SEM structural analysis showed that MgO had a crystalline character and that it was distributed uniformly in the epoxy matrix. The dielectric properties revealed that dielectric constant ( $\epsilon'$ ) was maximum for composite with 5 wt.% of MgO, and the electrical modulus ( $M''$ )

was maximized at 10 wt.% of MgO. The AC conductivity increased with frequency and showed hopping conduction; the AC conductivity was the highest value observed with 5 wt.% MgO. In conclusion, the results of this study suggest that the MgO nanoparticles can modify the dielectric and conductive performance of epoxy in a beneficial way. The Epoxy/MgO polymer nanocomposites could have valuable potential for applications as sensors, capacitors and insulating materials.

## **A comprehensive review for catalytic potential of Schiff base metal complexes in oxidation reactions**

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### **Abstract**

Schiff base and their metal complexes are synthesized by condensation of an amino group with carbonyl group followed by complexation with metal ion have garnered significant attention for their versatile activities for biological as well as chemical process. The chemical catalytic potential of Schiff base metal complexes for oxidation reactions due to their versatile coordination chemistry and ability that enhance catalytic processes. Over the past few years, there have been several reports published for homogeneous and heterogeneous Schiff base metal catalyst for different chemical transformation. This review compiles the catalytic applications of these complexes, particularly in the oxidation of organic sulfides, toluene, alkanes, and benzylic alcohols. The complexes demonstrate remarkable stability and efficiency, with recent advancements and innovative approaches further improving their performance. These findings underscore the potential of Schiff base metal complexes as promising catalysts for sustainable oxidation technologies.

## **Layered double hydroxide for sustainable water clean-up –A review**

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### **Abstract**

Water pollution has emerged as one of the most critical environmental issues worldwide, primarily due to the rapid growth of population, industrialization, and urbanization. The continuous discharge of untreated effluents, agricultural runoff, pharmaceutical residues, and domestic sewage has led to the accumulation of harmful pollutants in aquatic ecosystems. These contaminants not only deteriorate water quality but also pose severe risks to human health, aquatic life, and ecological balance. Among the common pollutants, heavy metals such as arsenic, lead, cadmium, and chromium are highly toxic and persistent, while organic pollutants, including dyes, pesticides, antibiotics, and pharmaceutical compounds, contribute to antimicrobial resistance, bioaccumulation, and long-term ecological damage.

To address these challenges, advanced materials and technologies are being developed for efficient water treatment. Layered Double Hydroxides (LDHs), also known as hydrotalcite-like compounds, have gained significant attention as promising adsorbents and catalysts for pollutant removal. Additionally, LDH-based composites with biochar, metal oxides, or carbonaceous materials have shown enhanced stability, reusability, and adsorption capacity, making them suitable for large-scale water treatment applications. The integration of LDHs in water purification systems offers a sustainable and eco-friendly pathway for mitigating water pollution. By effectively addressing a wide spectrum of pollutants, LDH-based materials provide opportunities for safe water reuse, environmental protection, and the development of cleaner technologies to ensure global water security.

## **Characterisation of green-synthesised silver nanoparticles of *Murraya koenigii* along with their antioxidant property: a sustainable approach**

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### **Abstract**

Nanobiotechnology leverages nanoscale materials for a wide range of applications, including materials engineering, healthcare, and environmental remediation. Oxidative stress, caused by an imbalance of reactive oxygen species (ROS) and reactive nitrogen species (RNS), is a natural byproduct of cellular metabolism. When ROS and RNS are produced in excess and not sufficiently neutralised by the body's antioxidant defence system, they can lead to significant damage to lipids, proteins, and DNA, contributing to cellular injury and the onset of various chronic diseases. Maintaining a balance between free radicals and antioxidants is crucial for overall health, and effective regulation of oxidative stress plays a pivotal role in disease prevention and treatment. This study investigates the synthesis of silver nanoparticles using *Murraya koenigii* leaf extract (MKLE-AgNPs) through a green approach and characterises their properties via UV-Vis spectrophotometry, HR-TEM, FE-SEM, EDX, and FTIR. The UV-Vis spectrum confirmed nanoparticle formation with a surface plasmon resonance (SPR) peak at 450 nm. HR-TEM imaging and the selected area electron diffraction (SAED) pattern revealed that the nanoparticles were spherical, with a narrow size distribution (40–55 nm) and a crystalline structure. FE-SEM analysis showed spherical particles (90%), and EDX confirmed the presence of elemental silver (89.94 weight %). FTIR spectroscopy identified the functional groups involved in the reduction and stabilisation of the nanoparticles. The *in-vitro* antioxidant potential of MKLE-AgNPs was assessed through DPPH, ABTS, and FRAP scavenging assays, demonstrating dose-dependent scavenging activity with IC<sub>50</sub> values of almost 266, 134, and 112 µg/ml, respectively. These results highlight the eco-friendly synthesis of MKLE-AgNPs and suggest their moderate antioxidant properties.

# Investigation of the dehydrogenation reaction mechanism of catalyzed $\text{Mg}(\text{AlH}_4)_2$ by bimetallic oxides of alkali- transition metal

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## **Abstract**

Complex metal hydrides are also a fascinating choice as hydrogen storage materials because of their high gravimetric hydrogen capacity and variable thermodynamics properties. In this experiment, we have prepared a solvent-free  $\text{Mg}(\text{AlH}_4)_2$  matrix through a mechanochemical process of metathesis. To increase the sorption kinetics, 10 wt.% of  $\text{NaNbO}_3$  and  $\text{KNbO}_3$  were doped in the  $\text{Mg}(\text{AlH}_4)_2$  matrix. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM) confirmed the efficient incorporation of catalysts into the  $\text{Mg}(\text{AlH}_4)_2$  matrix. This wide mixing enhances the uniformity of the catalytic activities as it enhances the interface between the catalyst and the pure material. Thermal techniques, i.e. thermal desorption mass spectrometry (TDMS), thermal gravimetric analysis (TGA) and differential thermal analysis (DTA), indicated that both catalyzed and un-catalyzed systems desorbed in two steps. The desorption temperature dropped to 163.3°C and 171.0°C compared with 178.4°C (5°C/min) with the addition of  $\text{NaNbO}_3$  and  $\text{KNbO}_3$  respectively that indicate the justification of better desorption kinetics. The extent of structural and spectroscopic measurement was done through XRD, FTIR and XPS to identify the background reaction mechanism of the two decomposition reactions. In particular, the XPS demonstrated that the amounts of Na, K, Nb stay inactive at the surface, which suggests that the relationship between catalyst surfaces can be enhanced. Despite all these improvements, the positive Gibbs free energy ( $\Delta G$ ) of reverse reaction limits its ability to store hydrogen in a reversible form. The results are consistent and this implies that though there is an increment in the kinetics of desorption with the inclusion of catalysts, there is need to engage in more studies to understand the catalytic mechanism so that more can be done to improve.

# Advanced Catalysis Strategies for Improving Reversible Hydrogen Storage in $\text{Mg}(\text{BH}_4)_2$

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## Abstract

Magnesium borohydride ( $\text{Mg}(\text{BH}_4)_2$ ) is a promising material for hydrogen storage because it can grasp a very vast amount of hydrogen by weight. However, in its pure form it releases hydrogen only at high temperatures and often too slowly for practical use. It can also show poor reversibility (putting hydrogen back in) after cycling. To make  $\text{Mg}(\text{BH}_4)_2$  useful for real-world hydrogen systems, researchers add small amounts of catalysts that change the way the material breaks down and re-forms, so hydrogen can be released and stored at lower temperatures, faster, and with better long-term stability.

Two families of oxide catalysts that have shown particular promise are perovskites (crystal formula  $\text{ABO}_3$ , e.g.,  $\text{NaNbO}_3$ ,  $\text{KNbO}_3$ ,  $\text{CaTiO}_3$ ) and spinel oxides (general formula  $\text{AB}_2\text{O}_4$ , e.g.,  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ ). These catalysts work in several complementary ways: they provide surfaces and interfaces that weaken the chemical bonds holding hydrogen in the borohydride, they offer alternative lower-energy reaction pathways, and they can facilitate the transport of ions or electrons needed for the chemical transformations. Structurally, perovskites often supply flexible lattice sites and oxygen vacancies that interact strongly with hydrogen-containing species, while spinels offer robust, often mixed-valence metal sites that can participate in redox steps and stabilize intermediate products. Both types of catalysts can also prevent particle sintering, increase active surface area, and create nano-scale contact with  $\text{Mg}(\text{BH}_4)_2$  — all factors that enhance the rate and extent of hydrogen release and uptake. Experimental studies typically report that adding perovskite or spinel catalysts lowers the dehydrogenation temperature, increases hydrogen desorption rates, and improves the number of reversible cycles compared to uncatalyzed  $\text{Mg}(\text{BH}_4)_2$ . Remaining challenges include fully understanding detailed atomic-scale mechanisms, optimizing catalyst composition and loading for the best balance of performance and weight, and ensuring long-term cycling stability under down-to-earth conditions.

# **Track - III**

## **Materials Modelling & Simulation**

# Impact of Electric Vehicle Charging Loads on Radial Distribution Networks: A Power Flow and Cost Analysis

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## Abstract

The rapid uptake of electric vehicles (EVs) poses enormous challenges to current power distribution systems, particularly with respect to voltage stability, network losses and operational costs. This study examines clustered EV charging stations on a 33-bus radial distribution feeder using a backward–forward sweep (BFS) power flow algorithm. A set of realistic EV load profiles were used to inject into the system model to assess the variations in bus voltages, total system losses, and daily charging costs over the baseline without EV load. The results show a marked decrease in minimum bus voltages and an overall increase in network losses from the baseline of zero EV loads providing strong evidence of potential stress on the existing distribution infrastructure. The conclusions drawn from these findings indicate that utility operators could benefit from some form of EV charging management, increased infrastructure reinforcement, and demand-side initiatives in order to offer reliable and cost-effective operation of the grid with an influx of EVs onto the networks.

