International Conference
on
Next-Gen Materials for Sustainable Future
(ICNMSF–2026)

Abstract Proceedings

04–06 May 2026

Organized by

Department of Physics
Akal University, Talwandi Sabo, Punjab, India

in Association with

Department of Physics
Eternal University, Baru Sahib, Himachal Pradesh, India

With Financial Support From

Anusandhan National Research Foundation
CSIR-INDIA
सीएसआईआर CSIR भारत का नवाचार इंजन The Innovation Engine of India
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Editors

Dr. Ramandeep Kaur
Dr. Janpreet Singh

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Preface

The International Conference on Next-Gen Materials for Sustainable Future (ICNMSF–2026), organized by the Department of Physics, Akal University, Talwandi Sabo, Punjab, India, from 04–06 May 2026, brings together researchers, academicians, industry professionals, and students working in different areas of materials science. The conference aims to provide a common platform for the presentation of research work, exchange of ideas, and discussion on recent developments in advanced and sustainable materials.

The focus of ICNMSF–2026 is on materials and technologies relevant to energy, environment, electronics, photonics, magnetism, functional materials, and computational materials science. The conference includes themes such as Energy Materials; Electronic, Photonic and Magnetic Materials; Advanced Functional Materials; and Computational and AI-Driven Materials Science.

This Book of Abstracts contains the abstracts of the papers accepted for presentation at the conference. The contributions included in this volume reflect current research activities, new findings, and continuing efforts in the field of next-generation materials. This volume is intended to serve as a useful reference for participants and as a record of the scientific work presented during **ICNMSF–2026**.

It is hoped that ICNMSF–2026 will encourage meaningful scientific discussions, academic interaction, and future collaborations in the area of materials science for a sustainable future.

Dr. Ramandeep Kaur
Convenor, ICNMSF–2026

Dr. Janpreet Singh
Co-Convenor, ICNMSF–2026

Acknowledgement

The Organizing Committee of the International Conference on Next-Gen Materials for Sustainable Future (ICNMSF–2026) expresses its heartfelt gratitude to the funding agencies, Anusandhan National Research Foundation (ANRF), Council of Scientific and Industrial Research (CSIR), and Board of Research in Nuclear Sciences (BRNS), for their generous financial support. Their support has been instrumental in the successful organization of this conference and in strengthening our efforts to provide a meaningful platform for academic exchange, research discussion, and scientific collaboration.

We express our deep gratitude to H.E. Dr. Davinder Singh Ji, Hon'ble Chancellor, Akal University, for his blessings, inspiration, and visionary guidance. We are sincerely thankful to Prof. Gurmail Singh, Hon'ble Vice Chancellor, Akal University, for his constant encouragement, institutional support, and leadership in promoting research and academic excellence at the university.

The Organizing Committee also extends sincere thanks to Maj. Gen. (Dr.) G. S. Lamba, Dean Academic Affairs, Prof. Sawarn Singh, Registrar, Prof. Sukhjeet Singh, Director IQAC, Dr. Bubun Banerjee, Associate Dean Research, and Dr. Sandeep Singh, Associate Dean Research, for their valuable guidance, cooperation, and support throughout the planning and execution of the conference.

We warmly acknowledge Dr. Sushil Kumar, Head, Department of Physics, and all faculty members of the Department of Physics for their wholehearted involvement, encouragement, and valuable contributions. We also sincerely appreciate the administrative staff and technical staff of Akal University for their cooperation, timely assistance, and dedicated support in ensuring the smooth conduct of the conference.

We express our sincere gratitude to all invited speakers, authors, reviewers, advisory board members, sponsors, and participants for their invaluable contributions, active engagement, and generous support. Their scholarly inputs and participation have greatly enriched the academic quality and spirit of ICNMSF–2026.

We also deeply acknowledge the dedicated efforts of the organizing team, research scholars, student volunteers, and supporting staff, whose commitment, enthusiasm, and teamwork played a vital role in the successful execution of the conference.

Finally, we thank all delegates and contributors for making ICNMSF–2026 a memorable and meaningful academic gathering dedicated to advancing research in next-generation materials for a sustainable future.

About the Conference

The International Conference on Next-Gen Materials for Sustainable Future (ICNMSF–2026) is being organized by the Department of Physics, Akal University, Talwandi Sabo, Punjab, India, from 04–06 May 2026 in hybrid mode. The conference aims to bring together researchers, academicians, industry experts, and students to share recent advancements and exchange ideas in the field of advanced and sustainable materials. ICNMSF–2026 focuses on emerging trends and innovations addressing global challenges in energy, environment, and technology. The conference includes invited talks, oral presentations, and poster sessions, providing a platform for scientific interaction and collaboration. The conference encompasses a broad spectrum of research areas in next-generation materials, organized under the following thematic tracks:

Energy Materials

- Hydrogen Generation and Storage
- Renewable and Sustainable Energy Materials
- Photovoltaic and Thermoelectric Materials
- Battery and Advanced Electrode Materials
- Supercapacitors

Electronic, Photonic & Magnetic Materials

- Electronic and Optoelectronic Materials
- Photonic Materials
- Magnetic Materials and Phenomena
- Superconducting and Spintronic Materials

Advanced Functional Materials

- Functional 2D Materials and Their Applications
- Advanced Nanomaterials
- Smart and Multifunctional Materials
- Polymers, Ceramics, Glasses, and Composites
- Sensors, Actuators, and Sensing Devices

Computational & AI-Driven Materials Science

- Computational Physics, Modelling, and Simulation
- Machine Learning and AI-Driven Approaches for Materials Discovery, Prediction, and Optimization

About the University

Akal University, Talwandi Sabo, Punjab, India, is a premier institution established under the Punjab Government Act No. 25 (2015) and recognized under Section 2(f) of the UGC Act (1956). The University is dedicated to promoting excellence in higher education through a harmonious blend of scientific knowledge and spiritual values. Founded under the visionary leadership of H.E. (Late) Padma Shri Baba Iqbal Singh Ji, with the blessings of Sant Baba Attar Singh Ji Maharaj, the University strives to realize a mission of value-based education and societal transformation. It is committed to fostering academic excellence, research, and innovation while nurturing ethical and socially responsible individuals. Akal University offers a wide range of undergraduate, postgraduate, and doctoral programmes across disciplines including Physical Sciences, Life Sciences, Social Sciences, Commerce, Management, Education, Languages, and Sri Guru Granth Sahib Studies. The University provides a peaceful, disciplined, and drug-free campus environment equipped with modern infrastructure, laboratories, and research facilities to support holistic development.

About the Department of Physics

The Department of Physics at Akal University is committed to delivering high-quality education and promoting cutting-edge research in both theoretical and experimental domains. The department offers undergraduate, postgraduate (M.Sc.), and doctoral (Ph.D.) programmes in Physics in alignment with the NEP 2020 framework. The research activities of the department span diverse areas such as Condensed Matter Physics, Nuclear Physics, High Energy Physics, and Atmospheric Physics. With a team of dedicated and experienced faculty members, the department aims to create a dynamic academic environment that encourages innovation, critical thinking, and scientific inquiry. The department actively engages in organizing conferences, workshops, and training programmes, providing students and researchers with opportunities to interact with experts and stay updated with recent advancements in the field.

Message from Chief Patron

H. E. (Dr.) Davinder Singh Ji
Chancellor
Akal University

It gives me immense pleasure to learn that the Department of Physics, Akal University, is organizing the International Conference on Next-Gen Materials for Sustainable Future (ICNMSF–2026) from 04–06 May 2026. In the present era, where sustainable development and technological advancement are of paramount importance, the role of next-generation materials has become increasingly significant. This conference, focusing on energy materials, advanced functional materials, and AI-driven materials science, is both timely and relevant. It reflects a strong commitment towards addressing global challenges through scientific innovation and collaborative research. The initiative to bring together scientists, academicians, industry experts, and young researchers from across the globe will not only promote knowledge exchange but also strengthen interdisciplinary research and innovation ecosystems. Such platforms are essential for nurturing scientific temperament and fostering solutions aligned with national priorities like clean energy, self-reliance, and technological progress. I commend the organizing committee for their dedicated efforts in conceptualizing and organizing this important scientific event. I am confident that ICNMSF–2026 will serve as a catalyst for meaningful discussions, collaborations, and advancements in the field of materials science. I extend my best wishes for the grand success of the conference.

Message from Patron

Prof. Gurmail Singh
Vice-Chancellor
Akal University

It is a matter of great pride and honor for Akal University to host the International Conference on Next-Gen Materials for Sustainable Future (ICNMSF–2026).

The conference focuses on navigating emerging energy trends and the complexities of modern materials science. It will address key challenges and opportunities in the field, particularly in areas such as renewable energy materials, nanomaterials, electronic and photonic materials, and computational approaches. These themes are closely aligned with national missions and global sustainability goals, making the conference highly significant in the present scientific and technological context.

ICNMSF–2026 provides a valuable platform for researchers, academicians, and students to engage in meaningful scientific dialogue, exchange innovative ideas, and explore collaborative opportunities. Such initiatives play a crucial role in strengthening research capabilities, enhancing academic excellence, and promoting interdisciplinary approaches to problem-solving. I appreciate the efforts of the Department of Physics and the organizing committee in bringing together a distinguished gathering of experts and young minds. I am confident that the conference will inspire participants and contribute significantly to the advancement of scientific knowledge and innovation. I wish the conference great success and hope it achieves its intended objectives.

Message from Dean Academic Affaris

Maj. Gen. (Dr.) G. S. Lamba
Dean Academic Affairs
Akal University, Talwandi Sabo

It is a matter of immense pride for Akal University to have successfully hosted the International Conference on Next-Gen Materials for Sustainable Future from May 4–6, 2026. Organized by the Department of Physics, this seminar marks a significant milestone in our institutional commitment to fostering high-quality research and global scientific collaboration. The theme of this conference is profoundly relevant as we face global challenges that require innovative, sustainable solutions in energy storage, hydrogen generation, and advanced functional materials. By bringing together distinguished international speakers and young researchers in a hybrid format, this event provided a vital platform for discussing real-time challenges in the design and application of materials from both experimental and theoretical perspectives. In alignment with Akal University's mission to provide value-based scientific education, this seminar has undoubtedly inspired our academic community to push the boundaries of materials science. I extend my heartiest congratulations to the Convenor, Dr. Ramandeep Kaur, and the entire organizing committee for their meticulous execution of this event. I am confident that the insights documented in this report will serve as a valuable catalyst for future research and innovation.

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Keynote Speaker Sessions

K-01

Role of Charge Carriers in the Optoelectronic Properties of Two-Dimensional Nanocrystalline Semiconducting Materials

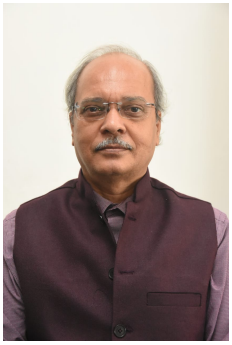
Prof. S. K. Tripathi

Department of Physics, Panjab University, Chandigarh-160 014 (INDIA)

Abstract

2D semiconducting materials are demonstrated to exhibit highly tunable bandgaps, achieved via the control of layers number, heterostructuring, strain engineering, chemical doping, alloying, intercalation, substrate engineering, as well as an external electric field. Semiconducting materials are the heart of electronics and optoelectronic devices and are helpful regarding devices due to their amplification properties, energy changing properties, etc. In present years, there has been considerable attention in the area of the II–VI group nanocrystalline semiconducting thin films because of their large range of applications. Charge transport in 2D semiconductors plays an important role in the optimization of optoelectronic devices. Particularly, charge transport in an epitaxially-grown thin films will dramatically influence its optical and electronic properties. Studies on the carrier diffusion length and carrier diffusion coefficient provide the figure of merit for these devices. In the present talk, the role of charge carriers in the opto-electronic properties of such nanocrystalline semiconducting layers which are determined, by the steady-state photocarrier grating method (SSPG) and steady-state photoconductivity ($\mu\tau$) measurements, in a coplanar configuration will be discussed. The conditions for the validity of the procedure for determining the ambipolar diffusion length, Lamb, from SSPG measurements are carefully examined and found to hold in these thin films by taking certain precautions. These results will be compared with the results obtained from the time-of-flight (TOF) technique. Some very recent interesting results obtained in the laboratory will also be discussed during the talk.

Biography



Prof. S. K. Tripathi
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Dr. Surya Kant Tripathi is a Professor and Chairperson of the Department of Physics, Panjab University, Chandigarh. He holds an M.Sc. and Ph.D., and completed postdoctoral work at the Department of Physics, IIT Kanpur. His research expertise lies in experimental condensed matter physics, nanoscience and nanotechnology, thin films, and device fabrication. He has published more than 400 research papers in SCI journals and over 100 papers in proceedings published by reputed publishers such as Elsevier, Springer, and AIP. With more than 12,300 citations and an h-index of 48, he has guided 55 Ph.D. scholars and 40 M.Tech. students. He has also completed 26 research projects funded by agencies including DST, CSIR, UGC, and IUAC. Prof. Tripathi has been listed among the Top 2% World Scientists by Stanford University, USA, and has delivered several invited talks at national and international conferences. He has edited books, contributed chapters to internationally published volumes, organized numerous conferences, and served as a reviewer for several reputed international journals.

K-02

Interface-Driven Properties of Two-Dimensional Materials

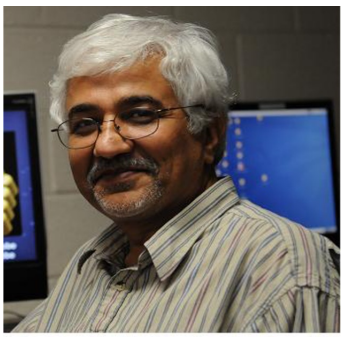
Prof. Ravindra Pandey

Physics Department, Michigan Technological University, Houghton, MI, USA

Abstract

The discovery of graphene has sparked significant interest in two-dimensional (2D) materials due to their unique properties. Graphene-based heterostructures, considered for novel applications, consist of interfaces. In this talk, we will highlight how interfaces govern the electronic, mechanical, and optical properties of these heterostructures, using state-of-the-art first-principles methods. Examples such as two-terminal electronic devices, graphene/polymer composites, and van der Waals heterostructures demonstrate that a fundamental understanding of interfacial interactions is important for advancing the applications of atomically thin 2D materials.

Biography



Prof. Ravindra Pandey
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Dr. Ravindra Pandey holds the position of Professor of Physics and serves as the Chair of the Department of Physics at Michigan Technological University, Houghton, MI, USA. He received his undergraduate and graduate degrees from Dr. Hari Singh Gaur University, Sagar; the National Physical Laboratory, Delhi; the Atomic Energy Research Laboratory, UK; and the University of Manitoba, Winnipeg, Canada.

Engaging in multidisciplinary research, both theoretical and experimental, he has contributed significantly to the development of programs focused on crystals, surfaces, and nanostructures. His highly cited research includes bulk alkaline-earth sulfides and Ga_2O_3, low-dimensional materials such as graphene, BN monolayers, phosphorene, antimonene and their heterostructures, transition metal–benzene complexes, and bioconjugated nanomaterials.

Prof. Pandey has played a pivotal role in organizing and contributing to several international conferences and workshops on materials modelling and nanoscale science. He is also recognized as a Fellow of the American Physical Society.

K-03

World Record in Green Hydrogen Production by Hydroelectric Cells: India's Gift to the World—Globally Recognized and Validated!