# Design and Theoretical Analysis of a Bi-Core Hexagonal Photonic Crystal Fiber Sensor for Refractive Index-Based Chemical Detection

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## Abstract

In this paper, we propose and theoretically analyze a refractive index–based bi-core hexagonal photonic crystal fiber (BC-PCF) sensor for detecting chemical analytes with refractive indices ranging from 1.33 to 1.38. In this work, water, propane, ether, ethanol, acetic acid, and propanol with different refractive indices are considered as chemical analytes, as their RI values play a crucial role in determining the sensing performance of the proposed sensor. In this sensor, two independent waveguides are created because of the presence of a central elliptical hole and two solid cores. This elliptical hole acts as a sensing channel where different chemical analytes are placed. As a result, variations in the refractive indices of the chemical analytes cause a shift in the peak wavelength within the transmission spectrum, which can be explained by the mode coupling theory. The performance of the proposed PCF sensor has been numerically analyzed using the full-vector finite element method (FV-FEM) across the wavelength range of 1.5 – 2.2  $\mu\text{m}$ . The numerical analysis of the proposed sensor demonstrates a maximum wavelength sensitivity of 8000 nm/RIU under x-polarization with less coupling length and better than published previous works, which is the main feature of the proposed sensor. Additionally, maximum effective mode index difference values for x-polarization are  $4.95 \times 10^{-3}$ ,  $5.24 \times 10^{-3}$ ,  $5.56 \times 10^{-3}$ ,  $5.92 \times 10^{-3}$ ,  $6.32 \times 10^{-3}$  and  $6.76 \times 10^{-3}$  for water, propane, ether, ethanol, acetic acid, and propanol respectively and

the highest coupling length values for x-polarization are  $2.21 \times 10^{-4}$  m for water,  $2.09 \times 10^{-4}$  m for propane,  $1.97 \times 10^{-4}$  m for ether,  $1.85 \times 10^{-4}$  m for ethanol,  $1.73 \times 10^{-4}$  m for acetic acid, and  $1.85 \times 10^{-4}$  m for propanol. This sensor design offers high sensitivity and a short coupling length, making it suitable for various applications in the chemical field.

## Charge-Transfer Interactions of 4-Amino-1,2,4-Triazole Derivatives with DMAD: A Combined Spectroscopic and Computational Study

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### Abstract

Six new charge-transfer (CT) complexes of 4-amino-1,2,4-triazoles [1–3] with dimethyl acetylenedicarboxylate (DMAD) [4] were synthesized and systematically investigated in DMF and DMSO solvents at room temperature. The synthesized complexes were characterized by UV–vis, FT-IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, HRMS, and conductivity measurements. Spectrophotometric analysis revealed distinct absorption bands in the visible region (434–537 nm), attributed to  $n \rightarrow \pi^*$  transitions, along with additional  $\pi \rightarrow \pi^*$  transitions in the ultraviolet region (249–404 nm). These spectral features confirmed the charge-transfer nature of the complexes. Job's continuous variation method indicated the formation of stable 1:1 CT complexes. The formation constants and molar extinction coefficients, determined by the mole-ratio method and the Benesi–Hildebrand equation, showed a clear dependence on the substituent present on the triazole ring. Among the three donors, 4-amino-5-(4-pyridyl)-1,2,4-triazole-3-thiol [3] produced the most stable CT complex, followed by 4-amino-5-phenyl-1,2,4-triazole-3-thiol [2], while the unsubstituted 4-amino-1,2,4-triazole [1] gave comparatively weaker complexes.

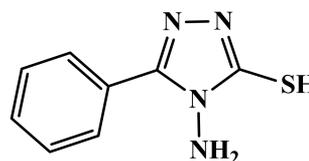
In both DMF and DMSO solvents, higher formation constant values and more negative free energy ( $\Delta G^\circ$ ) were observed for the pyridyl-substituted derivative, confirming its spontaneous and strong complexation with DMAD. In contrast, the unsubstituted triazole showed less negative  $\Delta G^\circ$  values, consistent with its weaker donor capacity. The lower transition energy ( $E_{\text{CT}} = 2.43$  eV) obtained for the pyridyl-substituted system, compared to the phenyl-substituted and unsubstituted analogues, further reflected stronger donor–acceptor interactions. The donor strength of the studied triazoles was also examined theoretically at the B3LYP/6-31+G(d) level using the Gaussian 16 program. Consistent with experimental findings, 4-amino-5-(4-pyridyl)-1,2,4-triazole-3-thiol exhibited the highest HOMO energy, the lowest HOMO–LUMO energy gap ( $\Delta E$ ), and the most favourable global reactivity descriptors—chemical softness and chemical potential—demonstrating its superior electron-donating ability. The phenyl-substituted triazole showed intermediate donor strength, while the unsubstituted 4-amino-1,2,4-triazole was the weakest donor of the series.

The higher values of formation constants recorded in DMSO compared to DMF indicated the formation of more highly stable complexes in this solvent. This enhanced stability can be attributed to the stronger solvation ability and higher polarity of DMSO, which better stabilizes the charge-separated donor–acceptor species, thereby favoring complex formation.

The combined spectroscopic and theoretical results thus highlighted a clear substituent effect, establishing the order of donor capacity as: pyridyl-substituted > phenyl-substituted > unsubstituted triazole. This trend underlines the potential of pyridyl-substituted triazole derivatives as highly efficient

donors for CT complex formation, with promising applications in sensing, molecular electronics, and functional material development.

**Donors**

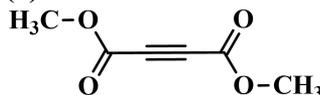


(1)

(2)

(3)

**Acceptor**



(4)

**Solvents**

DMF, DMSO

## Fenton Oxidation Optimization for Effective Decolorization of Congo Red and Reactive Yellow 84: A Comparative Study

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### Abstract

This study investigates and compares the efficiency of the Fenton oxidation process for the decolorization of two structurally different textile dyes: Congo Red (CR), an anionic azo dye with a relatively simple molecular structure, and Reactive Yellow 84 (RY84), a more complex bifunctional reactive dye. Batch experiments were systematically conducted to evaluate the influence of key process variables, including initial dye concentration (50–150 mg/L), ferrous ion (Fe<sup>2+</sup>) dosage (0.002–0.01 M), hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) concentration (0.01–0.05 M), solution pH (2–4), and reaction time (0–60 minutes).

The optimal decolorization conditions for both dyes were found to be an acidic pH of approximately 3, Fe<sup>2+</sup> concentration around 0.005–0.01 M, and H<sub>2</sub>O<sub>2</sub> concentration near 0.02 M. Under these conditions, Congo Red achieved a maximum decolorization efficiency of about 95% within 60 minutes, while Reactive Yellow 84 reached approximately 92% over the same period. The results highlight that the simpler molecular structure of Congo Red makes it more susceptible to oxidative degradation compared to the bulkier, more complex RY84. This comparative study underscores the effectiveness of the Fenton process for treating structurally diverse dyes and emphasizes the need for process optimization based on dye characteristics. The findings provide practical insights into improving advanced oxidation processes for textile wastewater treatment, particularly in scenarios involving mixed dye effluents.

# Squirmers Dynamics Near Convex Obstacle: A Combined Simulation and Far-Field Approach

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## Abstract

Microswimmers are microscopic objects that have the ability to convert environmental energy into locomotion. Their applications include biomedical uses, targeted drug delivery, microsurgery, cell manipulation, as well as environmental and materials science uses. Locomotion of the microswimmers is very well understood experimentally and theoretically for uniform, homogeneous environments. However, active swimming usually involves complex conditions such as complicated geometries, obstacles, chemical gradients, external stimuli, and fluid flow. Investigating the characteristics of the microswimming in these challenging conditions is essential for designing real-life applications. Using Multi-Particle Collision Dynamics (MPCD), the hydrodynamics of a spherical microswimmer, squirmer, near an irregular boundary characterised by a convex bump is explored. We observe that the motion of a squirmer is a combination of movement near a flat wall and a spherical obstacle. The neutral squirmer always moves away from the surface. In comparison, the pusher can stick to the front part of the obstacle as well as the back of the bump. Depending on the value of the  $\beta$ , the puller shows a variety of trajectories. For the theoretical analysis, the flowfield generated by the squirmer near the boundary is constructed using the far-field approximation. The squirmer is considered a combination of force-dipole, source dipole, and force quadrupole. No-slip boundary conditions are satisfied using the method of images by combining Blake image, and spherical obstacle image with the squirmer's flowfield. Comparison between simulation and analytical outcomes reveals that the near-field forces play an important role in the squirmer's motion. We incorporated lubrication terms to obtain trajectories identical to the simulated motion. We measured the scattering angle from simulation, which agrees with analytical calculations done using Faxen's law and far-field approximation.

# First-Principles Investigation of Structural, Mechanical and Optoelectronic Properties of Ca<sub>3</sub>PI<sub>3</sub>

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## Abstract

This piece of work is a systematic examination of the structural, electronic, optical, and mechanical behaviour of Ca<sub>3</sub>PI<sub>3</sub> perovskite type substance, utilizing WIEN2k simulation package via density functional theory using PBE\_sol exchange-correlation functional. The computed lattice parameter was found to be 6.10 Å, while the bulk modulus was estimated to be 35.00 GPa, showing the medium structural rigidity. The electronic band structure indicates a direct bandgap of 1.32 eV, indicating good potential for opto-electronic applications. The optical parameters yield distinctive results with static dielectric constant,  $\epsilon_1(0) = 0.63$ , static refractive index,  $n(0) = 0.25$ , and reflectivity of 18% at zero photon energy. In addition, the elastic constants were also determined to examine the mechanical stability of Ca<sub>3</sub>PI<sub>3</sub>, and potential for practical application. These results clearly indicate that Ca<sub>3</sub>PI<sub>3</sub> is a promising candidate for future applications in opto-electronic and photonic devices.

## Performance Enhancement of Perovskite Solar Cells Using Al<sub>2</sub>O<sub>3</sub> Anti-Reflection Coating: A Simulation Study

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## Abstract

In this work OghmaNano simulation tool is used to compute the optical performance of perovskite solar cell, a renewable energy device, designed with the following structure: FTO/TiO<sub>2</sub>/MAPbI<sub>3</sub>/Spiro-OMeTAD/Au. For this device structure, the computed results show a Fill Factor (FF) = 0.686, a Power Conversion Efficiency (PCE) = 25.37%, an Open-Circuit Voltage (Voc) = 1.044 V, and a Short-Circuit

Current Density ( $J_{sc}$ ) = -354 mA/cm<sup>2</sup>. To further increase light harvesting and mitigate optical reflection losses off the front surface, a 10 nm Al<sub>2</sub>O<sub>3</sub> Anti-Reflection coating was included as top layer of the device. After this modification the device performance improved significantly and the modified FF, PCE, Voc, and  $J_{sc}$  were found to be 0.433, 46.18%, 1.074 V, and 990 mA/cm<sup>2</sup>, respectively. Thus, this work shows significant improvement in the performance (~80% increment in the PCE) of the device based on the introduction of the Anti-Reflection layer of Al<sub>2</sub>O<sub>3</sub>.

## **First-Principles Investigation of the Structural, Optoelectronic, and Thermoelectric Properties of Lead-Free Cs<sub>2</sub>AgSbBr<sub>6</sub> Halide Double Perovskite**

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### **Abstract**

The halide double perovskite Cs<sub>2</sub>AgSbBr<sub>6</sub>'s structural, electronic, and optical properties are studied in detail with first-principles density functional theory (DFT) in the local spin-density approximation (LSDA) using WIEN2k simulation code. The optimized lattice constant is determined to be 10.95 Å. The bulk modulus is 33.89 GPa, implying moderate mechanical stability. The computed electronic band structure displays an indirect bandgap of 1.67 eV (L–X), which compares favorably to available experimental data, establishing confidence in the methods, as well as potential applicability in optoelectronic and photovoltaic devices. The optical analysis corresponds to a static dielectric constant  $\epsilon_1(0) = 0.42$ , refractive index  $n(0) = 0.20$ , and reflectivity  $R(0) = 12\%$ . Further, the thermoelectric figure of merit (ZT) is comparatively higher at lower temperatures and decreases as temperature increases, indicating relatively good thermoelectric performance at lower temperatures. These results show that Cs<sub>2</sub>AgSbBr<sub>6</sub> is a promising lead-free multifunctional optoelectronic and thermoelectric material.

# Substrate Effects on Performance Enhancement in a Gap Coupled E-Shaped Microstrip Antenna with Air gap for S-Band Applications

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## Abstract

This study presents the design, simulation, and comparative analysis of an E-shaped gap-coupled microstrip patch antenna incorporating a 5.9 mm air gap between dual substrates, tailored for S-band applications. The insertion of the air gap is intended to enhance impedance matching and broaden the usable bandwidth by reducing effective permittivity and altering field distributions. We investigate the effect of three substrate materials—RT/Duroid 5880, RO 4003, and FR-4—on key performance metrics: bandwidth, gain, radiation efficiency, and axial ratio. Through detailed electromagnetic simulations, we examine how the differing dielectric constants and loss tangents influence current distribution, field confinement, surface-wave excitation, and coupling behavior. Our comparative results demonstrate that the low-permittivity, low-loss RT/Duroid substrate yields superior radiation efficiency and gain, and delivers the broadest fractional bandwidth, whereas the higher- $\epsilon$ , higher-loss FR-4 exhibits significantly degraded performance. RO 4003 offers an intermediate tradeoff. These findings provide practical design guidelines for substrate selection in S-band patch antennas, especially in configurations employing air-gap coupling, and underscore the critical interplay between dielectric properties and antenna performance.

# Polyamine Modified Metal Organic Frameworks MIL-101(Fe)-NH<sub>2</sub> for CO<sub>2</sub> Adsorption Applications

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## Abstract

MIL-101(Fe) based MOFs were successfully synthesized and modified with amine functional groups using solvothermal reaction of FeCl<sub>3</sub>·6H<sub>2</sub>O in DMF at 110 °C. Structural, thermal, morphological, and textural analyses confirmed successful incorporation of amines while preserving the MOFs framework. The elemental analysis of the prepared MIL-101(Fe)-NH<sub>2</sub> product was found as C, 38.35%; H, 1.98%; N, 5.61%. Then 500 mg of methanol exchanged MIL-101(Fe)-NH<sub>2</sub> was activated by heating in oven for 2 hr at 100 °C. Subsequently, the PEI solution containing 50 wt% water was added to the dispersed material to achieve 10, 25, 35, 50, 75, and 100 wt% PEI vs MIL-101(Fe)-NH<sub>2</sub>. The mentioned proportions were

prepared with different number of PEI-X monomer units (X= 800, 1200, and 2000). Then the samples were collected and grinded and the samples were noted as MIL-101(Fe)-NH<sub>2</sub>-PEI-X-Y (X=800, 1200, 2000; Y=10,25, 35, 50, 75). Before the adsorption studies, the samples were activated by evacuation at 100°C for 24h to remove the guest molecules from the cavities. The nitrogen adsorption isotherm for desolated samples were collected in a relative pressure range from  $p/p_0 = 0.005$  to 1. Based on the nitrogen adsorption isotherms, the BET specific surface areas ( $S_{BET}$ ) and pore volumes ( $V_p$ ) of the samples were evaluated. CO<sub>2</sub> adsorption at low pressures revealed that optimal uptake was achieved and amine modified MIL-101(Fe) has excellent potential as an CO<sub>2</sub> absorber.

## **Finite Element Analysis on the Tunability of Thermomechanical Properties in Cu doped NiTi Shape Memory Alloy**

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### **Abstract**

This investigation evaluates the thermomechanical behavior of NiTi Shape Memory Alloys (SMAs) with varying copper additions (i.e. NiTi, NiTiCu<sub>1</sub>, NiTiCu<sub>3</sub>, NiTiCu<sub>5</sub>, NiTiCu<sub>7</sub>, and NiTiCu<sub>10</sub>) through comparative finite element method (FEM) modeling within the ANSYS platform. The study is specifically aimed at measuring the Shape Memory Effect (SME) hysteresis and energy dissipation capacity for both tensile (equivalent stress) and shear loading. Results show a clearly delineated, progressive trend that as copper content increases, functional stability improves. Quantitatively, the maximum stress applied to achieve deformation progressively decreases as in the case where peak equivalent stress decreased from a maximum of 1135.9 MPa for NiTi to 1083.8 MPa for NiTiCu<sub>10</sub> for all loading modes, while the area within hysteresis loop decreases significantly (tensile energy dissipation decreased by approximately 57% from NiTi to NiTiCu<sub>10</sub>). Additionally, residual deformation observed at the end of mechanical unloading decreased significantly following the initial addition of copper. This discovery indicates that Cu is an effective element to control the transformation profile of NiTi. Therefore, this research supports Cu's inclusion in customizing thermomechanical properties of NiTi for specific engineering applications to provide some trade-off between low energy loss and functional stability versus high energy dissipation.

# **Track - IV**

## **Biomaterials and Technology**

# Nanoparticles for Latent Fingerprint Development – A Review

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## Abstract

The advancement of forensic science relies heavily on the ability to effectively visualize latent fingerprints, which are crucial for criminal identification and investigation. Traditional fingerprint development techniques often involve chemical reagents that are hazardous, costly, and environmentally damaging. In light of these challenges, there has been a growing interest in the green synthesis of nanoparticles using plant waste materials as an innovative and sustainable alternative. This review paper comprehensively examines the current state of research on the green synthesis of nanoparticles for latent fingerprint development, emphasizing the utilization of plant waste. The review explores various types of plant waste, such as fruit peels, leaves, and stems, highlighting their potential as natural reducing and stabilizing agents in nanoparticle synthesis. The biochemical mechanisms underlying the reduction process and the properties of the resulting nanoparticles are discussed in detail. Characterization techniques, including UV-Vis spectroscopy, X-ray diffraction (XRD), and electron microscopy (SEM and TEM), are evaluated for their effectiveness in confirming the size, morphology, and crystalline nature of the synthesized nanoparticles. A critical analysis of the application of these biogenic nanoparticles in fingerprint development is provided, with a focus on their performance across different substrates such as glass, metal, and plastic. Comparative studies reveal that nanoparticles derived from plant waste offer enhanced visualization of fingerprint ridges with improved contrast and detail, outperforming some conventional methods. The review also addresses the environmental and economic benefits of using plant waste, underscoring the alignment with green chemistry principles and the potential for cost savings in forensic laboratories. Challenges and limitations in the current research are identified, including variability in plant waste composition and the need for standardization in synthesis protocols. Future directions are proposed, emphasizing the need for further optimization of synthesis processes, exploration of diverse plant waste sources, and extensive field testing to validate the practical applicability of this technology. In conclusion, the green synthesis of nanoparticles from plant waste presents a promising and sustainable approach for latent fingerprint development. This review highlights the dual benefits of environmental sustainability and forensic efficacy, advocating for continued research and development in this innovative field. The adoption of plant waste-derived nanoparticles could revolutionize fingerprint development techniques, making them more eco-friendly and accessible worldwide.