R K Kotnala

Chairman New Science Creators Institute, New Delhi, India

Abstract

A Dual Disruptive Technology: Green Hydrogen and Clean Electricity Generation by a Hydroelectric Cell invented by Prof R. K. Kotnala & Dr Jyoti Shah, which is the biggest invention of the 21st century in the green energy domain. Hydroelectric Cell is based on oxygen-deficient nanoporous ferrite/metal oxide (Sustinable Material), achieving spontaneous water splitting without using any catalysts, acid, alkali, electrolyte, or light. What sets the Hydroelectric Cell apart from every existing energy technology is its dual disruptive capability: its solar cell current density and its Green Hydrogen generation surpass modern electrolyzer capabilities. It simultaneously generates Green Hydrogen—the fuel of the future—and Clean Electricity, both from the simplest substance on Earth: water and it is radically simpler, safer, and more cost-effective than Solar Cells, Fuel Cells, or conventional electrolyzers. Hydroelectric Cell technology offers safe, clean, low-cost, and reliable power generation. This technology applies to a wide range of portable, stationary, and transport applications—from battery chargers and low-power devices to domestic energy needs and automotive power sources—with the potential to significantly reduce urban pollution. Moreover, the Hydroelectric Cell is Biocompatible, supports Circular Economy, and contributes to net-zero carbon accomplishments. Unlike lithium-ion batteries and conventional fuel cells that generate hazardous chemical waste, the Hydroelectric Cell is designed with the planet in mind from the beginning. The cell is a potential alternative to solar cells and fuel cells for achieving a net-zero carbon goal. Its materials are biocompatible, its by-products—Zinc hydroxide nanoparticles and hydrogen gas—are non-toxic and industrially valuable, and its end-of-life disposal poses no environmental hazard. This makes the HEC a perfect fit for a circular economy, where energy generation leaves no harmful footprint.

Biography

Prof. R. K. Kotnala
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Dr. R K Kotnala is an Indian scientist, who is world-renowned for his spectacular work in Net Carbon Zero, Hydroelectric Cell, Water Splitting by Non-Photocatalytic process, Nanomaterials, Multiferroic, Spintronics, Magnetics & Biomedical Devices Metrology. With his constant hard work and dedication Dr. Kotnala, along with Dr. Jyoti Shah, has contributed exceptionally, a path-breaking invention of a green and clean energy device-Hydroelectric Cell. The hydroelectric cell is an astounding, miraculous, and incredible invention in the green energy domain and a panacea towards achieving Net Carbon zero. Dr. Kotnala is well known in the science fraternity for his outstanding contributions in the field of Solar cells, Multiferroics, Spintronics, Clean Energy, Environmental sciences, and Values of Scientific Ethics. He has written many books, chapters and delivered countless scientific lectures in diversified areas. He is also creating awareness for science among youth through numerous invited talks and YouTube videos on simple scientific concepts.

PLENARY TALK

Distinguished Speaker Sessions

P-01

DFT Calculations to Explore Materials for Thermoelectric Applications

Ranjan Kumar

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Abstract

Energy in any form is global index of prosperity of a nation. With growing population need for energy also grows exponentially. In this scenario it is not possible and good to rely on single source of energy. Fossil fuel has been and will remain major source of energy for domestic and industrial use. There has been constant quest for alternative sources of energy. Thermoelectricity is one such area which exploits the waste heat and convert it to electricity. Although it has been discovered long back theoretically as well as experimentally. The issue of low efficiency always limits its application to real world scenario. In last 2 decades the research in this area has got a boost to explore materials and devices with high efficiency to convert heat to electricity. DFT calculations have been a great success to predict structure and transport properties of materials. In this talk we will explore some materials which are potential thermoelectric materials.

P-02

Engineering 2D Nanomaterial Interfaces: From Defect-Induced Physics to Plasmon-Enhanced Sustainable Applications

Anirban Chakraborti

School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi, India

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Abstract

This talk presents a unified framework for understanding and engineering two-dimensional (2D) nanomaterials, with a particular focus on MoS_2-based systems, through the interplay of defects, interfaces, and resonance phenomena. By integrating ab initio computational insights with systematic experimental investigations, this talk elucidates how defect engineering, plasmonic coupling, and heterostructure design collectively govern charge transfer, energy transfer, and optical enhancement mechanisms. These fundamental principles are harnessed to demonstrate high-efficiency photocatalysis, ultrasensitive surface-enhanced Raman scattering (SERS) detection, and tunable bio-nano interactions. Collectively, the findings establish a coherent design pathway toward next-generation multifunctional nanomaterials with promising applications in sustainable wastewater remediation, chemical sensing, and advanced biomedical technologies.

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P-03

Tailoring Noble Metal Atomic Wires for Enhanced TE Performance and Spin Seebeck Effect via Alloying and Decoration: First-Principles Simulations

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Abstract

Recent advances in nanoscale techniques, viz. mechanically controlled [1] and scanning tunnelling microscopy [2] break junction methods, have enabled transport measurements through nanowires (NWs) of varied length and geometry. Novel effects emerge in transport (such as quantization of electrical [3] and thermal [2] conductance, oscillatory thermopower [4], etc.) in the course of stretching bulk NWs down to atomic-sized contacts, suggesting its control via manoeuvring of atomic-scale geometry. Recently, we have carried out extensive simulations of coherent transport in free-standing ultrathin noble metals (Cu, Ag, Pt, Au) NWs along different crystallographic directions using a non-equilibrium Greens function based first-principles approach, with focus on improving thermoelectric (TE) performance. Topological manipulation [5], and composition alteration via alloying [6] and decoration [7] of NWs with Pt are found to be effective means of improving TE efficiency. Remarkably, Pt alloying induces ferromagnetism and some topologies develop half-metallic conduction, with alloying also introducing energy gap(s) in the phonon spectra. Consequently, alloyed NWs exhibit spin Seebeck effect, and a reduction in the electronic and phononic conductance over pristine NWs, which yields significantly improved charge (ten-fold) and spin figures of merit. Furthermore, our simulations show that Pt-decoration brings in dramatic changes in the electronic structure of NWs, and it may be an alternative to alloying to achieve spin caloritronics. In this talk, I would share how topological tailoring can be exploited together with alloying and decoration for achieving an improved TE performance.

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INVITED TALKS

Distinguished Speaker Sessions

IN-01

Tetrapods based Advanced Materials for Advanced Technologies

Yogendra Kumar Mishra

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Abstract

Considering the size dependent utilization complexities of nanoscopic dimensions tin real technologies, the focus of nanomaterials community is converging to three-dimensional (3D) smart nanomaterials which are built out of interconnected nanostructures building blocks. This talk will briefly introduce the importance of tetrapod nanostructures towards smart 3D ceramic nanostructuring via a simple and single step flame-based approach for synthesis of zinc oxide tetrapods. These ceramic tetrapods have already demonstrated their potential roles in many different technologies. These zinc oxide tetrapods can be used as solid backbone or sacrificial templates to design hybrid or new tetrapods as smart materials. These smart 3D nanomaterials offer many applications in engineering and advanced technologies. Application examples of 3D ceramic tetrapods in nanosensing, optical sensing, whispering gallery mode resonances, light trapping and guiding, composite engineering, antiviral candidates, water purification, piezotronics, agriculture, and in several other applications will be demonstrated [1-10]. The integration of tetrapods in electrospun fibers offer many advantages in biomedical engineering and few examples about nano-engineered electrospun fibers will be presented as recent developments.

Keywords: Zinc Oxide Tetrapods, Smart Materials, Advanced Technologies

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IN-02

Emergent Multiferroicity in Certain Two Dimensional Rare-Earth Halide Based Monolayers

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Abstract

There is a huge surge in research activities, of late, to achieve multiferroicity in two-dimensional materials due to their enormous potential for applications in nanoelectronic and spintronic devices. I will discuss our recent work [1, 2] on Eu-substituted GdX_2 (X = Cl, I) monolayers. In Eu-substituted $GdCl_2$ we predict, based on our first-principle calculations, a triferroic phase with three ferroic orders—ferromagnetism, ferroelectricity, and ferroelasticity— coexisting simultaneously whereas in Eu-substituted GdI_2 we observe a polar metallic phase which is both ferromagnetic as well as ferroelastic. This is achieved in the GdX_2 monolayers (ferromagnetic semiconductor) by hole doping via substitution of $1/3^{rd}$ of the $Gd^{2}+$ ions with Eu^{2+}. The emerging metallic state in $GdCl_2$ undergoes a bond-centered charge ordering which makes it semiconducting again as well as ferroelastic. Further, the associated lattice distortions break the lattice centrosymmetry leading to a noncentrosymmetric charge distribution, which makes the monolayer ferroelectric, at the same time. The two ferroic orders, ferroelectricity and ferroelasticity, present in the Eu-substituted $GdCl_2$ monolayer are found to be strongly coupled, making it a promising candidate for device applications whereas simultaneous coexistence and coupling of the ferroic orders in a metallic 2D material makes the Eu substituted GdI_2 monolayer an incredibly rare material for nano-electronics and spintronics applications. Finally, I would like to discuss, a mechanism we proposed recently, in Gd-substituted $EuCl_2$ monolayer and Li-intercalated $CrBr_3$ monolayer, where the valley splitting is caused by an in-plane electric polarization and the coupling between the two makes it possible for an electric field to control the valley degree of freedom[3].

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IN-03

Photovoltaic Solar Cells for Sustainable Energy Development

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Abstract

Sustainable development requires long-term solutions to growing environmental and energy challenges. Renewable energy technologies, particularly solar photovoltaic (PV) systems, offer a promising pathway toward clean and sustainable energy production. This study highlights the role of photovoltaic solar cells in addressing global energy demand, which is projected to double by 2050. Solar energy, as the largest renewable resource, provides an abundant and environmentally friendly alternative to fossil fuels, which are finite and associated with significant environmental impacts. PV technology directly converts sunlight into electricity and is increasingly being adopted for residential, commercial, and industrial applications due to its scalability and declining costs. Ongoing advancements in photovoltaic materials and device engineering are improving efficiency and reducing production costs, strengthening the role of solar cells in the global transition to low-carbon energy systems.

Keywords: Photovoltaic solar cells, renewable energy, sustainable development, solar energy, clean energy

IN-04

Solar Energy Breakthrough: Hybrid Halide Perovskite Solar Cells with Enhanced Efficiency and Stability

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Abstract

Currently, the non-renewable energy resources are the main source to fulfil the demand of energy in the world. But the rapid degradation of these traditional resources and several environmental effects associated with them created a need to find alternate ways to harness energy for securing the future of coming generations. In order to develop the advanced renewable and clean energy resources, harnessing solar energy has always been a top choice. Amongst the available solar energy harnessing materials, Hybrid Halide Perovskite (HHP) solar cells, belonging to 3^{rd} generation, may likely be able to reach at 30 % power conversion efficiency (PCE) with extremely low cost and be ready for industrial usage in the next 10-15 years. It is expected by observing the increase in PCE of these cells that these perovskite solar cells will be available as an alternative of Silicon-based solar cell technology (which is most common in market today). Further the scientists are making good efforts in reducing the toxicity and enhancing stability of perovskite based solar cells as well. In this regard, there is a lot of scope for further improvement and realization of high performance hybrid halide Perovskites solar cells with flexibility. In the talk, both, wet and dry lab techniques to design and demonstrate HHP solar cells will be discussed. The overview of the discovery of perovskites as PV materials, followed by discussions on their performance, their stability, present challenges, and future prospects will be covered. Some results from our group will be shown to justify the potential of these HHP based solar cells.

Keywords: Photovoltaics; Perovskites; Power Conversion Efficiency; Renewable Energy

IN-05

Hybrid Supercapacitors: Fundamentals and Future of Energy Storage Devices

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Abstract

The energy storage devices like supercapacitors (SCs) are getting the most noteworthy consideration from researchers and industrialists because of their superior power density, excellent rate capability, long cycle performance, and less repairing than other energy storage devices. The characteristics of the electrode material are the key parameter for the electrochemical performance of supercapacitors. According to the charge storage mechanism of supercapacitors, the electrode materials are divided into two classifications: faradic materials and electric double layer materials. In previous studies, it has been reported that specific capacitance (Cs) value offered by faradic materials is much higher than electric double layer-based materials. Further, relative to single metal oxides, transition metal oxides (TMOs) exhibits more prominent electrochemical properties because of synergistic redox reactions of different cations which leads to high capacitance and long-term cyclic stability. In this talk, we will discuss the fundamental of the supercapacitors with the main focus on the classification and charge storage mechanisms. Then, important performance parameters and their interrelation will also be presented followed by crucial characterization techniques to examine supercapacitors performance. Further, the fabrication process of hybrid supercapacitor device will be discussed along with potential of hybrid supercapacitors as an energy storage device.

Keywords: Renewable Energy, Energy Storage, Hybrid Supercapacitors.

IN-06

New Functionalities Derived by Tailoring Multiferroics for Sustainable Wastewater Purification

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Abstract

Bismuth ferrite ($BiFeO_3$) is gaining significant attention as an efficient photocatalyst for wastewater purification due to its narrow band gap (~2.4–2.8 eV), good chemical stability, and strong absorption in the visible region. These properties enable effective utilization of solar energy for the degradation of organic pollutants in water. In this work, we highlight the role of band gap engineering in enhancing the photocatalytic performance of $BiFeO_3$. Through strategies such as nanostructuring and aliovalent ion substitution, the band structure can be tuned to improve light absorption, charge carrier separation, and redox efficiency. This tuning allows better alignment of conduction and valence band positions with respect to pollutant degradation reactions, leading to enhanced generation of reactive species. As a result, modified $BiFeO_3$ demonstrates improved photocatalytic activity, and good reusability, making it a promising material for sustainable wastewater treatment. This study emphasizes the potential of tunable band gap $BiFeO_3$ as a cost-effective and environmentally friendly solution for real-world water purification challenges.

IN-07

Many-Body Electron Correlation Effects in Quantum Materials

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Abstract

We investigate the stability and phase structure of electron–hole pairing in a strictly one-dimensional biwire system using diffusion Monte Carlo simulations. By varying both the carrier density and the interwire separation, we map out an exotic quantum phase diagram spanning the excitonic regime, the two-component plasma, and a correlated Wigner-crystal-like state. At sufficiently small separations, the ground state exhibits robust excitonic order, reflected in strong electron–hole correlations and a suppressed two-component plasma response. Increasing the separation drives a sharp crossover into an unbound two-component plasma at high density, whereas at low density the system instead enters a quasi-Wigner-crystalline phase. The resulting phase boundary shows that excitonic binding persists over a surprisingly wide range of parameters, exceeding mean-field expectations.These results provide a fully many-body, nonperturbative benchmark for exciton formation in one-dimensional electron–hole systems and establish quantitative constraints for realizing 1D excitonic phases in semiconductor nanowire heterostructures.

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IN-08

Atomic Clusters for Energy Applications

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Abstract

Atomic clusters serve as highly efficient catalysts for hydrogen production and hydrogenation of CO_2 by leveraging their quantum size effects and high surface-to-volume ratios to activate and convert CO_2 into fuels and chemicals. Their discrete electronic structures enable the adsorption of CO_2 and reaction intermediates, while atomically precise compositions and ligand environments allow for the rational tuning of activity and selectivity toward products such as CO, formic acid, and methanol. To this end, I will discuss the structural and electronic properties of atomic cluster catalysts consisting of 3d and 4d transition-metal elements. The interaction of CO_2 with these systems has been thoroughly investigated to identify optimal compositions for efficient capture and activation. I will further discuss the fundamental connection between electronic back-bonding and CO_2 adsorption mechanisms, highlighting configurations that promote effective activation. The systematic evaluation of d-orbital contributions, back-bonding effects, and activation pathways in transition-metal clusters provides key design principles for developing efficient catalysts aimed at carbon dioxide mitigation.