# Biosynthesis of silver Nanoparticles using *Lagenaria siceraria* peel extract and their antimicrobial effects

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## Abstract

The green synthesis of silver nanoparticles (AgNPs) offers an eco-friendly alternative to conventional physicochemical methods that often involve hazardous chemicals. In this study, *Lagenaria siceraria* (bottle gourd) peel extract, a low-cost agricultural waste rich in bioactive phytochemicals, was employed as a reducing and stabilizing agent for AgNPs biosynthesis. The synthesis was confirmed by UV-Vis spectroscopy, functional group analysis via FTIR, morphological examination by SEM, and surface charge determination through zeta potential analysis. The antimicrobial potential of the biosynthesized AgNPs was evaluated against bacterial (*Bacillus subtilis* (*B. subtilis*), *Escherichia coli* (*E. coli*), *Pseudomonas aeruginosa* (*P. aeruginosa*), *Klebsiella pneumonia* (*K. pneumonia*), *Staphylococcus aureus* (*S. aureus*)) and fungal (*Candida albicans* (*C. albicans*), *Aspergillus niger* (*A. niger*)) strains using the agar well diffusion method. The nanoparticles exhibited significant, dose-dependent antimicrobial activity, with maximum inhibition observed against *B. subtilis* (zone of inhibition:  $21 \pm 0.6$  mm) followed by *E. coli*, *P. aeruginosa*, *K. pneumoniae*, and *S. aureus*. Among the fungi, *C. albicans* showed greater susceptibility ( $18 \pm 0.4$  mm) compared to *A. niger*, which may be attributed to structural differences in their cell walls. The results indicate that *L. siceraria* peel-derived AgNPs possess broad-spectrum antimicrobial properties, while providing a sustainable route for the valorization of agro-waste. This approach aligns with circular economy principles, offering potential applications in biomedical formulations and environmental disinfection strategies.

## Biosynthesis of Silver Nanoparticles using *Lagenaria siceraria* (Bottle gourd) Seed Extract and their Antimicrobial Effects

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## Abstract

Nanotechnology has significantly advanced various scientific domains by leveraging the distinctive properties of nanoparticles. The green synthesis of silver nanoparticles (AgNPs) offers an environmentally sustainable alternative to conventional chemical and physical methods, utilizing plant-derived biomolecules as natural reducing and stabilizing agents. This study explores the biosynthesis of AgNPs using *Lagenaria siceraria* (*L. siceraria*, bottle gourd) seed extract, an underutilized agricultural byproduct, and evaluates their antimicrobial properties. AgNPs were synthesized by reacting a silver nitrate ( $\text{AgNO}_3$ ) solution with the seed extract under controlled conditions. Characterization techniques, including UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDS), and zeta potential analysis, were employed to assess the physicochemical properties of the nanoparticles. Their antimicrobial

efficacy was tested against five bacterial strains (*Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*) and two fungal species (*Candida albicans*, *Aspergillus niger*) using agar well diffusion and minimum inhibitory concentration (MIC) assays. Formation of AgNPs was confirmed by a strong surface plasmon resonance (SPR) peak at 420 nm. FESEM imaging revealed spherical nanoparticles with diameters ranging between 20 and 50 nm, while EDS analysis indicated 98.5% elemental silver content. FTIR spectra confirmed the presence of hydroxyl, carbonyl, and amine functional groups, which contributed to nanoparticle stabilization. Zeta potential measurements recorded a charge of  $-28.5$  mV, indicating high colloidal stability. Antimicrobial testing demonstrated inhibition zones ranging from 8 to 15 mm, with *S.aureus* (12 mm) and *E. coli* (14 mm) exhibiting the highest susceptibility. MIC values varied between 50 and 250  $\mu\text{g/mL}$ , while *C. albicans* (15 mm) exhibited slightly greater inhibition than *A. niger* (14 mm). These findings highlight the potential of *L. siceraria* seed extract as a cost-effective and sustainable bioresource for AgNP synthesis. The study underscores its applicability in antimicrobial treatments, agriculture, and food preservation, contributing to agricultural waste valorization and promoting eco-friendly nanotechnology.

## Study of antibacterial behavior of chitosan-gelatin based hydrogels and its characterization

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### Abstract

Wound healing remains a clinical challenge due to infection risk and the limited effectiveness of conventional dressings. Hydrogels, with high water absorption, biocompatibility, and capacity for drug delivery, have emerged as promising alternatives. This study was to develop chitosan–gelatin composite hydrogels incorporated with bioactive agents, such as quercetin and catechol. The hydrogels were optimized to evaluate its physicochemical and antimicrobial properties. It was examined for solubility, gel fraction, swelling behavior, and water retention capacity under physiological conditions, with statistical analysis performed using ANOVA followed by Tukey’s test. Structural characterization was carried out using Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) to assess chemical bonding and molecular interactions, while scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDAX) were employed to investigate surface morphology and elemental composition. Antimicrobial activity was evaluated using disc diffusion and *in vitro* antibacterial assays against drug-resistant bacterial strains including *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, and *Bacillus subtilis*. The bioactive-loaded hydrogels demonstrated enhanced performance compared to controls. The catechol-incorporated formulation exhibited water absorption of 730%, solubility of 94.57%, gel fraction of 64.11%, and water retention capacity of 86.48%. FTIR confirmed the functional group peaks of the hydrogel matrix, and both quercetin- and catechol-loaded hydrogels showed measurable antibacterial activity, with variations between formulations. In conclusion, the developed chitosan–gelatin composite hydrogels incorporated with bioactive agents combine

desirable physical stability with effective antibacterial properties against multi drug resistant bacterial strains. These findings suggest their potential application as advanced wound dressing materials with multifunctional performance.

## **Stability evaluation of Lysozyme coated gold nanoparticles in acidic, neutral and basic conditions and their bioactivity assessment to combat E.coli and Staphylococcus aureus**

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### **Abstract**

Lysozyme is a common enzyme found in the tears, saliva and the chicken egg white which possess strong antimicrobial potential, along with anti-inflammatory and anti-oxidant properties, efficiently functional at pH 6-7 and temperature 45 °C-60 °C. The Lysozyme breaks down the glycosidic bonds in the 1,4-β-linkages between N-acetylmuramic acid (NAM) and N-acetylglucosamine (NAG) in the peptidoglycan layer. Therefore, lysozyme is found to be more effective on Gram-positive bacteria.

In the current research, we have synthesized lysozyme coated gold nanoparticles, with lysozyme acting both as reducing agent and stabilizing agent. This represents a green-synthesis approach forming biocompatible surface corona on the AuNPs. The prepared AuNPs (AuNPs-Lys) has been characterized for size, shape, effective surface charge, and FTIR. The stability of the AuNPs-Lys has been checked in acidic, basic, and neutral pH in BSA (2%) and salt solutions (0.1M), at 37 °C. Further, the antimicrobial activities have been checked with Kirby-Bauer antimicrobial assay on Gram-positive and Gram-negative bacteria and its antioxidant potential is determined by DPPH activities. The antimicrobial potential of lysozyme has been found to be superior on the nanoparticle surface owing to its stability at varied conditions (acidic, basic, and neutral). In future, AuNPs-Lys can be tested for anti-cancerous potential.

# Water-Based Graphene-Biopolymer Ink for Sustainable Printed Electronics

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## Abstract

The growing demand for sustainable alternatives in printed electronics has led to significant interest in exploring eco-friendly conductive inks for applications such as sensors, antennas, smart packaging, displays and supercapacitors. Advancements in printing technologies have made it possible for the deposition of functional inks on various substrates. In this work, a water-based graphene conductive ink was formulated using the water-soluble biopolymer sodium alginate as both binder and additive, for screen printing on flexible substrates. The ink formulation was carefully optimized by varying the biopolymer concentration and the number of printed layers to evaluate its influence on the electrical properties of the printed structures. The resulting printed films exhibited sufficient electrical conductivity and mechanical flexibility, making it suitable for the development of lightweight, flexible devices. These findings highlight the potential of water-based carbon conductive inks to minimize the use of toxic materials which are commonly used in conventional printed electronics and thereby produce environmentally friendly, low-cost disposable electronics. The findings also demonstrate that the biopolymer concentration and the number of print layers can significantly impact the final performance and should be tailored based on the intended applications. In conclusion, this study demonstrates the potential of water-based carbon conductive inks as a sustainable alternative to conventional conductive inks for producing next-generation flexible, sustainable, low-cost printed electronic devices.

## Plasmonic Printed Nanostructures under White-Light Assistance for Optothermal Tweezing

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## Abstract

The ability to trap and manipulate single biological cells plays a vital role in understanding cellular behaviour, interactions, and responses at the microscale. Controlling the position of individual particles with high precision is essential for research in areas such as cellular biology, diagnostics, drug delivery, and the controlled assembly of micro- and nanostructures. Conventional techniques like optical tweezers,

microfluidics, and plasmonic traps allow non-contact manipulation of cells and molecules, enabling advanced single-cell studies.

Plasmonic nanostructures are particularly powerful in such applications due to their localized surface plasmon resonances (LSPRs). When illuminated, metallic nanostructures generate strong electromagnetic fields, producing optical forces capable of trapping small biological entities. By positioning cells near these structures, enhanced field gradients provide spatial control over movement and confinement, offering a non-invasive means of cellular manipulation with high precision.

In this work, we demonstrate a direct-write printing approach for fabricating plasmonic nanostructures using a colloidal solution. The setup employs a commercial projector coupled with an inverted microscope. When a colloidal silver solution is exposed to broadband white light, the spectrum includes the silver absorption band (~425 nm). The resulting plasmonic interaction drives photon-phonon conversion, creating localized heating and strong temperature gradients at the focus. These gradients induce nanoparticle migration through convection, overcoming electrostatic repulsion and enabling pattern formation on substrates via van der Waals forces.

The printed plasmonic patterns serve as optothermal traps for microparticles and biological cells. Unlike conventional high-power trapping methods, this technique requires low optical energy, minimizing the risk of particle damage and expanding the range of trappable species. Using yeast cells as a model, we successfully demonstrated optothermal trapping and lateral manipulation. Cells migrated toward illuminated printed patterns and could be transferred between trap sites by sequential illumination of different structures.

This method represents the first demonstration of white-light-assisted optothermal manipulation of yeast cells, highlighting its potential for applications in cellular research, microbiology, diagnostics, and drug delivery.

## **Forensic Electrochemical Detection of Promethazine as a Misused OTC Sedative Mimicking Club Drugs Using Ag/MWCNT Modified Electrodes**

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### **Abstract**

Promethazine, a commonly available over-the-counter (OTC) antihistamine with sedative and hypnotic properties, has emerged as a substance of interest in forensic toxicology due to its potential misuse as an alternative to club drugs. Its easy accessibility in pharmacies and ability to induce sedation, relaxation, and drowsiness make it susceptible to recreational abuse, mimicking some effects of traditional club drugs. This study presents a sensitive voltametric method for detecting promethazine in various solvent systems using Ag/MWCNT-modified glassy carbon electrodes. The Ag/MWCNT modification enhances electron transfer rates and surface area, significantly increasing detection sensitivity. Optimised cyclic voltammetry techniques offer nanomolar-level detection limits, with rapid response times and minimal interference. The highly portable and robust design of the sensor positions it as an ideal tool for future forensic on-site applications, enabling the fast and reliable screening of promethazine in pharmaceutical formulations, biological fluids, and seized drug samples with minimal sample preparation. This addresses

a growing forensic need to detect not only illicit substances but also increasingly misused OTC compounds. The technology supports law enforcement and forensic experts in monitoring promethazine misuse, mitigating public health risks, and providing reliable evidence in judicial processes. By combining advanced electrochemical sensing with forensic applicability, this research offers a crucial tool for combating novel drug abuse patterns involving OTC medications like promethazine.

## **Nanoparticles a New Boon For Various Crops - A Review)**

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### **Abstract**

Metal nanoparticles that are synthesized in a green environment are anticipated to enhance the growth and yields of plants in agriculture. They have demonstrated the potential to improve nutrient availability, photosynthetic efficiency, disease resistance, and stress tolerance. AgNPs, ZnONPs, Fe<sub>3</sub>O<sub>4</sub>NPs, AuNPs, and CuNPs have demonstrated substantial benefits in a variety of commodities, resulting in increased growth and yields. These nanoparticles have the potential to address global agricultural challenges, including sustainability, resource optimization, and food security, as green synthesis continues to evolve. Nevertheless, their implementation is hindered by regulatory concerns, environmental consequences, and application methodologies. A multifaceted approach is required to overcome these constraints, which includes the development of standardized synthesis protocols, the optimization of application methods, and the investigation of environmental impact and toxicity. It is essential to collaborate with regulatory agencies, industry stakeholders, and researchers in order to advance the use of green-synthesized metal nanoparticles in agriculture as well as vegetable crops. Long-term environmental effects assessment, optimization of application techniques, and scalability and reproducibility of synthesis methods should be the primary focus of future research.

## **Pt, Au, and Ru complexes in Medicinal Chemistry: Coordination Strategies and Biological Activities**

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### **Abstract**

Metal complexes are vital to pharmaceutical sciences because of their numerous and significant functions. So Schiff bases can create chelating complexes with many metals such as Platinum, Ruthenium, and Gold in varying oxidation states, making them versatile pharmacophores. After that, the generated Schiff base and metal complexes were examined by FTIR, Electronic data and etc. Additionally, the

characterization investigation illustrates that the Pt (II) and Au (III) complexes exhibit square planar structures, while the Ru (III) exhibits distorted octahedral geometry. There are various biological activities like: antibacterial, antimicrobial, antitumour of aforementioned metal complexes have been examined. Along with it, these metal complexes show various physical and chemical properties which are discussed in this review paper

## **Kinetic and Isotherm Modeling of Methyl Red Dye Adsorption from Aqueous Solution Using Copper Nanoparticles Functionalized *Cicer arietinum* Peel Powder as a Sustainable Biosorbent**

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### **Abstract**

This research investigated the adsorption kinetics and isotherm modeling of methyl red (MR), a representative azo dye, using biosorbent derived from *Cicer arietinum* (chana) peel powder. Agricultural by-products such as chana peels often remain underutilized, contributing to waste generation; however, their natural composition makes them promising materials for environmental remediation. The biosorbent chana peel powder (CPP) was prepared in powder form and further functionalized with copper nanoparticles synthesized via biosorbent extracts. Adsorption trials examined the influence of initial dye concentration, adsorbent mass, and nanoparticle incorporation on MR removal efficiency at 30°C temperature and pH as 7. Kinetic modeling revealed that adsorption behavior aligned better with pseudo-second-order kinetics than with pseudo-first-order, indicating that chemisorption processes were predominant involving stronger adsorbate–adsorbent interactions. Isotherm modeling showed that both Langmuir and Freundlich models adequately described the adsorption, with maximum adsorption capacities as 1.77mg/g for CPP. The adsorption showed a good fit with the Langmuir model, indicating monolayer coverage on a homogeneous surface. The findings demonstrate that *Cicer arietinum* peel waste can be effectively repurposed as a green biosorbent for dye removal, providing an eco-friendly approach to wastewater treatment. The applicability of the Langmuir model was supported by the calculated  $R_L$  value as 0.21 for CPP, which ranged between 0 and 1, indicating favorable adsorption across all tested concentrations. The study report functionalization of CPP with copper nanoparticles (CuNps) in liquid phase for the first time using green synthesis for removal of MR dye from aqueous solution. CPP was characterized by FTIR and FESEM techniques. EDX characterization was also done for CuNps synthesized by CPP extract. The findings highlight the potential of *Cicer arietinum* peel powder as an eco-friendly and effective biosorbent for dye-laden wastewater treatment, offering a viable approach to sustainable environmental management.

# Phytogenic Silver Nanoparticles from *Carissa carandas*: Synthesis, Characterization, and Antimicrobial Efficacy

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## Abstract

The alarming rise of antimicrobial resistance (AMR), responsible for millions of deaths annually and projected to worsen, underscores the critical need for innovative therapeutic strategies that can circumvent conventional resistance mechanisms. Silver nanoparticles (AgNPs) have emerged as a potent alternative due to their broad-spectrum antimicrobial activity and ability to induce lethal oxidative stress in bacterial cells through the generation of reactive oxygen species (ROS). While AgNPs can be synthesized by various methods, plant-mediated green synthesis offers a superior, eco-friendly approach by utilizing phytochemicals as reducing and capping agents, enhancing biocompatibility and stability. This study leverages the phytochemical diversity of two fruit variants of *Carissa carandas* (green and pink seeds) for the sustainable synthesis of AgNPs, and its successful formation of nanoparticles was confirmed by UV-Vis spectroscopy, for both green and pink seed extracts, respectively. Dynamic light scattering (DLS) revealed mean hydrodynamic diameters, while zeta potential measurements indicated moderate colloidal stability with surface charges. Crucially, the AgNPs demonstrated significant antibacterial efficacy against *Escherichia coli* in Kirby-Bauer assays, with nanoparticles from green seeds exhibiting superior activity, whereas the crude plant extracts showed no effect. The AgNPs also exhibited concentration-dependent colloidal stability in physiological-like buffers. This research confirms that *C. carandas* is an effective platform for generating stable and bioactive AgNPs, positioning these phytogenic nanomaterials as promising, sustainable candidates for combating antibiotic-resistant infections.

## Article Title: Role of Biodegradable Nanoparticles for Detection and Bioremediation of Environmental Pollutants

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## Abstract

Environmental pollution caused by heavy metals, pesticides, plastics, dyes, and industrial effluents poses serious risks to ecosystems and human health. Conventional remediation techniques are often costly and generate secondary waste, creating demand for safer and sustainable alternatives. Biodegradable nanoparticles (BDNPs) have emerged as an innovative solution for pollution detection and remediation. Made from natural or synthetic polymers such as chitosan, polylactic acid, and alginate, BDNPs degrade

into non-toxic products, reducing long-term environmental impact. In detection, BDNPs are employed as biosensors for highly sensitive monitoring of pollutants including pesticides, dyes, and heavy metals. In remediation, they enhance pollutant removal via adsorption, biodegradation, and catalytic mechanisms, often supporting enzymes or microbes to improve efficiency. Green synthesis approaches using plant extracts and microbes further add to their eco-friendly potential. Despite these advantages, challenges such as large-scale production, economic feasibility, and long-term ecological safety remain. This review highlights the principles, applications, limitations, and future prospects of BDNPs in sustainable environmental management.