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IN-09

Study of Lithium Lanthanum Zirconate Thin Films using X-ray Absorption Spectroscopy

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Abstract

Rechargeable batteries are challenged by the safety and size issues. These issues are related with the liquid nature of electrolytes used for these batteries. Therefore, efforts to replace such electrolytes with solid state electrolytes (SSE) are underway. Incorporation of these SSEs in rechargeable batteries has added advantage of size miniaturization as batteries can be designed in thin film form. This enables the integration of rechargeable batteries in microelectronic devices. Despite these advantages, SSEs faces issues of the poor ionic conductivity. Therefore, design of SSEs with ionic conductivity needed for effective ion migration from anode to cathode and vice versa is essentially required. As ionic conductivity is influenced by the synthesis condition, stoichiometry, doping ions, hence, this work is focussed on the growth of lithium lanthanum zirconate (LLZO) for thin film battery. LLZO has potential to be utilized for Li ion rechargeable because of it's moderate value of ionic conductivity. This material when grown in thin film form faces several challenges. Hence, this work presents systematic investigations on the growth of lithium lanthanum zirconate (LLZO) by using radio frequency (RF) sputtering.

To study the substrate dependence, growth of LLZO is studies on different substrates such as glass, quartz and Si. Impact of deposition parameters such as sputtering power, sputtering power durations is also studies on the stoichiometry and crystalline phase of LLZO film. Effect of post-deposition annealing on the growth of LLZO film is also investigated. All these investigations are carried out using X-ray absorption spectroscopic (XAS) study to throw light on the mechanistic understanding of film growth.

Acknowledgement

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IN-10

Designing of Transparent Broadband Photodetectors

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Abstract

Futuristic electronics require the development of flexible and transparent electronic devices. Flexible electronics provide the utility of devices in bending and stretched conditions, like in wearable devices, phone displays, and strain gauges in bridges etc. [1,2]. On the other hand, transparent electronics enables us to see through devices, which is an emerging and state-of-the-art technology for the development of the next generation of electronic and optoelectronic devices like transparent displays, solar cells, LEDs, photodetectors (PDs), sensors, Li-ion batteries, etc. [3–4]. The broadband (BB) or broad spectral (BS) or multispectral (MS) PDs are essential for the development of the high quality and hyperspectral image systems and thereby boost the performance and capabilities of the devices of its area of applications in safety and security, smart phone cameras, night vision, automotive sensor systems, innovative band switches, food and pharmaceutical inspection, and memory storage etc. [5, 6]. Additionally, the MS/BB PDs may reduce the complexity and cost of an electronic circuit by reducing the number of single/specific colour PDs. Indeed, the designed PDs that employ sole photoactive material (SPM) are limited to detecting a narrow spectrum and hardly respond under a broad spectrum ranging in UV-Vis.-NIR. To overcome the limitations of SPMs, heterostructure (HS) is one of the broadly used approaches. In practice, the choice of heterogeneous materials, their bandgap, electrical conductivity, and band alignment are very critical for the development of high-performance BB PDs.

Keywords: Metal oxides and Metal sulfide nanostructures, Doping, Heterostructures, Broad Band Photodetectors.

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IN-11

AI-Driven Monte Carlo Modeling for Radiation Damage and Reliability in Sustainable Materials

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Abstract

The extent of the radiation damage of a material strongly depends not only on its properties but also on the irradiation condition. In the present study, an artificial intelligence-driven Monte Carlo framework has been established to examine radiation damage in various irradiation cases by means of simulation data obtained via the JA-IPU code. Radiation effects of 1 MeV photons on iron (Fe) and of silicon ions on 3C-SiC are investigated, allowing the comparison between electronic and nuclear radiation damage processes. By adopting machine learning-based surrogate models, radiation damage can be predicted effectively with high prediction efficiency, where the test R^2 and cross-validation R^2 are 0.816 and 0.812, respectively, in case of Fe. By means of feature importance analysis, it is found out that the electronic stopping power plays an important role in photon-irradiated Fe. On the other hand, atom–atom collision cross-section and PKA-related parameters play a dominant role in ion-irradiated 3C-SiC. Furthermore, a classification model is adopted to distinguish the responses of silicon and carbon atoms in 3C-SiC, where the cross-validation accuracy reaches 0.936. Overall, the difference in irradiation condition leads to a shift in the governing mechanism of radiation damage from electronic energy loss to nuclear atom–atom collisions.

Key words: Radiation Damage, Monte Carlo Simulation, Machine Learning, Photon and Ion Irradiation, Silicon Carbide (3C-SiC)

IN-12

Turning Waste into Function: Flash-Polymer Composites for Photocatalytic Dye Degradation

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Abstract

Growing levels of discharge of effluents from industries loaded with dyes pose environmental hazards and adversely impact public health; therefore, developing sustainable solutions for such waste management becomes imperative. This study involves valorization of fly ash, a widely available industrial waste material, into functional polymer composites to be used for photocatalytic degradation of dye-loaded effluents. Fly ash-polymer composites were prepared through simple synthesis methods to ensure adequate mixing and distribution of inorganic particles in the polymer. Various structural, optical and morphological analyses have confirmed enhanced surface area, improved light harvesting and photoinduced charge separation properties.

Degradation capability of the prepared composites has been assessed by conducting experiments on selected organic dyes under UV and/or visible light irradiation. Enhanced efficacy was observed during the process, due to synergistic effects arising from fly ash particles and polymer matrix. Improved efficacy was a result of improved adsorption of dyes and faster generation of reactive oxygen species. Kinetics involved in the process followed first order kinetics, demonstrating catalytic ability. Moreover, the composites exhibited stability and repeatability, thereby demonstrating the potential utility in real-world applications.

Key words: Fly Ash, Photocatalysis, Dye Degradation, Wastewater Treatment, Sustainable Materials, Organic Pollutants

IN-13

Quantum Devices and Circuits

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Abstract

Quantum devices exploit quantum-mechanical carrier transport mechanisms such as superposition, entanglement, and tunneling to overcome the fundamental limitations of conventional devices like MOSFET. In this talk, we will cover quantum mechanics principles and basics quantum electronic devices which include Tunnel FET, Quantum dots and Spin-based devices. To comment on quantum computing and specifically the quantum circuit model of computation, we will discuss key terms including unitary matrix, reversibility, qubit, quantum logic gates such as Pauli, CNOT, SWAP and Toffoli etc.

IN-14

Nano Semiconductor Materials and Devices

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Abstract

The continued scaling of conventional CMOS technology is approaching its fundamental physical and technological limits, posing critical challenges for realizing next-generation high-speed, ultra-low-power, and cost-effective electronic systems. As the traditional trajectory of Moore's law slows, there is an urgent need to explore alternative paradigms rooted in nano semiconductor materials and devices. This talk focuses on the emerging landscape of nano semiconductor materials, including low-dimensional systems such as nanowires, 2D materials, and quantum-confined structures, which offer superior electrostatic control and enhanced carrier transport properties. At the device level, novel architectures based on these materials are being actively investigated to overcome short-channel effects, variability, and power dissipation challenges inherent in deeply scaled CMOS technologies. Furthermore, the discussion highlights the importance of physics-based modeling and simulation frameworks that accurately capture process-induced variations and short channel effects in nanoscale devices. The integration of nano semiconductor devices into advanced computing architectures, including bio-sensor and optical applications, is also explored, emphasizing their potential in enabling energy-efficient memory and logic solutions for complex computational tasks. Overall, nano semiconductor materials and devices represent a promising and evolving frontier, offering transformative opportunities for the future of electronics beyond the CMOS era.

IN-15

Attosecond-XUV Photon Pulse Generation Using Mid-Infrared Laser in Argon Gas

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Abstract

Attosecond time-resolved spectroscopy is one of the most powerful techniques for observing electron motion in real time domain. To understand chemical bonding, ionization, charge transfer, or ultrafast electronic relaxation, you need sources with attosecond resolution. Typical chemical reactions happen in femtoseconds (10^{-15} s), but the underlying electron rearrangements occur much faster, in attoseconds. Moreover, isolated attosecond pulse with broad spectral bandwidth are indispensable for probing ultrafast electronic dynamics in atoms and molecules. In this work, we investigate high-harmonic generation (HHG) in argon driven by a two-colour laser field and examine its effectiveness for generating stable isolated attosecond pulses. The two-colour field is synthesized by fixing the wavelength of the primary laser while varying that of the secondary laser. Our analysis shows that the HHG cutoff and the resulting attosecond pulse characteristics depend sensitively on the electric-field composition, pulse durations, relative time delay between the two pulses, carrier-envelope phase (CEP), and laser intensities. Compared with conventional single-colour HHG, the two-colour approach offers several important advantages, including extension of the harmonic cut-off into the water-window spectral region, significant enhancement of the harmonic yield, and improved control over isolated attosecond pulse generation. Using laser pulses with durations of 5–10 fs (FWHM), we demonstrate the generation of a stable isolated attosecond pulse with central photon energy of 341 eV and a pulse duration of 125 attoseconds (FWHM). Such pulses provide an exceptional ultrafast probe for directly observing electron dynamics in atoms, molecules, solids, and other systems evolving on the attosecond timescale.

Keywords: High Harmonic Generation, Isolated Attosecond Pulse, Argon Gas, Dipole Approximation, Two-Colour Laser Field

IN-16

Solid State Cold Spray Deposition: Introduction, Evolution, Applications and Future

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Abstract

Thermal spray (TS) refers to a group of coating technologies used to deposit materials in the form of molten or semi-molten particles through the application of high thermal and kinetic energy. As an evolving field, TS has witnessed the development of several processes over the years, including Arc Spray, Flame Spray, Plasma Spray (PS), Detonation Gun (D-gun) Spray, High-Velocity Oxy-Fuel (HVOF) Spray, and Cold Spray (CS), all aimed at producing coatings with enhanced properties. CS is a relatively recent addition to the TS family. Unlike conventional TS processes, where deposition occurs through molten or semi-molten particles, CS relies on the kinetic energy of solid particles accelerated to high velocities to form coatings upon impact with the substrate. This unique mechanism enables the production of oxide-free coatings with properties comparable to bulk materials, making CS particularly attractive for depositing low-melting-point and thermally sensitive materials, especially in healthcare and aerospace applications. Furthermore, due to its effective bonding mechanisms and ability to produce thick deposits, CS extends beyond traditional surface engineering and is increasingly recognized as a competitive technique for additive manufacturing (AM) and repair applications. Another significant advantage of CS is the convenience of employing simulations to understand coating behavior prior to experimental trials. This talk will introduce the fundamentals of Cold Spray, highlight its evolution as a competitive technology within the TS domain, and explore its potential in surface engineering and additive manufacturing applications.

IN-17

Harnessing Visible–Solar Light for Sustainable Energy, Environmental Remediation, and Fine Chemical Synthesis through Green Photocatalysis

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Abstract

Green photocatalysis under visible–solar light irradiation has emerged as a powerful and sustainable approach to address global challenges related to energy scarcity, environmental pollution, and fine chemical synthesis. The integration of visible-light-active materials with green chemistry principles minimizes energy consumption, reduces hazardous by-products, and promotes eco-friendly chemical processes, making visible–solar-driven photocatalysis a key technology for sustainable development. This presentation will focus on the fabrication, and application of a series of advanced hybrid nanostructures (1-10) such as Au/Ag/Cu-loaded TiO_2, CdS, ZnS, graphene oxide/reduced graphene oxide coated Ag–TiO_2, C3N4-passivated Au–TiO_2 and bimetallic core–shell Pd@Ni deposited on TiO_2, photocatalysts. Photocatalytic green H_2 production, catalytic hydrogenation of industrially important selective hydrogenation of carbonyl compounds and unsaturated aldehydes will be emphasized in details. These hybrid nanomaterials demonstrate superior photocatalytic performance in diverse applications, including hydrogen (H_2) evolution via water splitting, dehydrogenation of waste alcohols, reduction of nitroorganics, and degradation of toxic pollutants in wastewater under UV, visible, and solar irradiation. The talk will highlight detailed insights into their surface morphology, structural, and physicochemical properties as characterized by different instrumental techniques. Special emphasis will be placed on the role of (i) metal co-catalyst deposition, (ii) graphene oxide integration, (iii) core–shell composition, and (iv) semiconductor choice, in enhancing photocatalytic efficiency. Collectively, these findings provide valuable insights into the rational design of multifunctional nanocomposites for sustainable energy production and environmental remediation.

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IN-18

Next-Generation Food Packaging Using 0D–2D Nanocomposites: A Route to Extended Shelf Life and Eco-Friendly Solutions

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Abstract

The growing demand for sustainable and high-performance food packaging has accelerated the development of advanced nanocomposite materials. In this study, we report the design and fabrication of next-generation poly(vinyl alcohol) (PVA)-based 0D–2D nanocomposite films incorporating MoS_2 nanosheets and carbon quantum dots (CQDs). The synergistic integration of 0D CQDs and 2D MoS_2 within the PVA matrix results in a multifunctional packaging material with significantly enhanced physicochemical and functional properties. The developed PVA/MoS_2–CQDs nanocomposites exhibit excellent ultraviolet (UV) blocking capability, effectively protecting food products from photo-induced degradation. Oxygen transmission rate (OTR) measurements reveal a substantial reduction in oxygen permeability due to the tortuous path created by the well-dispersed nanofillers, thereby minimizing oxidative spoilage. Mechanical analysis demonstrates notable improvement in tensile strength and structural integrity, ensuring durability and handling stability during packaging applications. Furthermore, the nanocomposite films display strong antimicrobial activity against common foodborne pathogens, attributed to the reactive oxygen species generation and surface interactions of CQDs and MoS_2. These combined properties contribute to a marked extension in the shelf life of perishable food items, as validated through storage studies on fresh-cut produce. Overall, this work highlights a sustainable and scalable strategy for developing multifunctional biodegradable packaging materials. The PVA/MoS_2–CQDs nanocomposite films offer a promising solution for next-generation food packaging by integrating enhanced barrier, mechanical, UV-protective, and antimicrobial functionalities, thereby improving food quality, safety, and longevity while reducing environmental impact.

Keywords: 0D–2D nanocomposites; PVA/MoS_2–CQDs; Food packaging; UV-blocking; Oxygen barrier (OTR); Antimicrobial activity

IN-19

Tiny Materials With Huge Potential: Nanoparticle Reinforced Hydrogels for Osteoporotic Bone Repair

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Abstract

There are very few regenerative biomaterials in the orthopaedic commercial space. The most successful, Medtronic's InFUSE® bone graft, targets anabolism via rhBMP-2 soak-loaded onto a collagen sponge at a supraphysiological concentration, but has been associated with a number of risks. For minimally invasive procedures, bone cements (e.g. PMMA) are commonly used but are non-reparative and have been linked to adverse complications in patients. Whilst hydrogels provide an ideal platform for tissue regeneration in terms of biocompatibility and biodegradability, their mechanical and structural properties often deem them unsuitable for bone. There is a major unmet clinical need for minimally invasive regenerative biomaterials. The aim of this work is the development of thermoresponsive hydrogel platforms, functionalised with therapeutic nanoparticles (NPs), designed to repair or replace tissue via minimal invasive techniques. Specifically, this work focuses on producing natural polymeric networks incorporating carbon nanotubes, ceramic and metal based nanoparticles to develop mechanically robust hydrogels with regenerative properties.

IN-20

Quantum Dots from Fundamental to Sustainable Technology Development

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Abstract

As the global community accelerates its transition toward sustainability, nanoengineering has emerged as a transformative force across the clean energy and smart agriculture sectors. At the heart of this innovation are colloidal quantum dots (QDs), solution-processable nanocrystals whose optoelectronic properties can be finely tuned by size, shape, and composition, thanks to quantum confinement. Their exceptional properties, including broadband absorption (300–2000 nm), large absorption cross-section, potential for multiple exciton generation (MEG), and hot-carrier extraction, position QDs as versatile building blocks for next-generation photovoltaic devices, solar-driven hydrogen production, and smart agriculture technologies. However, the performance of QD-based clean energy and smart agriculture devices is still lower than the expected theoretical value, which is mainly due to slow charge injection/transfer rates from QDs to scavengers and fast non-radiative carrier recombination within the QDs and at the QDs/metal oxide/electrolyte interface. To address these challenges, surface engineering of QDs, in which the QD core surface is passivated by a shell layer of varying thicknesses and compositions, is an effective approach. This talk will cover the journey of colloidal QDs from fundamental research to practical product development. A detailed discussion of the impact of advanced surface engineering of colloidal QDs via shell growth, composition, and interfacial layers between the core and shell on the optoelectronic properties of QDs will be presented. Finally, the integration of optimized colloidal QDs into clean energy technologies such as photovoltaics, green hydrogen production systems and smart agriculture technologies will be presented, and possible pathways for future innovation and commercialization will be outlined.

Keywords: Nanoengineering, Quantum Dots, Carrier-Dynamics, Clean Energy, Smart Agriculture

IN-21

Hybrid Supercapacitors: A Smart Energy Storage Solution for Sustainable Development

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Abstract

Humanity faces major challenges, including rising energy demand, pollution, water scarcity, food insecurity, and poverty. Among these, energy is most critical because industries, healthcare, education, transport, and communication depend on reliable electricity. However, excessive use of fossil fuels has led to climate change, air pollution, and resource depletion. Therefore, renewable energy and efficient storage systems are essential for a sustainable future. In this regard, hybrid supercapacitors have emerged as a promising solution. Hybrid supercapacitors are advanced energy storage devices that combine the fast charging, high power density, and long cycle life of supercapacitors with the higher energy density of batteries. As a result, they store more energy and deliver power rapidly, making them ideal for modern applications.

Their importance increases when integrated with intermittent renewable sources such as solar and wind energy. They can store excess energy and supply it during peak demand, improving efficiency and grid stability. Applications include electric vehicles, portable electronics, backup systems, and smart grids. Environmentally, hybrid supercapacitors reduce dependence on fossil fuels, lower carbon emissions, and decrease electronic waste due to their long lifespan. Economically, they can improve rural electrification, generate employment, and support sustainable growth. Although challenges such as cost and material development remain, continued research can overcome these barriers, making hybrid supercapacitors vital for future clean energy systems.

IN-22

Machine Learning Assisted Study of Materials for Energy Applications

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Abstract

The rising demand for clean and green energy sources has sparked global interest in sustainable energy conversion and storage technologies driven by solid state materials. The conventional first principles calculations are computationally intensive for solid state materials as number of atoms increases in the system of study. Incorporating a machine learning (ML) workflow into the conventional first principles method could significantly reduce the time and resources needed. Also, the size of the dataset for high-throughput computation is often in the order of hundreds or thousands; exploring each of them poses a huge challenge. However, machine learning-assisted screening solves this constraint to a great degree. In this talk, machine learning assisted first principles study will be demonstrated for energy conversion such as photocatalytic water splitting using van der Waals heterostructures and energy storage such as NASICON-type solid state electrolytes for Na-ion batteries. These studies demonstrate the usefulness of a hybrid ML-DFT strategy in accelerating the search for promising water splitting photocatalysts and solid-state electrolytes for Na-ion batteries.

IN-23

Polypyrrole Based Electrodes for Supercapacitor Devices: Significance of Mass Loading on Electrochemical Performance

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Abstract

Supercapacitors are promising energy storage devices of recent era that are designed to make efficient energy storage devices with fast charging capacity and considerable energy and power density. Conducting polymer such as Polypyrrole (PPy) electrode material is explored for its high conductivity, reversible doping–dedoping behaviour with easy synthesis methodology. In this work, we have synthesized PPY by electrochemical oxidation method and investigated for structural, morphological and electrochemical properties. The mass loading plays an effective role in deciding the performance of the electrode as well as supercapacitor devices. The electrochemical study revealed that the gravimetric capacitance does not simply decrease with increasing mass loading; instead, electrodes with moderate mass loading exhibited the highest gravimetric capacitance. The gravimetric capacitance is improved by 20% at 1 A/g current density on increasing the mass loading from 2.3 to 3.1 mg. However, the increase in mass loading leads to reduction in capacitance. Therefore, the mass loading has a critical influence on achieving scalable performance in PPy-based supercapacitors.

Keywords: Energy Storage Technology, Batteries, Materials manufacturing, Characterization techniques

IN-24

Multiscale Computational Insights into Irradiation-Induced Defect Evolution in Functional Oxides

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Abstract

This talk presents multiscale computational insights into irradiation-induced defect evolution in functional oxides, focusing on Ga_2O_3 polymorphs and actinide dioxides. Using ab initio molecular dynamics, we investigate defect formation and electronic structure changes in Ga_2O_3, revealing oxygen-related defects as the dominant contributors to band-gap modulation. For actinide oxides, a Monte Carlo and molecular dynamics framework is used to study swift heavy ion irradiation, identifying track formation thresholds and associated mechanical degradation. The results reveal distinct radiation tolerance across materials, with UO_2 showing the highest resistance.These findings provide atomistic understanding of defect evolution and property degradation, offering guidance for designing radiation-tolerant oxide materials for nuclear and electronic applications.

IN-25

Magnetic Nanostructures: Nanoscale Properties and Recent Applications

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Abstract

The advancements in the field of magnetic materials and their practical uses in daily and industrial life have been shaping the human life. This talk reviews different classes of magnetic materials, their properties on nanoscale and their applications, with an emphasis on multifunctional applications, where magnetic materials can bring the most spectacular benefits to society. The distinctive characteristics of magnetic nanostructures such as exchange bias effect, large uniaxial magnetic anisotropy (UMA) as compared to bulk materials have opened avenues for the evolution of novel devices like magnetic supercapacitors, ultrahigh density data storage devices and recording media. In past few years, magnetoelectric tuning in ferroelectric materials is one of the hot topics aiming at the development of new generation low-power spintronics and microelectronics. Hybrid supercapacitors may tune the magnetism which involves electrostatic and electrochemical doping. In view of recent research, focus is on hybrid magnetic supercapacitors and suitable magnetic materials (bulk as well as nanocrystalline) for the formation of these supercapacitors. The talk concludes with promises for the future of magnetic materials at nano scale and technologies as important as ever for humanity.

IN-26

From Materials to Devices: Chalcogenide Thin Films for Future Solar Energy Applications

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Abstract

Tin-based chalcogenide absorbers are emerging as strong candidates for sustainable photovoltaics; however, achieving an optimal balance between voltage and current remains a critical challenge. Here, we report the controlled synthesis of high-quality $SnSxSe_{1-x}$ thin films via vapor transport deposition, enabling systematic tuning of composition from S-rich to Se-rich regimes. Structural analysis confirms alloy formation with lattice expansion driven by Se incorporation. Device investigations reveal a distinct trade-off: S-rich compositions deliver higher VOC, while Se-rich films enhance JSC, limiting overall efficiency in both extremes. By strategically engineering composition, we achieve an optimized $SnS_{0.70}Se_{0.30}$ absorber that overcomes this limitation, delivering a peak efficiency of 3.75% (JSC = 23.96 mA cm^{-2}, VOC = 0.293 V, FF = 0.53). This work highlights the critical role of bandgap and defect engineering in ternary chalcogenides and establishes a clear pathway for performance enhancement in earth-abundant thin-film solar cells.

IN-27

AI-Assisted Modeling of Defect-Mediated Dark and Photoconductive

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Abstract

This work investigates the dark and photoconductive behavior of amorphous Se–Te–Pb thin films using an artificial intelligence (AI)-based framework that integrates experimental data with predictive modeling. Thin films of Se–Te–Pb with Pb concentrations of 0, 0.6, 1.1, and 1.4 at.% were fabricated by thermal evaporation, and current–voltage characteristics were measured under both dark and illuminated conditions. The resulting conductivity and activation energy data were used to train and validate machine-learning models, including polynomial regression, adaptive boosting (AdaBoost), and multilayer perceptron (MLP).

Among the tested models, the MLP achieved the highest predictive accuracy, with average R^2 values of 0.982 for dark conductivity and 0.975 for photoconductivity. For the Pb = 0 at.% sample, the AI-predicted dark conductivity ($1.6 \times 10^{8\ 1}\ cm^1$)closely matched the experimental value ($1.55 \times 10^{8\ 1} cm^1$). Under illumination, the predicted conductivity enhancement of 3.1× was in strong agreement with the experimental increase of 3.3×. At higher Pb concentrations, particularly 1.1 and 1.4 at.%, the model successfully captured the reduction in activation energy from 0.48 eV to 0.32 eV, with an overall deviation below 4%.

The close agreement between AI-predicted and experimental curves across all compositions demonstrates that the framework accurately reproduces both the sublinear and saturation regimes of photoconductivity. Feature-importance analysis further showed that Pb concentration is the dominant factor controlling dark resistivity, while illumination intensity most strongly influences photoconductive gain.

Overall, this study demonstrates that combining AI-driven analytics with experimental validation provides a rapid and scalable strategy for understanding complex defect-mediated transport in amorphous chalcogenide thin films. The strong correlation between model predictions and experimental results ($R^2 > 0.97$)highlights the potential of data-driven approaches for the predictive design of next-generation photoconductive and optoelectronic materials.

IN-28

Pressure-Induced Emergence of Dual Topological Phases in $PbSnX_2$ (X = S, Se, Te) Chalcogenides

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Abstract

The ability to controllably engineer topological phases is central to advancing next-generation quantum and electronic devices. In this context, transitions between topological insulator (TI) and topological crystalline insulator (TCI) phases are particularly compelling, as TCI states offer symmetry-driven tunability beyond conventional topological protection. In this talk, I will present our recent first-principles investigation of Sn-based ternary chalcogenides, $PbSnX_2$ (X = S, Se, Te), demonstrating the emergence of dual topological phases under externally applied hydrostatic pressure. This family have a topologically trivial ground state with direct band gap values 0.338 eV, 0.183 eV and 0.217 eV for $PbSnS_2$, $PbSnSe_2$ and $PbSnTe_2$, respectively. The first TPT i.e., TI phase for these materials is observed, under the effect of external pressure of 5 GPa, 2.5 GPa and 3.5 GPa, with a single band inversion at F-point in the bulk band structure and an odd number of Dirac cones along the (111) surface. A further increase in pressure to 5.5 GPa, 3 GPa and 4 GPa results in another band inversion at Γ-point and an even number of Dirac cones along the (111) plane. These even number of band inversions suggest that $(\bar{1}2\bar{1})$ surface has mirror symmetry around $(10\bar{1})$ plane and hence, the TCI phase is obtained. This TCI phase is further corroborated with even value of mirror Chern number calculated using winding of Wannier charge centers. These materials, which are topologically trivial at ambient conditions with finite direct band gaps, undergo a sequence of pressure-driven topological phase transitions while remaining dynamically stable. These findings establish pressure as a powerful tuning parameter for accessing and switching between distinct topological regimes within a single material platform, opening new avenues for designing symmetry-controlled quantum devices.

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IN-29

Applications at Terahertz Frequency

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Abstract

Exploring the potential of terahertz radiations lying between microwave and infrared frequency regions, is emerging as a dynamic discipline today. Here, various advancements at terahertz frequency are discussed in terms of sensors, modulators, switches, lasers, tunable devices etc. This can pave the way to address novel research directions in materials and photonics.

Keywords: Terahertz, Devices, Photonics, Materials

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IN-30

Green Multifunctional Materials for EMI Shielding and Energy Storage Applications

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Abstract

The proliferation of 5G/6G communication technologies, Internet of Things (IoT) platforms, and wearable electronics has, in turn, heightened concerns about electromagnetic pollution, signal interference, and the overall reliability of devices. Traditional electromagnetic interference (EMI) shielding materials, which are largely rigid, dense, and characterized by a reflection-dominant response, are becoming less suitable for the demands of flexible, lightweight, and multifunctional electronic architectures. This lecture will discuss the deliberate engineering of hybrid micro–nano architectures designed to provide both effective electromagnetic interference (EMI) shielding and energy storage. The focus will be on sustainable material design, specifically on using cellulose nanofibers (CNFs) from sugarcane bagasse as an environmentally friendly, flexible support structure. The lecture will highlight the combined role of polydopamine (PDA) as an interfacial binder and redox mediator, enabling the controlled integration of silver nanostructures, including one-dimensional silver nanowires (AgNWs) and zero-dimensional silver nanoparticles (AgNPs). In addition, the shift from traditional reflection-based shielding to absorption-dominant mechanisms will be thoroughly examined, demonstrating how porous, hierarchical architectures improve multiple internal reflections, interfacial polarization, and conductive loss. The synthesized AgNWs@PDA/CNF structures demonstrate superior performance, achieving an electromagnetic interference (EMI) shielding effectiveness of approximately 82.5 dB within the X-band (8–12 GHz) and a remarkable specific capacitance of roughly 1038 F g^1. Furthermore, the lecture presents a green method for electron-beam-induced reduction of graphene oxide on cellulose paper, yielding flexible films with a shielding effectiveness of up to 60.8 dB while completely avoiding toxic reducing agents. The hybrid films also exhibit mechanical robustness and environmental stability, maintaining their electrical and shielding performance after more than 500 bending and twisting cycles. Thus, these findings establish sustainable hybrid micro–nano architectures as a promising platform for next-generation flexible electronics, multifunctional EMI shielding, and integrated energy storage systems. Keywords: Flexible Electronics; EMI Shielding; Energy Storage; Cellulose Nanofibers; Silver Nano Architectures, Graphene Oxide

IN-31

Metal Oxide Based Chemiresistive Sensors

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Abstract

Accelerated demographic and economic growth has resulted in a rise in hazardous gas emissions (NOx, NH_3, CH_4, SO_x, CO). Gas sensors are essential to monitor and mitigate these gases. Further, in industrial settings such as chemical plants, manufacturing units, oil refineries, mining operations etc., gas sensors serve as essential safety tools for detecting leakage of toxic and explosive gases. Amongst different kind of sensors used, Chemiresistive gas sensors which rely on changes in electrical resistance induced by interactions between the target gas molecules and the sensing material are particularly promising due to their simple device architecture, fast response times, and resistance-based signal readouts, which enable easy electronic integration. Generally, metal oxides are used as chemiresistive material as these materials exhibit higher sensor response and are cost-effective. Metal Oxides however encounters practical limitations such as cross-sensitivity to other gases, poor long-term stability, and operation at elevated operating temperature. To address these challenges, various strategies such as surface functionalisation, elemental doping, structural modifications, defect engineering and heterojunction formation etc have been implemented. In this talk, I will discuss the gas sensors developed and recent work being carried out at Gas sensing devices section.