## **From Seeds to Nanomaterials A Systematic Literature Review on the Antimicrobial Applications and Bioactive Potential of *Jatropha curcas***

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### **Abstract**

*Jatropha curcas*, a multipurpose medicinal plant, has attracted considerable interest for its antimicrobial properties, with reported activity against a wide range of bacterial and fungal pathogens, including multidrug-resistant (MDR) strains. Its bioactive potential is attributed to diverse phytochemicals present in different plant parts—particularly seeds, latex, leaves, bark, and roots—as well as its suitability for green synthesis of antimicrobial nanoparticles. Following the PRISMA 2020 guidelines, 12 peer-reviewed in vitro studies published between 2016 and 2024 were systematically reviewed to evaluate the antimicrobial applications of *J. curcas*. The *In Vitro* Quality Evaluation Instrument was used to assess methodological rigor and risk of bias, revealing that all included studies exhibited low risk of bias, with quality scores ranging from 78.57% to 100%. The findings demonstrate that *J. curcas* derivatives, including seed oil, seed kernel extracts, latex, essential oils, and plant-mediated nanoparticles (silver, zinc oxide, copper oxide/silver, and magnetite), show strong antibacterial effects against Gram-positive bacteria such as *Staphylococcus aureus*, *Bacillus subtilis*, and *Enterococcus faecalis*, and Gram-negative bacteria including *Escherichia coli*, *Klebsiella pneumoniae*, *Salmonella enterica*, and *Pseudomonas aeruginosa*. Some preparations also exhibited antifungal activity against *Candida albicans*, *Candida tropicalis*, *Aspergillus niger*, and *Aspergillus fumigatus*. However, resistance was noted in certain pathogens, particularly *P. aeruginosa* and some *Candida* species, depending on the extract type and formulation. Seed-based products frequently showed notable potency, and nanoparticle formulations often outperformed crude extracts. Variations in antimicrobial activity across studies appear linked to differences in plant part, extraction solvent, synthesis method, strain susceptibility, and testing conditions. This review synthesizes current evidence on *J. curcas* as a natural antimicrobial agent and highlights its potential role in combating antimicrobial resistance. Further research should focus on expanding antifungal testing, elucidating mechanisms of action, and evaluating clinical safety and efficacy for therapeutic development.

# Comparative Physicochemical Evaluation of Textile Effluents and Soil Samples from Sanganer and Bagru Industrial Regions of Jaipur

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## Abstract

The textile industry is one of the major contributors to environmental pollution, especially through the discharge of untreated dye-laden effluents into nearby water bodies and soils. The present study undertakes a comparative physicochemical evaluation of textile effluents and adjoining soil samples from two major textile industrial hubs of Jaipur—Sanganer and Bagru—to assess their pollution load and environmental impact. Water and soil samples were collected from four sites in each region and analyzed for key physicochemical parameters, including pH, electrical conductivity (EC), total dissolved solids (TDS), total suspended solids (TSS), total hardness (TH), biological oxygen demand (BOD), chemical oxygen demand (COD), dissolved oxygen (DO), phosphate, nitrate, fluoride, and selected heavy metals (Fe, Zn, Mn, Cr, and As), following standard BIS and APHA methods.

The results revealed marked variations between the two regions. Effluents from Bagru exhibited higher EC ( $3.0\text{--}4.0 \times 10^6$   $\mu\text{S/cm}$ ), TDS (6300–10176 mg/L), TH (689–2362 mg/L), and COD (1706–2176 mg/L) than those from Sanganer, indicating greater ionic and organic loads. Soil samples from both sites reflected the cumulative impact of effluent discharge, with pH values ranging from 7.72–9.53 in Sanganer and 5.72–9.62 in Bagru, and elevated concentrations of Fe, Zn, and Mn. Although Cr and As were either absent or within permissible limits, other parameters frequently exceeded WHO and CPCB standards for discharge and irrigation. Correlation analysis showed strong positive relationships among EC, TDS, and COD, suggesting a common industrial origin of contamination.

The study concludes that effluents from both Sanganer and Bagru significantly deteriorate surrounding soil and water quality, with Bagru showing comparatively higher pollution intensity due to denser dyeing and printing operations. Continuous monitoring, effective effluent treatment, and enforcement of zero-liquid discharge practices are essential to mitigate the environmental impacts and safeguard local ecosystems and agricultural productivity.

# Institutional and Legal Reforms Are Essential for Strengthening India's Biosafety Governance in Biotechnology

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## Abstract

The convergence of biotechnology and environmental law presents complex governance challenges, particularly in regulating the environmental release of genetically modified organisms (GMOs) and related biotech products. This paper critically examines India's legal and institutional framework governing the environmental release of such organisms, situating it within a comparative global context. The analysis identifies regulatory gaps, institutional overlaps, and enforcement deficiencies that undermine biosafety and environmental protection in India.

Employing a doctrinal and comparative legal methodology, the study evaluates India's regulatory structure under the Environment (Protection) Act, 1986, and the Rules of 1989, comparing it with the process-based precautionary approach of the European Union and the product-based regulatory model of the United States. The findings reveal that India's biosafety regime remains fragmented, with overlapping mandates between the Genetic Engineering Appraisal Committee (GEAC), the Review Committee on Genetic Manipulation (RCGM), and sub-national bodies such as State Biotechnology Coordination Committees (SBCCs) and District Level Committees (DLCs). This institutional fragmentation contributes to regulatory inefficiency, limited transparency, and weak post-release monitoring mechanisms.

Judicial interventions, notably in *Aruna Rodrigues v. Union of India*, alongside sustained civil society activism, have significantly shaped India's cautious stance on GMO approvals. However, the absence of a dedicated biosafety statute, clearly defined liability provisions, and an independent oversight authority continues to impede the development of a coherent and enforceable biosafety framework. While India's adherence to the Cartagena Protocol on Biosafety reflects its formal commitment to international standards, domestic implementation remains inconsistent and inadequately supported by institutional capacity or public participation mechanisms.

The paper concludes that ensuring biosafety within India's rapidly expanding biotechnology sector requires comprehensive legal and institutional reform, including the establishment of a unified and transparent regulatory framework that integrates scientific evaluation with environmental accountability. Establishing an independent National Biosafety Authority, enacting a comprehensive Biosafety Law, integrating public consultation mechanisms, and strengthening post-release monitoring are essential to align India's regulatory practices with global benchmarks, thereby ensuring a governance framework that balances technological innovation with ecological sustainability and public accountability.

# **Track - V**

**Materials in Engineering and Technology**

# Agri waste Generated in Indian Agriculture, Difficulties and Resolutions Faced by The Government: A Review

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## Abstract

Agricultural wastes are described as leftovers from agricultural activities which includes waste created by farming, planting, harvesting, fertilizer run off from fields, pesticides go to fields, slaughterhouse, livestock waste, post-harvest waste. Agricultural waste has the ability to harm the environment and expose personnel to biohazards, which are dangerous biological materials. Every year India produces a vast amount of agricultural waste. Over 500 million tonnes of agriwaste is produced by India every year, most of it remains non-utilized or is discarded through harmful practices like open burning that creates both an environmental problem (production of harmful gases during burning) and an economic opportunity (bioenergy, compost, animal feed, industrial feedstock). This review paper states the types and sources of agriwaste generated in India by agriculture practices, the challenges faced by stakeholders and government in managing the waste like lack of infrastructure, low awareness. The review highlights the need for a more integrated and scalable approach, involving public-private partnerships, farmer education, and investment in decentralized waste management systems to transform agriwaste from a liability into a resource for sustainable development. This review comprises the scale and sources of agricultural waste in India, the main challenges governments face in handling the waste, the preventive measures taken so far, observed rifts and problems in execution, and practical advices to ameliorate outcomes also future aspects like technical innovation, bioenergy production, integration of circular economy are discussed in the review paper.

## Strain-Induced Modulation of Electronic and Catalytic Properties in 2D Janus TMDs

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## Abstract

Janus transition metal dichalcogenides (TMDs) have attracted considerable attention as promising electrocatalysts for the hydrogen evolution reaction (HER) owing to their broken out-of-plane symmetry, intrinsic dipole moments, and chemically versatile surfaces. Nevertheless, their basal planes are typically catalytically inert, which restricts their overall activity. In this study, we employ density functional theory (DFT) to systematically investigate the effect of biaxial strain on the catalytic performance of a representative Janus NbSSe monolayer. Strain ranging from  $-4\%$  (compressive) to  $+4\%$  (tensile) is

applied to probe its influence on the electronic structure, hydrogen adsorption free energy ( $\Delta G_H$ ), and charge redistribution at the active sites. Our results demonstrate that strain induces significant modifications in the local density of states and alters the interaction strength between hydrogen and the chalcogen atoms. Specifically, compressive strain enhances the binding interaction, whereas tensile strain weakens hydrogen adsorption, leading to near-optimal  $\Delta G_H$  values close to the thermoneutral condition. These findings establish strain engineering as an effective strategy to activate the basal plane of Janus TMDs and optimize their HER activity. This work provides a fundamental theoretical framework for guiding the rational design of strain-modulated, cost-effective 2D electrocatalysts for sustainable hydrogen production.

Selective Hydrogen Detection at Reduced Temperatures Using WO<sub>3</sub> Nanorods Functionalized with Pd–Pt Alloy Nanoparticles

Hydrogen (H<sub>2</sub>), with its high energy density and clean utilization, is expected to play a vital role in sustainable energy systems, but its low ignition energy and wide flammability range necessitate reliable detection. Here, we report a hydrogen sensor based on WO<sub>3</sub> nanorods functionalized with Pd:Pt alloy nanoparticles prepared by ascorbic acid reduction. By systematically tuning the Pd:Pt atomic ratio, we optimized the sensor's performance, with Pd<sub>2</sub>:Pt<sub>1</sub>@WO<sub>3</sub> achieving the highest response ( $R_a/R_g = 29.15$ ) toward 100 ppm H<sub>2</sub> at the remarkably low operating temperature of 125°C. The optimized sensor further demonstrates excellent sensitivity across a wide H<sub>2</sub> concentration range (2.5–500 ppm), outstanding repeatability, and superior selectivity over interfering gases. These results highlight that precise Pd:Pt alloy ratio engineering on WO<sub>3</sub> nanorods provides a promising strategy for low-temperature, high-performance hydrogen sensing.

## Smart Sustainable Healthcare through Medical Image Processing and Ultra-Wideband Integration

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### Abstract

Medical Image Processing (MIP) has emerged as a critical healthcare tool of today, facilitating improved disease detection, diagnostic accuracy, and individualized treatment planning. Its capabilities can be significantly boosted with integration from Ultra-Wideband (UWB) technology, which provides high-resolution sensing, precise localization, and power-efficient wireless communication. This research investigates the merging of AI-supported MIP methods such as image improvement, segmentation, feature extraction, and classification with UWB-based systems for non-invasive diagnosis, real-time patient monitoring, and safe data exchange. The strategy is complemented by IoT-powered and cloud-enabled infrastructures that enhance scalability, maximize computational efficiency, and increase telemedicine availability in remote areas. UWB's ability to operate in non-line-of-sight environments guarantees consistent operation in sophisticated clinical environments, while energy-conserving algorithms and transportable UWB hardware facilitate sustainable use in resource-constrained environments. Augmenting these digital solutions are advances in material science that further contribute

to sustainable healthcare. Some examples include biodegradable polymers used for the reduction of medical waste, nanomaterials used for the creation of highly sensitive biosensors, and bioresorbable implants that obviate secondary surgeries. These innovations support SDG 12 (Responsible Consumption and Production) by means of circular design approaches and SDG 3 (Good Health and Well-Being) by making biomedical devices safer. Together, the combination of AI-based MIP, UWB technology, and green material innovations enables several United Nations Sustainable Development Goals (SDGs), such as SDG 3, SDG 9, SDG 10, and SDG 12. Together, this combination creates a comprehensive smart healthcare model that improves diagnostic precision, reduces environmental impact, and provides universal access to sophisticated medical technologies across the globe.

## CO<sub>2</sub>-to-Hydrocarbon Conversion Enabled by Van der Waals o-B<sub>2</sub>N<sub>2</sub> Metal-Free Photocatalyst

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### Abstract

The efficient conversion of carbon dioxide (CO<sub>2</sub>) into value-added products offers a dual benefit of mitigating greenhouse gas emissions while supporting renewable energy development. Photocatalysis has emerged as a sustainable strategy for this transformation, with the design of stable, metal-free catalysts being of particular interest. In this work, the focus is on the recently predicted orthorhombic boron nitride (o-B<sub>2</sub>N<sub>2</sub>), a two-dimensional van der Waals monolayer polymorph of boron nitride that exhibits a direct band gap of 0.78 eV, placing it within the visible light absorption range and making it a potential candidate for photocatalytic CO<sub>2</sub> reduction reactions (CO<sub>2</sub>RR). Using first-principles density functional theory calculations, both pristine and defective o-B<sub>2</sub>N<sub>2</sub> are investigated as photocatalysts for CO<sub>2</sub>RR. The analysis reveals that pristine o-B<sub>2</sub>N<sub>2</sub> interacts only weakly with CO<sub>2</sub> molecules, limiting its catalytic efficiency. In contrast, defective o-B<sub>2</sub>N<sub>2</sub> demonstrates significantly enhanced adsorption behavior, with a calculated adsorption energy of -3.75 eV, thereby activating CO<sub>2</sub> molecules for subsequent reduction processes. The reaction pathways are systematically explored, focusing on two key mechanisms: the formate (\* OCOH) pathway and the carboxylic (\* COOH) pathway. Among these, the formate pathway is identified as the most favorable for methanol (CH<sub>3</sub>OH) production. The \* OCOH intermediate readily converts into \* HCOOH, with a limiting potential (U<sub>l</sub>) of 1.10 V required for CH<sub>3</sub>OH formation. This relatively low overpotential indicates that defective o-B<sub>2</sub>N<sub>2</sub> can effectively drive CO<sub>2</sub> reduction under moderate conditions. By contrast, the carboxylic pathway is less energetically favorable for hydrocarbon formation on this system the results highlight the crucial role of defects in modulating the catalytic activity of o-B<sub>2</sub>N<sub>2</sub>, transforming it from a weakly interacting surface into an efficient photocatalyst capable of driving multi-electron reduction processes. The favorable band gap, strong CO<sub>2</sub> adsorption, and pathway selectivity for CH<sub>3</sub>OH production collectively position defective o-B<sub>2</sub>N<sub>2</sub> as a promising, sustainable, and metal-free photocatalyst for CO<sub>2</sub>-to-fuel conversion. This study not only provides fundamental insight into the catalytic mechanism of o-B<sub>2</sub>N<sub>2</sub> but also contributes to the broader effort of developing cost-effective and environmentally friendly catalysts for renewable energy applications.

# Graphene–Diamane Interfaces for Enhanced Silicon Solar Cell Performance.

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## Abstract

In this work, we present a comprehensive study of diamane's role as an emitter and carrier collection layer in crystalline silicon heterojunction (SHJ) and heterojunction with intrinsic thin layer (HIT) solar cells, using systematic simulations performed with AFORS-HET version 2.5.

We first explored the application of n-type diamane as an emitter layer in SHJ solar cells modelled as ITO/n-diamane/p-cSi/Ag. The simulations revealed that by optimizing key parameters such as bandgap, donor concentration, and thickness, a maximum efficiency of 16.84% could be achieved for a 100  $\mu\text{m}$  thick crystalline silicon wafer. The study also showed that efficiency is slightly sensitive to diamane layer number and to the use of commercially available silicon wafers, demonstrating the practical feasibility of such designs. Building on this foundation, we investigated a novel graphene/diamane interface in HIT solar cells. In this configuration, graphene acted as the transparent conducting electrode (TCE) owing to its high optical transparency and tunable work function, while n-type diamane served as the emitter layer. With the insertion of an intrinsic hydrogenated amorphous silicon passivation layer, the optimized device achieved an efficiency of 24.15%, significantly higher than conventional ITO-based counterparts. This result confirmed that carbon allotropes alone can act as both efficient electrodes and emitter layers in next-generation solar architectures. Most recently, we introduced doped diamane as both the electron and hole collection layers in HIT solar cells, functioning respectively as the emitter and back surface field (BSF) layers. Careful optimization of band alignment, texturing angle, and front-contact absorption losses enabled a record simulated efficiency of 27.88%. The results demonstrated that doped diamane not only reduces parasitic absorption but also enhances carrier separation and transport, outperforming conventional amorphous silicon-based HIT cells.

Overall, this work establishes diamane as a highly versatile material with multiple roles across solar cell architectures. Its tunable electronic properties, high carrier mobility, and compatibility with graphene-based electrodes underscore its transformative potential in achieving next-generation high-efficiency silicon photovoltaics.

# Sustainable Space and NOMA-Enabled Wireless Systems through Materials Science Innovations.

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## Abstract

Non-Orthogonal Multiple Access (NOMA) is growing as the fundamental technology for future wireless communications that provides better spectral efficiency, massive connectivity, and ultra-reliable low-latency services. Meanwhile, space communication systems need high-performance materials to guarantee durability, energy-saving, and long-term sustainability in extreme environments. Materials science has an important function supporting both areas by providing innovations with improved electromagnetic, structural, and thermal characteristics. Nanostructured semiconductors, high-k dielectrics, and two-dimensional (2D) materials like graphene and MoS<sub>2</sub> are being designed to minimize propagation losses, increase antenna efficiency, and allow ultra-low-power miniaturized NOMA transceivers. Metamaterials and reconfigurable intelligent surfaces (RIS) enhance spectrum use and adaptive beamforming even further, with a direct implication for SDG 7 (Affordable and Clean Energy) as they reduce the energy profile of massive wireless networks. In space technology, lightweight composites, ceramic matrix materials, and radiation-hardened alloys increase the lifespan of satellites as well as provide more strength in harsh operating environments, in line with SDG 9 (Industry, Innovation, and Infrastructure) as they facilitate resilient worldwide communication infrastructures. Moreover, the use of biodegradable substrates, recyclable polymers, and green fabrication processes also fulfills SDG 12 (Responsible Consumption and Production) by reducing electronic waste and enabling circular material lifecycles. All these innovations collectively emphasize materials science as a pillar for supporting sustainable innovation in both space and NOMA-based wireless systems, linking technological advancements directly with the United Nations Sustainable Development Goals.

## Improved Voltage Regulation in Microgrids Using a Honey Badger Algorithm Tuned Anfis Controller for STATCOM.

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## Abstract

Voltage stability and power quality are major challenges for microgrids with hybrid renewable energy sources (such as wind and solar) because those sources are intermittent and stochastic. This paper proposes a novel approach of combining an Adaptive Neuro-Fuzzy Inference System (ANFIS) control framework with the Honey Badger Algorithm (HBA), to optimize a Static Synchronous Compensator (STATCOM) for reactive power compensation. The HBA-ANFIS hybrid controller tuned the non-linear

variables of the ANFIS model, which improved the STATCOM's ability to rapidly and efficiently stabilize voltage at the point of common coupling (PCC). Using a detailed microgrid model in MATLAB/Simulink, the microgrid system consisted of arrays of solar photovoltaic (PV) modules, a wind-driven doubly-fed induction generator (DFIG), and a diesel generator to simulate real-world conditions. The proposed control scheme with HBA-ANFIS was compared to conventional Proportional-Integral (PI) controllers and optimization-based adaptive controllers as benchmarks (PID-GA, PI-ACO, MPA-PIDA). Simulation results demonstrate that the HBA-ANFIS controller outperformed these solutions by being faster to settle, less voltage overshoot, and more efficient overall. More specifically, the proposed controller was able to achieve a settling time of 0.4671 seconds, voltage overshoot limited to 11% and efficiency of 99.1%. All of which indicates that the controller is superior for reactive power compensation and also voltage management. The findings presented in this study illustrate the capability of the hybrid HBA-ANFIS design as a means of developing better quality power and enhanced stability of intelligent microgrid systems, and thus facilitating the seamless integration of renewable energy sources.

## **Design and Comparative Analysis of Symbol-Inspired Frequency Selective Surfaces for C-, X-&Ku-Band Applications**

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### **Abstract**

The evolution of frequency selective surfaces (FSSs) has led to significant advancements in electromagnetic applications, including frequency selectivity, reduced radar cross section, enhanced gain, improved directivity, and sensitivity to the angle of incidence. In this comparison, three unique geometrical designs Swastik, Omega, and Jerusalem Cross [2,3]—are Simulated using Ansys HFSS 2019. Their performance is investigated in the C-band, X-band, and Ku-band in terms of return loss, bandwidth, gain, and angular sensitivity. These results demonstrate that these geometries offer distinct advantages across different frequency ranges, making them suitable candidates for multifunctional communication and sensing applications.