IN-32

Zinc-Ion Hybrid Capacitors: Mechanisms, Challenges, and Emerging Solutions

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Abstract

Electrochemical energy storage technologies have advanced significantly over the past decade to address escalating energy demands and environmental concerns. Lithium-ion batteries (LIBs) offer high energy density and stable operating voltages but are constrained by limited power density and cycling stability. In contrast, supercapacitors (SCs) exhibit excellent power capability and long cycle life, yet their low energy density restricts broader applications. Hybrid capacitors (HCs), which integrate battery-type and capacitive charge-storage mechanisms, have emerged as promising candidates by combining high energy density with rapid charge–discharge capability and superior cycling performance. Among various hybrid systems, zinc-ion hybrid capacitors (ZIHCs) have attracted increasing attention owing to the favorable electrochemical characteristics of zinc, including its high theoretical specific capacity (823 mA h g^1), suitable redox potential (0.76 V vs. SHE), low cost, and intrinsic safety. The relatively low chemical activity of zinc enables a two-electron transfer process, resulting in high energy density and fast ion transport kinetics compared with alkali-metal-based systems. ZIHCs are generally categorized into two configurations: (i) Zn//Cap systems, consisting of a zinc metal anode coupled with a capacitive carbon-based cathode, and (ii) Cap//ZBC systems, which employ a capacitive anode and a zinc-ion battery-type cathode. In Zn//Cap devices, energy storage relies on ion adsorption/desorption at the cathode and reversible zinc plating/stripping at the anode. However, the zinc anode suffers from parasitic side reactions and dendrite growth in aqueous electrolytes, leading to rapid performance degradation and limited cycle life. To address these challenges, asymmetric Cap//ZBC configurations have been proposed, eliminating metallic zinc anodes while expanding the operating voltage window and enhancing energy density compared with conventional zinc hybrid supercapacitors. Additionally, functional hydrogel electrolytes have shown promise in suppressing side reactions and stabilizing zinc interfaces. Overall, effective suppression of dendrite formation and optimization of charge-storage mechanisms are critical for realizing durable, high-performance ZIHCs for practical energy storage applications.

IN-33

Molecular Quantum Sensors Based on Organic Crystals

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Abstract

Quantum sensing harnesses the sensitivity of quantum states to their environment to measure physical parameters (such as magnetic fields, temperature, pressure, and strain) with exceptional precision[1]. In this talk, I will begin by introducing the basic principles of quantum sensing and reviewing the major types of quantum sensor platforms developed over the past decade. Widely used solid-state systems, such as nitrogen-vacancy centers in diamond and defect spins in silicon carbide, provide excellent optical spin interfaces but often exhibit limited sensitivity to mechanical perturbations due to the rigidity of their host lattices. Motivated by these limitations, I will present an alternative platform based on organic molecular crystals. In particular, pentacene-doped p-terphenyl (PDP) crystals can be interrogated by optically detected magnetic resonance (ODMR). These systems enable highly sensitive pressure detection. Our recent work demonstrates significantly enhanced pressure sensitivities compared with conventional defect-based platforms while offering additional advantages such as low-cost crystal growth, and high sensor densities [2,3]. I will conclude by discussing how chemically engineered molecular systems could enable new quantum sensing architectures, and molecular-scale quantum probes.

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IN-34

Next-Generation Solar Energy: From Nanostructured Photoanodes to Stable, Lead reduced Perovskite Devices

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Abstract

Achieving sustainable solar energy conversion requires continuous innovation in material design to balance efficiency, stability, and environmental compatibility. This talk presents a dual-pathway approach to developing high-performance photovoltaic materials. We begin by detailing our foundational research on nanostructured TZO (TiO_2/ZnO) photoanodes for dye-sensitized solar cells (DSSCs), highlighting how architectural control improves charge transport and device performance. Building upon these structural insights, we transition to the critical challenge of perovskite solar cell stability. We demonstrate how compositional engineering specifically through the development of lead-reduced and lead-free bismuth-,barium, and tin-alloyed perovskite systems effectively mitigates environmental degradation. By bridging these two research areas, this presentation offers a comprehensive perspective on the material design strategies necessary to advance next-generation, scalable, and durable solar energy technologies.

Keywords: TZO Heterostructures, Metal-Halide Perovskites, Charge Transport Dynamics, Bismuth, Barium Alloyed Systems, Structural Characterization

IN-35

Computational Materials Modelling

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Abstract

In this talk, I will present a brief overview of theoretical and computational overview of studying materials using ab-initio computational tools. Specifically, I will be presenting main components of density functional theory formalism and share some results demonstrating basic applications of density functional theory. I will also share some recent results from ongoing research by our group which include exploration of materials for superconductivity, hydrogen generation using photocatalytic water splitting, transport properties, battery applications.

IN-36

A Novel Approach for Fast Texture, Residual Stress and In-Plane Diffraction using an X-ray Lens with a Rotating Slit

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Abstract

In X-ray diffraction studies that use Eulerian cradles to tilt a sample continuously, beam defocusing and over-irradiating the sample during measurements are significant issues that affect the quality of the data and the analysis results. Among the applications most impacted are texture, residual stress, non-coplanar reciprocal space map, and in-plane measurements, where samples are positioned to predetermined Chi (χ) points and scans are conducted in Phi (ϕ), 2theta (2θ), or omega-2theta/phi-2theta (ω-2θ/ϕ-2θ) axis. It is customary to employ small beam (micro-spot) to prevent defocusing and over-irradiation. On the other hand, this also causes a considerable reduction in intensity and hence the measurement speed. In this contribution we introduce a novel beam-shaping tool that reduces over-irradiation and defocusing while also enabling much larger beam dimensions. The tool synchronously rotates the beam as a function of χ-tilt in the Eulerian cradle. As a result of this synchronous mode, beam projection remains consistent throughout χ-tilts. It also allows to fine-tune the incident angle for in-plane measurements utilizing the combined smart (χ + ω) axis. The findings displayed in this poster demonstrate the notable enhancement of particle statistics, and measurement intensity/speed, while maintaining the resolution in full range of χ-tilts.

Keywords: X-rays diffraction, X-ray optics, beam geometry, beam shaping, rotating slit, In-plane, texture

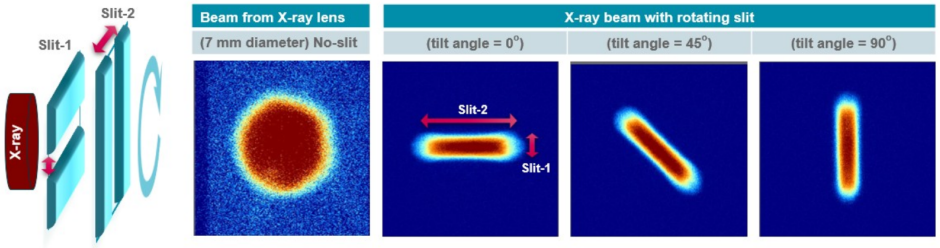

Figure 1: Functionality of rotating slit and corresponding direct beam images without slit as well as a (1/8)° divergence slit at 0°, 45° and 90° tilt.

IN-37

Ultrafast All-Optical Magnetization Dynamics for Spintronics

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Abstract

Our understanding of ultrafast laser control of magnetization has advanced significantly since the pioneering work of Beaurepaire et al. on femtosecond spin dynamics [1]. Harnessing light to manipulate magnetic order on ultrashort timescales is key for next-generation spintronic devices that combine ultrafast data processing and storage [2]. However, a comprehensive understanding of the parameters governing magnetization at fundamental time and length scales remains incomplete.

In this work, we present femtosecond laser-induced magnetization enhancement in FeNi/FePt exchange-coupled composite magnets [3], alongside the investigation of all-optical spin injection in silicon [4]. Using time-resolved magneto-optical Kerr effect (tr-MOKE) spectroscopy across the visible and extreme ultraviolet (EUV) regimes, we uncover the underlying mechanisms governing these phenomena. EUV tr-MOKE measurements were performed in a pump–probe configuration using FERMI free-electron laser pulses at the MagneDyn beamline (Elettra, Italy).

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IN-38

Beyond Passive Glass: Integrating Rare Earths for Photonic Applications

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Abstract

For decades, glass was primarily utilised in a conventional, passive role as a simple structural container or a transparent pathway for light. However, the integration of rare-earth (RE) ions has fundamentally transformed these amorphous networks into dynamic, multifunctional platforms capable of active electronic, photonic, radiation-shielding and sensing applications. The partially filled 4f orbitals of rare earth elements helps in sharp electronic transitions that yield high quantum efficiencies, long metastable lifetimes, and highly stable luminescence. This talk explores the impact of rare-earth elements as vital network modifiers within the glass. By strategically altering the glassy matrix, these dopants break bridging oxygen bonds to form non-bridging oxygens, precisely tuning critical physical and optical parameters such as the optical band gap, refractive index, polarizability, and metallisation criterion. The predictive power of Judd-Ofelt theory is also analysed in evaluating radiative transitions and oscillator strengths, which is essential for optimising the stimulated emission cross-sections of novel laser materials. The presentation will also highlight cutting-edge applications driven by specific rare earth elements doping. Furthermore, the deployment of multiple rare earth co-doped glasses for high-gain broadband optical fibre amplifiers (OFAs), solid-state lasers, white light-emitting diodes (w-LEDs), and smart radiation dosimetry will be discussed. Finally, the journey from passive glass to advance materials by engineering the local coordination environment of rare-earth elements illuminating the future of optoelectronics, advanced telecommunications, and robust radiation sensing technologies will be discussed.

IN-39

AI Driven Inverse Design of Metamaterials for Energy Harvesting Defence Platforms

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Abstract

Meta-materials are artificially made materials with properties notcaccessible to their naturally existing counterparts. The details of meta-materials and metasurfaces will be discussed. Electromagnetic meta surfaces will be highlighted from the perspective of defence applications. Few examples of meta-surfaces will be discussed including the concept of cloak. AI driven approach will be discussed for the forward design metasurface to mitigate design characteristics.

Keywords: Zinc Oxide Tetrapods, Smart Materials, Advanced Technologies

PAPER PRESENTATIONS

Contributed Research Papers

NMSF-AFM-001

Tween 20-Doped $LaF_3:Yb^{3+}$ ($LAYT_{20}$) Luminescent Nanoparticles: Structural & Optical Properties

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Abstract

Upconversion nanoparticles convert low-energy radiation to high-energy radiation. $LaF_3:Yb^{3+}$ nanoparticles doped with Polyoxyethylene sorbitan monolaurate (tween20) were synthesized using microwave. $LAYT_{20}$ was subjected to structural and optical characterisation using X-ray diffraction (XRD), EDAX, FTIR, UV/Vis & photoluminescence spectroscopy (PL). Composition was verified using EDAX and X-ray diffraction. Diffraction revealed the crystalline nature of $LAYT_{20}$ nanoparticles and the modified particle size. The diffraction peaks are readily indexed to those of the hexagonal LaF_3 phase, which are in good agreement with the literature (JCPDS: 320483). Surface analysis was performed using scanning electron microscopy (SEM), which confirmed the surface modification. FTIR studies revealed the presence of various bonds in the sample. The change in the band gap energy was observed by UV-absorption studies. PL spectra show an emission peak lying at 300 nm, indicating the upconversion luminescence. In addition, the studies show that Tween 20 may play a vital role in surface modification and substantially influences the band gap of $LaF_3:Yb^{3+}$ nanoparticles.

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NMSF-AFM-002

Oxygen Vacancies Assisted Photocatalytic Dye Degradation and Photoelectrochemical Water Splitting Performance in Ag and Mg-modified $NaNbO_3$

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Abstract

A lead-free $Na_{0.85}Ag_{0.15}Nb_{0.95}Mg_{0.05}O_3$ (*AM-NN*) polycrystalline ceramic was synthesized using the conventional solid-state reaction method, and its structural, dielectric, impedance, and optical properties were thoroughly investigated. X-ray diffraction (XRD) and Rietveld refinement of *AM-NN* confirmed that the material adopts a perovskite-type orthorhombic structure with the P_{21} ma space group. Introducing oxygen vacancies through AgO resulted in spectral changes observed in Raman spectroscopy and Photoluminescence. Dielectric and complex impedance measurements, taken from 10^2-10^6 Hz and room temperature to 500 °C, exhibited non-Debye behavior. *AM-NN* presented a reduced band gap of 3.12 eV compared to pure $NaNbO_3$ (NN) (3.4 eV) as obtained from UV-vis spectroscopy. *AM-NN* demonstrated a superior photocatalytic dye degradation percentage of 99% Methylene Blue (MB), 95% Crystal Violet (CV) and 60% Congo Red (CR) at 300 min with the rate constant (k) of 0.0128 min^{-1}, 0.0138 min^{-1} and 0.0027 min^{-1} (CR), respectively. PEC water splitting showed that the photoanode fabricated with *AM-NN* exhibits enriched photocurrent density (1.11 mA cm^{-2}). XRD showed no secondary phase after dye degradation, indicating the system's reusability. A detailed investigation into the electrical properties and photocatalytic mechanism was provided to account for the observed improvements in dye degradation and water splitting applications.

Keywords: *$NaNbO_3$, Oxygen Vacancy, Dielectric Study, Photocatalysis, Photoanode*

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NMSF-AFM-004

Shape Memory Phenomena and Diffusionless Phase Transformations Governing Reversibility in Shape Memory Alloys

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Abstract

Shape memory alloys are thermoresponsive materials and take place in a class of advanced smart materials by exhibiting dual memory characteristics, shape memory effect and superelasticity. Shape memory effect is initiated with thermomechanical processes on cooling and deformation and performed thermally on heating and cooling, with which shape of the material cycles between original and deformed shapes in reversible way, and this behavior can be called thermoelasticity. Shape memory effect is governed by diffusionless phase transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling with cooperative movement of atoms in $<110>$ -type directions on $\{110\}$ - type close packed planes of parent phase, and ordered parent phase structures turn into the twinned martensite structures, and twinned structures turn into detwinned martensite structures by means of stress induced martensitic transformations with deformation. Atomic movements are confined to the nearest atom distances, and martensitic transformations have diffusionless character. Superelasticity is performed with stressing and releasing the material in elasticity limit at a constant temperature in the parent austenite phase region, and shape recovery occurs immediately upon releasing, by exhibiting elastic material behavior. Superelasticity is also result of stress induced martensitic transformation, and the ordered parent phase structures turn into the detwinned martensite structures with stressing. Lattice twinning and detwinning reactions play important role in martensitic transformations, and they are driven by internal and external forces, by means of lattice invariant shears.

Copper based alloys exhibit this property in metastable β-phase region. Lattice twinning is not uniform in these alloys, and the ordered parent phase structures undergo the layered structures with martensitic transformation.

In the present contribution, x-ray and electron diffraction studies were carried out on ternary copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. A series of x-ray diffractogram were taken during aging. X-ray diffractograms taken in a long-time interval show that locations

and intensities of diffraction peaks change with the aging time at room temperature, and this result refers to the redistribution of atoms in diffusive manner.

Keywords: *Shape Memory Effect, Martensitic Transformation, Thermoelasticity, Superelasticity, Twinning, Detwinning*

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NMSF-AFM-005

Synthesis, Characterization, and Application of Psyllium–Epichlorohydrin-Tryptophan-Hydroxamate Biopolymer Resin for Solid Removal from Sewage Wastewater

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Abstract

The increasing load of sewage wastewater due to urban expansion necessitates the development of efficient, eco-friendly, and cost-effective materials for water purification. In this study, a novel bio-based chelating resin was synthesized using psyllium as a natural polysaccharide backbone, epichlorohydrin as a crosslinking agent, and tryptophan hydroxamate as a functional ligand. The incorporation of tryptophan hydroxamate introduces active chelating and adsorption sites, enhancing the biopolymer resin's affinity toward suspended and dissolved solids present in sewage wastewater. The synthesis was carried out under controlled alkaline conditions to form a stable, crosslinked polymeric network. The prepared psyllium-epichlorohydrin–tryptophan-hydroxamate resin was characterized using Fourier Transform Infrared Spectroscopy (FT-IR) to confirm functional group modification, Scanning Electron Microscopy (SEM) to study surface morphology, and X-ray Diffraction (XRD) to analyze structural properties. The results demonstrated significant improvement in solid removal efficiency due to the combined effects of adsorption, chelation, and coagulation facilitated by hydroxamate functional groups. The developed biopolymer resin exhibits excellent potential as a sustainable and biodegradable material for wastewater treatment. Its high efficiency, low cost, and environmentally benign nature make it a promising alternative to conventional synthetic coagulants. This study highlights the applicability of functionalized biopolymers in advanced water treatment technologies.

Keywords: *Psyllium Epichlorohydrin Tryptophan Hydroxamate, Biopolymer Resin, Wastewater Treatment, Solid Waste Removal, Adsorption, Sustainable Materials*

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NMSF-AFM-006

Design, Topology Optimization and Fabrication of Aerospace Bracket via FDM Printing Using Foxtail Palm Fibre Reinforced PLA Composites

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Abstract

The biodegradability and processing simplicity of polylactic acid (PLA) make it a popular choice for fused deposition modeling (FDM), but structural components made of this material are limited in their use owing to its low mechanical strength. This study details the process of developing, optimizing, and building a lightweight aircraft bracket out of PLA composites reinforced with foxtail palm fibers. Chemically treated foxtail fibers with an alkaline (NaOH) solution improved load transfer efficiency by strengthening the link between the fibers and the matrix. Fused filament manufacturing (FDM) was used to print the bracket after composite filaments were made by melt blending and extrusion. Significant weight reduction was achieved without compromising structural integrity by the use of topology optimization to eliminate low-stress sections.

Fiber treatment was found to improve interfacial adhesion, as indicated by increased thermal stability and decreased hydroxyl group content, as confirmed by thermal and chemical tests such as TGA, DSC, and FTIR. Mechanical testing showed that the material was more rigid and could support more weight than regular PLA, with a tensile strength of 37.35 MPa and a flexural strength of 101 MPa. The optimized bracket reduced weight by about 48–50% without compromising functional performance. Scanning electron microscopy (SEM) morphological investigation confirmed efficient fiber dispersion with minimal void formation characteristic of FDM. These findings point to the possibility of creating environmentally friendly, lightweight parts for optional aerospace uses by combining additive printing with topology optimization and natural fiber-reinforced composites.

Keywords: *Topology Optimization, PLA Composite, Foxtail Palm Fibre, FDM, Aerospace Bracket, Lightweight Design*

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NMSF-AFM-007

Enhancement of Mechanical, Tribological and Corrosion Properties of AZ91D Reinforced with WC and MoS_2 Using Random Forest

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Abstract

This study to evaluate the enhancement in strength, and wear resistance of the Mg-AZ91D matrix reinforced with 2 wt.% tungsten carbide (WC) and 2 wt.% molybdenum disulfide (MoS_2) for aerospace industrial components. Composite samples were fabricated using the stir casting technique and subjected to a comprehensive set of tests, including tensile, wear, impact, and hardness. Additionally, corrosion resistance was assessed to determine the material's behavior in corrosive environments. Among the tested composites, AZ91D +2MoS_2 demonstrated superior performance in wear resistance due to its excellent solid lubricating properties, which significantly reduced friction and improved sliding behavior. AZ91D + 2WC showed the highest hardness and improved tensile strength due to the presence of hard ceramic particles, which enhanced load-bearing capability and resistance to surface deformation. AZ91D + 2WC and AZ91D + 2MoS_2 composites exhibited better wear resistance and impact strength compared to the pure matrix. Microstructural analysis confirmed the uniform distribution of reinforcement particles and the formation of stable phases within the matrix. In Random Forest model showed limited predictivity accuracy for certain responses, especially wear rate (WR) and specific wear rate (SWR), indicating that the predicted optimal conditions should be interpreted. ANOVA results confirmed that load is the most consistently significant factor influencing wear WR and coefficient of friction (CF) while composite composition significantly affects SWR. The results reveal that the reinforced composites generally exhibited improved mechanical and tribological properties compared to the pure matrix. WC reinforcement significantly enhanced hardness and strength, while MoS_2 reinforcement improved lubrication and wear resistance. This study demonstrates the effectiveness of incorporating ceramic and solid lubricant reinforcements in improving the multifunctional performance of magnesium-based composites for lightweight engineering applications.

Keywords: *AZ91D, Tungsten Carbide, Molybdenum Disulfide, Mechanical Properties, Wear Rate, Corrosion Resistance*

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NMSF-AFM-009

Nanostructured Cu/C Catalysts Derived from Bio-Floral Waste for the Efficient Conversion of Levulinic Acid to γ-Valerolactone

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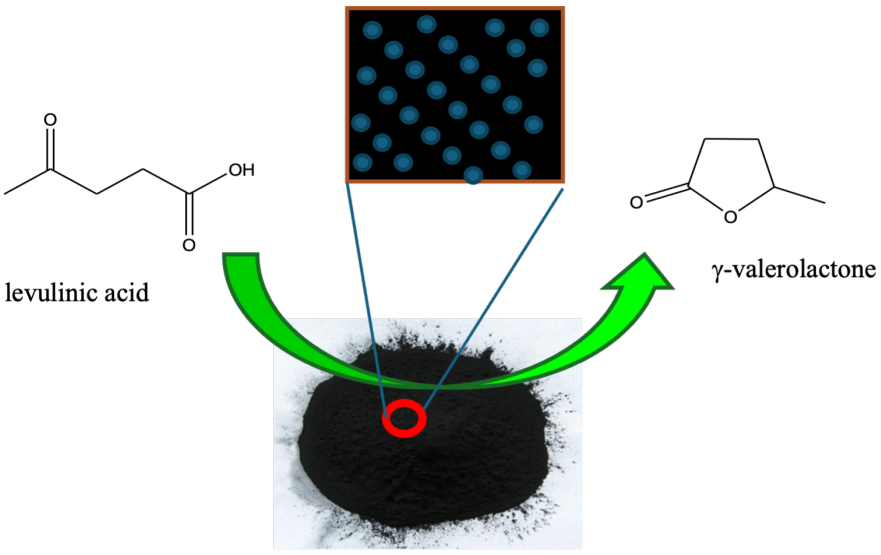
Abstract

Due to the diminishing of fossil fuels, people depends on other alternative energy sources. Among many alternative bio-derived platform chemicals, γ-valerolactone(GVL) is a versatile, an eco-friendly green solvent, sustainable fuel and food additive. The GVL has been effectively produced from bio-derived levulinic acid(LA) using Cu/C nanocatalysts which are synthesized using bio-char as the support. Bio-chars derived from cellulosic biomass are attractive functional carbon nanomaterials that are widely using nowadays as catalyst supports for the synthesis of metal, metal oxide nanoparticles. In this article, the synthesis, characterization and catalytic application of Cu/C nanocatalysts derived from red rose flowers is reported. Waste and used red rose flowers are collected from the temples, washed them thoroughly with distilled water and allowed to dry. The resulting mass was powdered and calcined in inert atmosphere to get functional carbon materials. Bio-derived carbon supported Cu nanoparticles were synthesized in wet impregnation method and characterized using XRD, ICP-OES and SEM and TEM techniques. The prepared catalysts were tested for hydrocyclization of bio-derived levulinic acid to γ-valerolactone, which is a versatile platform molecule and fuel additive. The catalysts showed superior catalytic activity in gas phase hydrocyclization of levulinic acid into γ-valerolactone at 265°C at atmospheric pressure. The uniform dispersion of Cu nanoparticles on carbon support might be the reason for high catalytic activity of the prepared catalysts.



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NMSF-AFM-010

Surface Characteristics Study Using Statistical Soft Computing Techniques During Facing of Hibiscus Rosa Sinensis / CNT / Epoxy Hybrid Composites

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Abstract

Recently, natural fiber reinforced nanomaterial incorporated hybrid polymer composites have demonstrated superior potential in industrial and manufacturing applications due to their enhanced machinability characteristics. Due to the heterogeneous nature of composite materials, processing method often leads to defects such as increased surface roughness, and dimensional inaccuracies. In contrast, among different conventional machining operation facing plays a critical role in plant fiber reinforced composites due to fact that it directly influences both mechanical performance and durability. Further this operation also enhances improved surface integrity by effectively removing surface irregularities and voids, thereby enhancing the overall finish and dimensional accuracy of the component. Hence this paper investigates the surface characteristics such as surface roughness and surface hardness induced during facing of Hibiscus Rosa-Sinensis/Carbon Nanotube (CNT) fiber/Epoxy-based hybrid composites and its morphological study. The experiments are conducted by varying key machining parameters, such as cutting speed, feed rate, and depth of cut using uncoated tungsten carbide tool. From the experimental investigation based on L_{27} orthogonal array it was observed that surface roughness (Ra) improved with increase in cutting speed and deteriorated as the feed rate increased which may be due to matrix cracking, fiber debonding, and fiber pull-out. Further, cutting speed plays a dominant positive role in enhancing the surface hardness of the composite, whereas increases in feed rate and depth of cut slightly reduce the surface hardness. Analysis of Variance revealed that feed rate is the significant factor on surface roughness with 94.07% of contribution and cutting speed is the dominant factor influencing surface roughness with 94.9% of contribution. The RSM model demonstrates high predictive accuracy with average error of 0.42% for surface roughness and 0.34% for surface hardness, confirming its effectiveness as a reliable tool for surface roughness analysis. However, the machining parameters significantly influence surface quality, with higher feed rates leading to increased surface damage, whereas optimized cutting conditions improve surface finish. Additionally, the microscopic analyses confirmed that CNT reinforcement

significantly improved the fiber matrix interfacial integrity, enhanced the surface finish of the composite and reduced the surface defects during facing. DFM analysis produced a high desirability value, confirming that the optimal machining parameter combination consists of a cutting speed of 101 mm/min, a depth of cut of 0.25 mm, and a feed rate of 0.11 mm/rev.

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NMSF-AFM-011

Electro-Mechanical Behavior of Self-Sensing Textile Reinforced Composites for In-Situ Structural Health Monitoring

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Abstract

Advanced engineering materials, such as glass-fibre-reinforced composites (GFRC), are commonly used in automotive components, civil structures, and the aviation industry. The unique anisotropic characteristics of composites pose challenges for accurately forecasting damage and failure under real-time loading conditions, in contrast to metals. This study utilises GFRC to demonstrate structural health monitoring using a piezoresistive sensor made from glass fabric coated with reduced graphene oxide (rGO). The sensor was integrated into the GFRC composite to monitor variations in fractional electrical resistance in response to flexural strain. The composite specimens that were developed underwent three-point bending tests to evaluate their piezoresistive performance. The evaluation involved examining how sensor width and their relative placements in the thickness direction of the composite specimen influenced strain and damage detection during testing. The test results indicated that these parameters were significantly linked to the piezoresistance of the developed sensor. The findings of this study indicate that the developed piezoresistive sensor can effectively detect strain and damage in glass-fabric-reinforced composite structures across various applications.

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NMSF-AFM-012

Defect-Tuned Conduction in Ultrathin $MoTe_2$ Field-Effect Transistors

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Abstract

Reduced dimensionality gives rise to rich and tunable electronic properties, making low-dimensional materials increasingly attractive for fundamental studies and device applications. Owing to their atomically thin nature, charge transport in these systems is often strongly governed by interfacial phenomena, with contacts, dielectric coupling, and adsorbed species playing a decisive role. In this work, we present a combined experimental and theoretical study of ultrathin p-type $MoTe_2$ field-effect transistors, where temperature- and pressure-dependent electrical measurements are used together with density functional theory to disentangle the role of defects and environmental exposure. Transport improves under vacuum, while low and nearly symmetric Schottky barriers are found. Both experiments and DFT calculations suggest Te and Mo vacancies as key sources of p-doping, while their passivation reduces both doping and conductivity. Overall, the results show that $MoTe_2$ transistor operation is jointly governed by vacancies, interface states, and environment, offering useful insight for the optimization of 2D semiconductor devices.

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NMSF-AFM-014

Synthesis and Tailoring of Structural and Optical Properties of g-C_3N_4/PANI/ZnO Ternary Nanocomposites for Antibacterial Applications

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Abstract

In this work, a novel Graphitic Carbon Nitride-Polyaniline-Zinc Oxide ternary Nanocomposite (g-C_3N_4/PANI/ZnO NCs) was successfully synthesized through a three-step process involving calcination, in situ polymerization, and coprecipitation. The nanocomposites with varying concentrations of g-C_3N_4 and PANI (1, 3, 5, and 10 wt.%) were synthesized. The synthesized NCs were characterized using X-ray Diffraction (XRD), UV-diffuse reflectance spectroscopy (UV-DRS), Photoluminescence Spectroscopy (PL), Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), Field Emission Scanning Electron Microscopy (FESEM), and X-ray Photoelectron Spectroscopy (XPS). XRD analysis indicates that the synthesized NCs are polycrystalline with hexagonal wurtzite structure. Morphological analysis using TEM and FESEM confirmed the uniform dispersion of g-C_3N_4 and PANI onto the ZnO matrix. FTIR, PL, UV-DRS, and XPS analyses further verified the chemical interaction and interfacial integration between g-C_3N_4/PANI and ZnO. Detailed characterization confirmed the uniform dispersion and successful integration of g-C_3N_4 and PANI onto the ZnO matrix. The antibacterial activity of the synthesized NCs was evaluated against both Gram-positive and Gram-negative bacteria, demonstrating their potential for antimicrobial applications.

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NMSF-AFM-016

Dielectric Response and Surface State Evolution in SnO_2 Nanoparticles: A Comprehensive Study Using XPS and Impedance Spectroscopy

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Abstract

Tin oxide (SnO_2), a widely studied n-type semiconductor, exhibits remarkable electrical and surface properties and can be effectively synthesized through various chemical routes such as the co-precipitation method for controlled nanostructure formation. Tin oxide (SnO_2) nanoparticles were synthesized via a simple co-precipitation method and annealed at three different temperatures, 250 °C, 500 °C, and 700 °C, to study the effect of thermal treatment on structural, morphological, and dielectric properties. X-ray diffraction (XRD) analysis confirmed the formation of the tetragonal cassiterite structure for all samples, with enhanced crystallinity and increased crystallite size observed at higher annealing temperatures. Field emission scanning electron microscopy (FESEM) revealed notable morphological evolution and grain growth with temperature, while X-ray photoelectron spectroscopy (XPS) provided insights into surface chemical states and oxygen vacancies. Dielectric studies, conducted using an Agilent 4294A precision impedance analyser, revealed temperature- and frequency-dependent behaviour of the dielectric constant and dielectric loss, highlighting the potential of these nanostructured materials for electronic and sensing applications. The observed variations are correlated with structural and microstructural modifications induced by annealing. These findings provide a comprehensive understanding of the influence of thermal treatment on SnO_2 nanoparticles for potential use in high-frequency microelectronic devices and gas sensor platforms.