# **Metal-Organic Frameworks: A positive outcome for efficient removal of water pollutants from point and nonpoint source of water pollution.**

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## **Abstract**

A serious environmental threat to animals, plants and human being is the relocation of organic and inorganic pollutants in water through different source of water pollution which can be point source or nonpoint source of water pollution. The release of pesticides, pharmaceutical products, radioactive substances, heavy metal ions, fertilizers, thermal pollutants from pharmaceutical, industrial, agricultural, sewage discharges, urban runoff and domestic activities causes a pitfall to human being and environmental bodies. With the flourishing growth and globalization, fossil fuels demand is also increasing which put pressure on natural resources which further results into environ-mental pollution and global warming. To address this challenging issue, we require cost effective and sustainable methods for effective removal and degradation of these pollutants from wastewater. Traditional and Conventional methods like precipitation, adsorption, coagulation, membrane filtration have some limitations like high-cost formation of secondary pollutants which limits their applications. In the recent era Metal-Organic Frameworks (MOFs) have offered an ultimate strategy for construction of photocatalysts for degradation of organic and inorganic pollutants in wastewater. MOFs are highly crystalline materials and porous crystalline structures, having high surface area and high thermal stability, high range of tunability, distinctive structural features and customizable properties. MOFs show high efficiency in adsorption, elimination, and degradation of organic and inorganic pollutants. In this review article the MOFs based removal, adsorption, degradation of organic pollutant which comes from point and nonpoint source of water pollution is summarized according to different process and opportunities and challenges can be discussed.

## **Kinetic, Isotherm, and Thermodynamic Studies on the Sorption of Malachite Green (MG) by Synthesized Iron Nanoparticles**

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## **Abstract**

Malachite green (MG) and other synthetic colours emitted from textile and industrial wastes are poisonous and persistent, posing a major risk to human health and aquatic ecosystems. Many physicochemical and biological treatment methods have been investigated. The adsorption method is the most effective among them all because of its high removal efficiency, simplicity of use, affordability, and material's capacity to be recycled. In this study, the ability of synthesised iron nanoparticles (FeNPs)

to adsorb malachite green dye from wastewater is examined. The impact of variables, including contact time, pH, adsorbent dosage, and initial dye concentration, on the sorption process were assessed by batch adsorption studies. With optimal conditions, the results showed that FeNPs had a high removal effectiveness of up to 83% dye removal. The pseudo-second-order model of kinetics suggested chemisorption as the dominant mechanism, while the Langmuir isotherm model of adsorption indicated monolayer adsorption on a homogenous surface. Thermodynamic analyses demonstrated that the process was endothermic and spontaneous. The results of this study demonstrate the potential of iron nanoparticles as an economical, environmentally benign, and efficient adsorbent for the treatment of wastewater contaminated with dyes, providing a long-term approach for resource recovery and environmental preservation.

## **A first-principles study of the electronic structure, and optical properties of ZnSnN<sub>2</sub> nitrogen base stable perovskite semi-conducting material.**

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### **Abstract**

This study presents a comprehensive first-principles analysis of the electronic structure, density of states (DOS), and optical properties of Zn-IV-N<sub>2</sub> heterovalent ternary nitride semiconductors, with a focus on zinc tin nitride (ZnSnN<sub>2</sub>), a stable nitrogen-based perovskite material. Utilising the Generalised Gradient Approximation (GGA-PBE) within density functional theory, the electronic band structure, DOS, and optical characteristics of ZnSnN<sub>2</sub> are calculated and compared with prior theoretical studies, demonstrating good agreement. The results reveal that ZnSnN<sub>2</sub> exhibits a direct bandgap, making it a promising candidate for optoelectronic applications. The electronic structure analysis highlights the contributions of constituent atoms to the valence and conduction bands, with nitrogen p-orbitals playing a significant role in the band edge properties. The DOS calculations further elucidate the distribution of electronic states, confirming the material's semiconducting nature. Optical properties, including the dielectric function, absorption coefficient, and refractive index, are evaluated to assess ZnSnN<sub>2</sub>'s potential for photovoltaic and photonic devices. The findings indicate strong optical absorption in the visible spectrum, attributed to the material's favorable bandgap and electronic transitions. This study underscores the potential of ZnSnN<sub>2</sub> as a high-performance semiconductor for next-generation optoelectronic technologies, providing valuable insights into its structural and functional properties through rigorous computational methods. These results contribute to the growing body of knowledge on ternary nitride semiconductors and their applications in sustainable energy and advanced electronics.

# Improved Energy-Efficient Deep Learning for Epilepsy Detection on the Bonn EEG Dataset: A Signal-Processing Guided Framework.

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## Abstract

Epileptic seizure detection from Electroencephalography (EEG) must reconcile high accuracy with tight energy budgets on edge devices. This paper presents an improved, energy-efficient deep learning framework guided by signal-processing priors and evaluated on the Bonn EEG dataset. The pipeline begins with lightweight preprocessing (0.5–40 Hz band-pass, notch, and z-score normalization) and adaptive segmentation, followed by multi-resolution wavelet decomposition to emphasize ictal-relevant rhythms while suppressing artifacts. We design a compact network using depthwise-separable temporal convolutions and linear attention, augmented with knowledge distillation, structured pruning, and quantization-aware training. A cascaded early-exit mechanism enables dynamic inference when confidence is high, further reducing compute. We report stratified train–test splits with strict intersubject separation. Performance is assessed using accuracy, sensitivity, specificity, F1-score, AUROC, FLOPs/MACs, latency, and estimated energy per inference. The proposed model achieves >98% accuracy with balanced sensitivity/specificity, while cutting multiply-accumulate operations by ~60% and end-to-end latency by ~3× compared to strong CNN baselines, enabling real-time screening on CPUs and low-power NPUs. Ablations isolate the contributions of wavelet guidance and compression. The framework demonstrates that principled signal processing coupled with modern efficiency techniques yields clinically meaningful performance under constrained power, and provides a reproducible path toward deployable EEG analytics at the edge in practical settings.

## Performance Evaluation of IRS-Based Energy Efficient Wireless Body Area Networks

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## Abstract

The wireless propagation environment can be intelligently controlled by Intelligent Reflecting Surfaces (IRS) that can significantly improve the signal strength at body-worn or implanted sensors in wireless body area networks (WBANs), enabling more efficient RF energy harvesting (EH). However, a significant challenge for WBAN devices is their short battery life and maintaining constant power

availability is necessary to prevent malfunctions and extend device life. In this paper, the potential of IRS in enhancing EH by Body Area Networks (BANs) devices is explored. IRS, which can intelligently reflect wireless signals towards EH nodes to increase wireless power transfer efficiency, is one such potential strategy. By dynamically modifying the phase shifts of IRS elements to increase received power at EH nodes, we evaluate the performance of IRS to enhance the sustainability of WBANs. In order to depict how IRS can improve energy efficiency in BANs, we further proposed a mathematical model for IRS-assisted EH and validate theoretical framework using MATLAB-based simulations by generating results showing the relation of controlling parameters such as phase shift, reflection amplitude, and distance between source and user. Further outage probability analysis of WBAN devices has been explored to examine the sustainability of proposed model

## **Improved Bandwidth in Insert-Fed Patch Antennas via U-Slot Techniques for 2.4 GHz Wireless Systems**

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### **Abstract**

Wireless communication applications like Bluetooth and Wi-Fi benefit from the design and analysis of an Insert-Feed Microstrip 2.4 GHz antenna. It draws attention to the advantages of microstrip patch antennas, such as its low profile and lightweight construction, which make integration with printed circuit boards easier. The study looks at important design elements such as feeding methods, patch sizes, and substrate composition. to enhance antenna performance, particularly regarding bandwidth and multiband capabilities. Innovative features like U-slots are introduced to improve bandwidth and support dual or triple-band operation. The importance of advanced electromagnetic simulation tools for optimizing antenna designs before fabrication. Overall, the proposed antenna design meets contemporary performance standards and helps create effective antennas for today's communication requirements.

## About the Editors



### Dr Pranav Saxena

Dr. Pranav Saxena currently serves as Professor and Head of the Department of Physics at JECRC University, Jaipur with more than 25 years of experience in higher education and research. He obtained his M.Phil. & Ph.D. degree from the University of Rajasthan with specialization in high-energy physics. His research interests encompass quantum field theory, gauge boson phenomenology, and applied electromagnetic in communication. Dr. Saxena has authored several research articles in reputed journals and international conferences.



### Dr Abhishek Sharma

Dr. Abhishek Sharma is an accomplished academic and researcher with 18 years of teaching experience at both undergraduate and postgraduate levels. His research expertise spans across the domains of optoelectronic devices and their applications, Dielectric/Metal/Dielectric (DMD) structures, material synthesis and characterization, and plasma processing techniques. He has contributed significantly to the advancement of functional materials and device fabrication through experimental research and interdisciplinary collaboration. Driven by a passion for innovation and academic excellence, he continues to guide students and young researchers while actively engaging in scholarly activities, publications, and academic development initiatives.



### Dr Hariom Pawar

Dr. Hariom Pawar is currently serving as an Assistant Professor in the Department of Physics at JECRC University, Jaipur, Rajasthan, India. His primary research focuses on the development of nanoferrites, ferroelectric materials, and ferrite-based nanocomposites, with an emphasis on studying their physicochemical properties and exploring their potential for sensing applications. In addition to his research pursuits, Dr. Pawar has made significant contributions to the teaching and mentoring of engineering undergraduates and M.Sc. Physics students.



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