Keywords: *Co-Precipitation, Cassiterite Structure, Microstructural*

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NMSF-AFM-018

Effect of K and Zr Substitution on the Functional Properties of BNT-Based Perovskite Ceramics

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Abstract

Concerns about the environment have led to the development of lead-free piezoelectric ceramics based on bismuth sodium titanate (BNT) as viable substitutes for traditional Pb-based materials. However, pure BNT exhibits limitations, including a high coercive field and relatively low piezoelectric performance, which limit its practical applications. The impact of simultaneous substitution of potassium (K^+) and zirconium (Zr^+) on the structural, microstructural, dielectric, and ferroelectric properties of BNT-based perovskite ceramics with the general formula $Bi_{0.5}(Na_{1-x}K_x)_{0.5}(Ti_{1-x}Zr_x)O_3$ (x = 0.1–0.2) has been thoroughly examined. The ceramics were synthesised using the solid-state reaction route, followed by calcination and sintering under optimised conditions to obtain dense and homogeneous samples. Phase formation and crystal structure were analysed by X-ray diffraction, which confirmed the presence of a single-phase perovskite structure with no detectable secondary phases. The incorporation of larger ionic radii K^+ at the A-site and Zr^{4+} at the B-site induces lattice distortion and modifies the crystal symmetry, influencing the overall phase stability of the system. Microstructural analysis using scanning electron microscopy revealed well-developed grains with relatively uniform distribution, while a slight increase in grain size was observed with increasing substitution concentration. The observed modifications in electrical properties are attributed to the disruption of long-range ferroelectric order and increased lattice heterogeneity caused by co-substitution at both A- and B-sites. Overall, the study demonstrates that K and Zr substitution is an effective strategy for tailoring the functional properties of BNT-based ceramics, making them suitable candidates for lead-free piezoelectric, dielectric, and energy storage applications.

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NMSF-AFM-019

Synthesis, Structural Characterization, and Gas Sensing Characteristics of Rare Earth Orthoferrite $DyFeO_3$ Prepared by the Sol-Gel Method

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Abstract

To address the growing need for detecting hazardous gas leaks and to supervise air pollution, it is essential to develop gas sensors that offer high sensitivity, stability, and selectivity. Due to their multifunctional properties and robust chemical structure, perovskite materials hold promise as a foundation for a wide range of device applications in engineering. This study investigates a room-temperature perovskite material with the chemical formula $DyFeO_3$ (DFO), also known as rare-earth orthoferrite. Polycrystalline $DyFeO_3$ nanoparticles have been produced using a sol-gel technique. The XRD and Rietveld analysis of the material revealed that DFO crystallizes in the Pbnm space group with orthorhombic symmetry. Dielectric measurements, taken at various frequencies and temperatures, suggest the material exhibits a high dielectric constant and low dielectric loss. The DFO pellet is evaluated for its potential in gas-sensing applications in a metal-insulator-metal configuration. The results show that DFO offers a sub- ppm detection limit and demonstrates high selectivity for NO_2 gas, operating effectively at temperatures ranging from 50 °C to 200 °C. Extensive and stable gas-sensing performance, coupled with exceptional adsorption and desorption properties, is demonstrated through a series of cyclic tests. These remarkable gas-sensing and dielectric characteristics suggest that ultra-sensitive gas sensors based on lead-free orthoferrites could become practicable. The $DyFeO_3$ (DFO) sensor showed a response of 7.35% at 250 °C to 150 ppm of NO_2 gas. This work highlights the DFO's high selectivity for NO_2 gas and demonstrates its superior gas sensing performance compared to basic DFO.

Keywords: *Sol-Gel, X-ray diffraction, Rietveld Analysis, Gas Sensor*

NMSF-AFM-021

Next-Generation Sulphide Based Cyan Phosphors for Energy-Efficient Solid-State Lighting: A DFT Study

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Abstract

The increasing demand for high-quality solid-state lighting has driven extensive research on phosphor-converted white light-emitting diodes (pc-WLEDs), as nearly 20% of global electricity consumption is attributed to lighting and display technologies. Among the various strategies for white light generation, the blue LED combined with a yellow phosphor remains the most widely employed due to its simplicity and high efficiency. However, this configuration suffers from a spectral deficiency in the 400–500 nm region, commonly referred to as the "cyan gap," which significantly limits the colour rendering index (CRI), correlated colour temperature (CCT), luminous efficacy, and visual comfort. The development of efficient cyan-emitting phosphors is therefore essential to bridge this gap and enhance white light quality. In this work, a comprehensive first-principles investigation of sulphide-based cyan phosphors $KGaS_2$, $LiGaS_2$, and $Ca(GaS_2)_2$ has been carried out within the framework of Density Functional Theory (DFT) using the pseudo-potential plane-wave method. The calculations were performed employing the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional, as implemented in the Quantum ESPRESSO and BURAI simulation packages. Structural optimization was conducted to obtain equilibrium lattice parameters, atomic configurations, and ground-state stability. The studied compounds crystallize in different symmetry groups: $KGaS_2$ (orthorhombic, Pnma), $LiGaS_2$ (orthorhombic, $Pna2_1$), and $Ca(GaS_2)_2$ (monoclinic, C_2/c). The optimized structural parameters show good agreement with available experimental data, validating the computational methodology. Electronic properties were analyzed through band structure, total density of states (TDOS), and partial density of states (PDOS), indicating semiconducting behaviour with direct band gaps and revealing the contributions of constituent atomic orbitals to the valence and conduction bands. Mechanical stability and rigidity were evaluated via elastic constants and bulk modulus calculations, confirming the structural robustness of these materials. Furthermore, optical properties were investigated through frequency-dependent dielectric functions, absorption coefficients, refractive indices, and reflectivity spectra. The results reveal strong optical responses in the visible region, highlighting their suitability for optoelectronic applications. Overall, the investigated compounds exhibit favourable

structural, electronic, mechanical, and optical characteristics, making them promising candidates for efficient cyan phosphors in next-generation pc-WLED technologies.

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NMSF-AFM-022

Vegetable Oil-Based Functional Materials: A Greener Approach to Combat Vehicular Pollution

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Abstract

The addition of chemical additives in lubricating oil (lube oil) also called base oil is essential for smooth functioning of modern engines. Lubricants (a combination of additive and lube oil) are generally liquids or semi–liquids which are used to lubricate the metal surfaces in-contact in automotive engine for their longevity and better performances. The key functions of a lubricant are to keep moving parts apart, reduce friction, protect against wear, transfer heat, prevent rust and corrosion, to act antioxidant, to act as detergents/dispersants etc. The acrylate/vinyl acetate based lubricants exhibit satisfactory performance but they are not environmentally benign. The research on vegetable oils as base stocks or their derivatives as additives for base stocks is increasing significantly due to their biodegradable property and availability in nature. Moreover, they show excellent Rheological, tribological and viscometric properties. Olive oil/Castor oil is widely used in different fields such as lubricants, pharmaceuticals, paints, adhesives, rubber, cosmetics, etc. The high flash point and the presence of polar functional group make them efficient candidate for the synthesis of additives for lubricating oil as well as bio lubricant. However, research articles regarding the application of vegetable oils or their copolymer as lubricant are very scanty.

Therefore, recently we have synthesized homopolymer of olive oil and copolymer of it with acrylate in different percentage ratios to get thermally stable, cost effective as well as eco–friendly lubricant additives. Acrylate was chosen because the incorporation of it enhances oil solubility and the thermal stability of lubricant. Performance evaluation of the prepared polymeric additives was carried out as viscosity index improver, pour point depressant and antiwear additive according to respective ASTM method.

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NMSF-AFM-023

Gate-Tunable Optoelectronic Synaptic Plasticity in 2D Tin Dichalcogenides for Neuromorphic Applications

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Abstract

As artificial intelligence continues to evolve, neuromorphic technologies that emulate biological neural networks are increasingly vital for energy-efficient computing. Two-dimensional semiconductors, particularly tin-based dichalcogenides such as SnS_2 and $SnSe_2$, have emerged as compelling candidates for optoelectronic synapses due to their strong light-matter interaction, environmental stability, and tunable properties. In this work, we investigate multilayer field-effect transistors based on 2D tin dichalcogenides, demonstrating highly controllable optoelectronic plasticity. Through systematic characterizations across a wide range of temperatures, ambient pressures, and illumination conditions, we reveal that the device photoresponse and persistent photoconductivity are strongly governed by trap-assisted photogating and interfacial dynamics. Rather than being detrimental, these intrinsic trap states and ambient adsorbates are actively exploited to emulate essential synaptic functionalities. We show that by finely tuning external parameters, such as gate voltage, thermal variations, and optical stimuli, it is possible to modulate the interplay between fast and slow charge recombination channels. This dynamic control enables a reversible and smooth transition between short-term memory and long-term potentiation, alongside cumulative learning capabilities with high reproducibility. Our results clarify the origin of plasticity in these materials and demonstrate their robustness under realistic operating conditions, highlighting the significant potential of 2D tin dichalcogenide-based synapses

for integration into scalable, next-generation neuromorphic architectures.

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NMSF-AFM-025

Synthesis of Fe-Cu Bimetallic Metal-Organic Framework-Based Macroscopic Beads for Adsorptive Adsorption of Rhodamine B

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Abstract

Recently, the adsorption process has been used at industrial level for the purification and chemical separation method gain a lot of attention due to their simplicity, ease of use, and environment friendly nature. In the given experimental study, metal-organic framework (MOF) obtained beads have been inspected to remove dye rhodamine B (RhB) from aqueous solutions via batch adsorption experiments. A bimetallic MOF namely Fe/Cu-BTC synthesized at room temperature was transformed into highly robust millimetre-sized beads using polyvinylidene fluoride (PVDF). The properties of the Fe/Cu-BTC @PVDF composite beads were determined using several characterization techniques. The effect of parameters such as initial pH, adsorption time, and initial RhB concentration on the adsorption process was also investigated. After -70 minutes of contact time, the dye adsorption equilibrium was achieved by dye removal of 91 %. The analysis of kinetic data of bimetallic MOF confirmed that the adsorption at dye followed the pseudo second order kinetics model with the best linearity (R_2=0.9899). The adsorption isotherm models of Bimetallic MOF finalize that the Langmuir model was better suited to describe dye adsorption on the beads. Regeneration studies showed that the reuse of adsorbent can be carried out effectively for at least five cycles without any substantial loss in the adsorption capacity of Bimetallic MOF.

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NMSF-AFM-027

Structural and Dielectric Characterization of ZnO–PMMA Nanocomposite Films

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Abstract

Polymer-based nanocomposites have gained significant attention due to their tunable electrical and dielectric properties. In the present study, nanocomposite films were prepared by incorporating zinc oxide nanoparticles (ZnO NPs) into a polymethyl methacrylate (PMMA) matrix with varying weight percentages. The objective of this work is to investigate the effect of ZnO nanoparticle concentration on the dielectric behavior of the ZnO–PMMA nanocomposite system. The prepared films exhibit an amorphous nature, as confirmed by structural analysis, which is advantageous for uniform dielectric performance. Different compositions were synthesized by varying the ZnO content, and their dielectric properties were studied at room temperature. The inclusion of ZnO nanoparticles significantly influences the dielectric constant and dielectric loss of the composite material. An increase in nanoparticle concentration enhances interfacial polarization, leading to improved dielectric permittivity, while maintaining acceptable loss characteristics. The amorphous structure of the ZnO–PMMA nanocomposites ensures reduced scattering and homogeneous dispersion of nanoparticles, contributing to stable dielectric behavior. These results indicate that ZnO–PMMA nanocomposites with optimized nanoparticle loading can be effectively utilized as promising dielectric materials for applications in capacitors, electronic devices, and energy storage systems.

Keywords: *ZnO–PMMA Nanocomposites, Dielectric Properties, Amorphous Materials, Zinc Oxide Nanoparticles, Polymer Matrix, Interfacial Polarization, Dielectric Constant, Energy Storage Materials*

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NMSF-AFM-028

Effective Removal of Lead Using Functionalized PAN/Zirconia Nanofibrous Mats

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Abstract

Heavy metal pollution, particularly lead (Pb^{2+}), is a major environmental concern due to its toxicity, persistence, and adverse effects on human health. This study presents the development of functionalized polyacrylonitrile PAN/Zirconia (ZrO_2) nanofibrous mats as an efficient material for lead removal from aqueous systems. The nanofibrous mats are fabricated using electrospinning, which produces a highly porous structure with a large surface area, suitable for adsorption applications. The incorporation of ZrO_2 nanoparticles enhances the chemical stability and provides active sites for metal ion binding, while PAN contributes to the mechanical strength and flexibility of the composite. Surface functionalization further improves the interaction between the adsorbent and lead ions. The work focuses on understanding the structural, morphological, and functional properties of the nano composite and its potential application in water purification. Such nanofibrous systems offer advantages including ease of handling, reusability, and environmentally friendly performance. Overall, the study highlights the significance of polymer–ceramic nanocomposites as promising materials for sustainable wastewater treatment and heavy metal remediation.

Keywords: *Polyacrylonitrile (PAN), Zirconia, Electrospinning, Heavy Metal, Environmental Remediation*

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NMSF-AFM-029

Development and Optimization of Carbon Black-CNT-Based Flexible Strain Sensor for Wearable Applications

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Abstract

Advancements in wearable technology demands stable and highly sensitive sensors capable of monitoring any physical parameter under robust conditions. Among the plethora of upcoming flexible sensors, strain sensors are becoming highly desirable in wearable technology, health monitoring, rehabilitation, robotics, etc. Carbon based strain sensors when integrated with polymers finds advantages of being both flexible as well display significant gauge factor required for high sensitivity applications. Present project aims at developing a low-cost, wearable and robust carbon black ink-based strain sensors with polyvinyl alcohol (PVA) as the binder along with effects of adding carbon-nanotubes (CNTs) in it. The study involves use of stencil printing, a cost-effective technique to generate reproducible sensors and assess its workability over various flexible substances like PET sheets and the nitrile gloves.

In the first configuration, different proportions of acetylene carbon black (ACB) (varying from 2%- 8%) were mixed with 10% PVA solution. The fabricated sensors (6cm x 3mm) formed agglomerations leading to non-uniformity in coating and resulting in greater instability along with issues of cracking and peeling-off. Thereafter, effects of adding CNT along with ACB and PVA was explored. ACB-CNT in various ratios (1:1, 1:2 & 2:1) were mixed along with PVA powder (optimized to 8%) and sodium dodecyl sulphate (SDS) as a dispersant to ensure a more uniform coating. ACB-CNT of ratio 1:1 ratio demonstrating very high resistance values whereas the ratio 1:2 resulted in frothing of the mixture due to the formation of CNT based cage structures trapping air molecules, resulting in quicker drying of samples and devices with air pockets, making them unsuitable for strain sensor applications. Finally, ACB-CNT of 2:1 ratio displayed good ink printability as well as showed increased change in resistance values under different bending and were used for all subsequent analysis. Performance testing also showed that sensors printed on pre-stretched nitrile gloves were more stable, with consistent increases in their resistance as bending increased, and did not generate any cracking or peeling -off that occurred with non-stretched structures. These results showed successful development of robust flexible strain sensors, as part of sustainable innovation in flexible electronics and preventative healthcare.

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NMSF-AFM-031

Smart Strategies for Harnessing Anisotropic Silver Nanoparticles in Green Energy Systems: A Review

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Abstract

Noble metal nanoparticles composed of silver, gold and platinum have drawn great focus in the antimicrobial research field due to their straightforward synthesis approaches and broad-spectrum efficacy. This review will highlight the synthesis approaches and bactericidal properties of anisotropic silver nanoparticles. It inspects how nanoparticle anisotropy affects the antibacterial activity against different test strains. Different synthesis approaches including chemical, physical and biological can be used to produce silver nanostructures. This review also explores the different aspects about shape dependent antibacterial properties, referencing recent research in this field. Notably, silver nanoparticles with greater degrees of anisotropy demonstrate superior bactericidal performance, particularly those possessing sharp corners and edges compared to round corners and edges. The review concludes with future prospects and potential applications in this field.

Keywords: *Silver Nanoparticles, Anisotropy, Antibacterial Activity, Synthesis Approaches*

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NMSF-AFM-032

Investigation of the Dielectric and Electrical Properties of $Pr_xSr_{1-x}TiO_3$ Synthesised via Solid–State Reaction

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Abstract

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

Keywords: *Green Nanomaterials, Perovskite Oxides, Praseodymium-Doped Strontium Titanate, Energy Storage Devices, Dielectric and Optical Properties*

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NMSF-AFM-033

Enhanced Optical Nonlinearities of Doped 2D MXene ($Ti_3C_2T_x$) by Z-Scan Technique

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Abstract

Two-Dimensional (2D) transition metal carbides, nitrides & carbonitrides have significant interest in the field of optoelectronics due to their extraordinary linear & non-linear optical, electronic and thermal properties. 2D MXene ($Ti_3C_2T_x$) is synthesized through chemical etching technique from MAX phase precursor (Ti_3AlC_2) by removing "Al" using HF solution. The structure and morphology of Pristine & doped (Fe_3O_4) MXene have been confirmed by X-Ray diffraction (XRD) & Scanning Electron Microscopy (SEM) respectively. The linear soptical properties of Pristine & doped (Fe_3O_4) MXene have been investigated by UV-Visible and Photoluminescence (PL) spectroscopy. These results indicate that it shows good optical quality with tunable band gap and luminescence indicates their broad range of applications. Thin films of Pristine & doped (Fe_3O_4) MXene are prepared by drop casting technique for studying its non-linear optical properties using Z-Scan technique (OA/CA). The non-linear parameters such as non-linear refractive index(n_2), absorption co-efficient (β) & third order susceptibility $\chi^{(3)}$ have been calculated. These results reveal intriguing non-linear optical properties of 2D Pristine & doped (Fe_3O_4) MXene films, highlighting their versatility and potential for implementing high-performance nonlinear photonic devices.

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NMSF-AFM-034

Effect of Fe-Co Co-Doping on Structural Dielectric and Ferroelectric Properties of $Na_{0.5}Bi_{0.5}Ti_{1-x}Fe_{x/2}Co_{x/2}O_3$ Ceramics

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Abstract

Lead free dielectric ceramics based on sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ have gained awareness in energy storage application. In this research, the effect of co-doping on structural, dielectric, optical, and ferroelectric characteristics of Fe-Co co-doped $Na_{0.5}Bi_{0.5}Ti_{1-x}Fe_{x/2}Co_{x/2}O_3$ ceramics were examined. All the samples are prepared using traditional solid state reaction method. X-ray diffraction was used to verify the formation of single phase rhombohedral perovskite structure with efficient incorporation of dopant ions. FTIR analysis showed local structural distortion without interfering with the perovskite structure. The dielectric response was highly dependent on frequency and temperature and co-doping resulted in an increase in the dielectric constant, owing to defect-assisted and interfacial polarization. The sample had the best balance of high dielectric constant with low dielectric loss over a wide frequency (1Hz-1MHz) and temperature (25–500 °C) range with diffuse phase transition and relaxor behaviour. Optical measurements showed non-monotonic change in band gap, which was dictated by the joint effect of the Burstein Moss effect on low doping concentrations and the effect of defect-generated electronic states at high concentrations. The measurements of polarization-electric fields indicated reduction in ferroelectric response with lower hysteresis loss, which is favourable in the application of dielectric energy storage. These results indicate that controlled co-doping is an efficient method to customize structure-property interaction in $Na_{0.5}Bi_{0.5}TiO_3$ -based ceramics that can be used in high-performance lead-free dielectric-based applications.

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NMSF-AFM-035

Investigation of Temperature Effects on the Rheology of Polyacrylamide Solutions

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Abstract

The integration of nanoparticles into polymer systems has emerged as a practical approach to enhance performance under demanding operational conditions, particularly in applications such as enhanced oil recovery and advanced fluid processing. This study examines the effect of silica nanoparticles on the rheological behaviour and thermal stability of aqueous polyacrylamide (PAM) solutions over a concentration range of 100–4000 ppm and a temperature range of 25–100 °C. Initially, the baseline rheology of pure PAM solutions was established to characterize intrinsic shear-dependent flow behaviour. The rheology of the polymer solutions was studied using Herschel-Bulkley model. Upon nanoparticle incorporation, a noticeable increase in apparent viscosity and enhanced shear-thinning behaviour was observed, indicating stronger intermolecular interactions and the formation of a transient network structure within the fluid matrix. The improvement in rheological properties is attributed to hydrogen bonding and physical adsorption between PAM chains and nanoparticle surfaces, which promote polymer chain entanglement and resistance to deformation under shear. Temperature-dependent analysis further revealed that nanoparticle addition significantly improves thermal stability, as evidenced by reduced viscosity loss at elevated temperatures compared to pure polymer solutions. This stabilization effect is primarily due to restricted polymer chain mobility and delayed thermal degradation in the presence of nanoparticles. A systematic stepwise methodology was adopted to isolate the individual and combined effects of concentration, temperature, and nanoparticle loading, enabling a clearer understanding of structure–property relationships. However, beyond an optimal nanoparticle concentration, a diminishing pattern effect in performance was observed, likely due to particle agglomeration and disruption of the polymer network. The findings demonstrate that controlled nanoparticle incorporation can effectively tailor the rheological and thermal characteristics of polymer systems, making them more suitable for high-temperature and high-shear applications. This work provides a more application-oriented insight into designing stable and efficient polymer-based nanofluids for industrial use.

Keywords: *Polyacrylamide, Silica Nanoparticles, Rheology, Thermal Stability, Shear Thinning, Nanofluids*

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NMSF-AFM-036

Biological Assessment of Copper-Doped Tin Oxide Nanoparticles: From Cytotoxicity to Antibacterial Action

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Abstract

Copper-doped tin oxide (Cu–SnO_2) nanoparticles have emerged as promising multifunctional nanomaterials owing to their tunable surface chemistry and enhanced bioactivity. In this study, Cu–SnO_2 nanoparticles were synthesized via coprecipitation method and systematically evaluated for their cytotoxic and antibacterial potential. Structural and physicochemical characterization confirmed successful copper incorporation into the SnO_2 lattice with nanoscale dimensions. The cytotoxic effects of the nanoparticles were assessed on cultured healthy (HEK-293) and cancerous (AGS – Gastric adenocarcinoma) mammalian cells using standard viability assay, MTT to determine dose-dependent responses and biocompatibility. Further, scratch assay was done to validate the anti-cancerous potency. Antibacterial activity was investigated against representative Gram-positive (B. *subtilis*) and Gram-negative (E. *coli*) bacterial strains using agar diffusion and growth inhibition methods. The Cu–SnO_2 nanoparticles exhibited significant antibacterial efficacy, attributed to enhanced reactive oxygen species generation. Comparative analysis indicated that copper doping substantially improved the biological activity of SnO_2 nanoparticles without inducing excessive cytotoxicity at optimized concentrations. These findings suggest that Cu–SnO_2 nanoparticles hold potential as effective antimicrobial agents with acceptable cytocompatibility towards healthy cells and toxicity effect towards gastric cancer, offering prospects for biomedical and therapeutic applications.

Keywords: *Nanomaterials, Cytotoxicity, Nanotherapeutics, Cancer*

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NMSF-AFM-037

Sustainable Future: Materials with Semiconducting Nanocoatings

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Abstract

Semiconducting nanocoatings represent a transformative approach toward sustainable material development. By integrating nanoscale semiconductor layers onto conventional substrates, materials gain enhanced functionality such as self-cleaning, energy harvesting, corrosion resistance, and environmental remediation. These coatings contribute significantly to sustainability by reducing energy consumption, extending material lifespan, and enabling green technologies. Sustainability in materials science focuses on minimizing environmental impact while maximizing efficiency and durability. The field of Nanotechnology has enabled the development of semiconducting nanocoatings that modify surface properties without altering bulk material composition. Semiconducting materials such as Titanium dioxide, Zinc oxide, and Silicon are widely used due to their unique optical and electronic properties. Semiconducting nanocoatings are thin films (1–100 nm) deposited on surfaces to impart functional properties like photocatalytic activity, antibacterial behavior, UV protection and electrical conductivity. These coatings exploit quantum confinement, which alters bandgap energy and enhances reactivity. They are required for sustainability as they improve solar cell efficiency via better light absorption, used in photovoltaics for renewable energy and reduce energy loss in buildings through thermal control coatings. They are applied in Environmental remediation as photocatalytic coatings degrade pollutants (air and water purification), TiO_2 coatings break down organic contaminants under UV light. They act as Corrosion resistance material and extend lifespan of metals and hence reduces resource consumption and replace toxic coatings (like chromates). They also have antibacterial and healthcare Applications as ZnO nanocoatings show antimicrobial properties and are used in medical devices and packaging. Sustainability also depends on fabrication methods which are green synthesis approaches such as sol-gel method (low temperature , green synthesis using plant extract. Semiconducting nanocoatings provide a powerful pathway toward sustainable materials by enhancing efficiency, reducing waste, and enabling environmentally friendly technologies. With advances in green synthesis and large-scale production, they are expected to play a crucial role in addressing global challenges related to energy, environment, and resource conservation.

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NMSF-AFM-038

Synthesis and Application of Biochar for Enhanced Photocatalytic Activity in Water Remediation

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Abstract

The industrial evolution has resulted to the continues release of pollutants such as dyes into water bodies. This has become a global concern as the conventional technologies are not highly effective in the treatment of this pollutants. Biochar a carbon-rich material obtained from the thermal decomposition of biomass offers an alternative solution. The study revealed recent advances in biochar preparation and application in water remediation. A facile one-step pyrolysis method was adopted using biomass and $ZnCl_2$ to form biochar/ZnO composites. This heightens the material desirability for use in environmental remediation due to its high photocatalytic activity, and reusability. Furthermore, the material demonstrated efficient degradation of dyes (methylene blue and crystal violet) under photocatalysis at 60 minutes run time. The enhanced performance is attributed to improved charge separation and reactive oxygen species generation facilitated by the biochar/ZnO synergy. This study expands knowledge on biochar composite research into scalable solutions for environmental remediation.

Keywords:

Biochar, Pyrolysis, Photocatalysis, Dyes, Nanomaterials

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NMSF-AFM-039

Structural and Optical Study of Pure and Modified Tin Selenide Nano-System

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Abstract

In this study, we introduce a fabrication method for composite materials with light-absorbing properties. A simple high-temperature and high-pressure method was used to fabricate these composites of $SnSe_2$–SnO_2 and $SnSe_2$–SnO_2–SnSe, along with pure SnO_2 and $SnSe_2$. XRD analysis was performed for all four samples, and the presence of these phases (with their percentages) is confirmed using Rietveld refinement with FullProf software. To study optical properties, UV–Visible analysis was carried out, and it was found that the composite materials exhibit more light absorption behaviour than their pure phases. This study shows potential future applications in optoelectronic devices like photodetectors and in environmental cleaning activities like synchronized photothermal–photocatalysis.

Keywords: *$SnSe_2$, SnSe, Photothermal- Photocatalysis*

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NMSF-AFM-041

PEGylation of Albumin Nanoparticles Loaded with the Antituberculosis Drug Isoniazid

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Abstract

PEGylated albumins are typically produced through a chemical reaction between an activated PEG fragment and reactive groups on the albumin, which include amino acid side chains or the N-terminal amino group and the C-terminal carboxylic acid group [1]. Therefore, to successfully PEGylate albumin, we 'activated' the PEG. The synthesis of polyethylene glycol dichloro-s-triazine ($PEGTC_2$) was carried out according to the method [2] using cyanuric chloride. The Taguchi method was used to optimise the PEGylation of bovine albumin nanoparticles loaded with isoniazid. The molecular weight and concentration of $PEGTC_2$, the concentration of BSA, pH, the concentration of INH, the rate of ethanol addition and the stirring rate were selected as factors influencing the particle size and PDI of the $PEGTC_2 - BSA - INH$ nanoparticles. PEGylated bovine albumin nanoparticles were prepared using 'activated PEG' via the desolvation method. Desolvation was carried out using ethanol, and cross-linking of the nanoparticles was performed using glutaraldehyde. The nanoparticles were prepared using 'activated PEG' with a molecular weight of 6000 and a concentration of 20 mg/mL; the concentration of albumin was 40 mg/mL and isoniazid was 4 mg/mL, the environment pH was 7, the ethanol addition rate was 1 mL/min, and the stirring speed was 200 rpm. The experimental result for the average particle size (226.9 ± 1 nm) showed reasonable agreement with the model.

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NMSF-AFM-042

Comparative Gas Sensing Performance of MWCNT-$MgCl_2$ Composite Towards Oxidising and Reducing Gases

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Abstract

This work presents a comparative study on the gas sensing performance of a multi-walled carbon nanotube–magnesium chloride (MWCNT-$MgCl_2$) composite towards oxidising and reducing gases. The composite was synthesised via a simple dispersion followed by a drop-casting technique. Comprehensive characterisation using UV-visible spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and field emission scanning electron microscopy (FESEM) confirmed the successful formation of the composite with enhanced surface activity and abundant adsorption sites. The sensing characteristics were systematically evaluated for nitrogen dioxide (NO_2) as an oxidising gas and ammonia (NH_3) as a reducing gas using current-voltage (I-V) measurements. A clear comparative behaviour was observed, where the sensor exhibited a significantly higher response towards NO_2 compared to NH_3. Key sensing parameters, including response, recovery time, sensitivity, and limit of detection (LOD) were analysed for both gases. The MWCNT-$MgCl_2$ composite demonstrated faster response and higher sensitivity towards oxidising gas (NO_2), while maintaining stable and reproducible performance for reducing gas (NH_3). The enhanced sensing behaviour is primarily due to the synergistic interaction between the high conductivity of MWCNTs and the adsorption capability of $MgCl_2$, which facilitates efficient gas adsorption and charge transfer. This comparative analysis highlights the potential of MWCNT-$MgCl_2$ as an effective sensing material for the selective detection of oxidising and reducing gases, making it a promising candidate for environmental and industrial gas monitoring applications.

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NMSF-AFM-043

Toward Sustainable Industrial Wastewater Treatment Using NKBT-based Piezocatalysis

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Abstract

Piezocatalysis, an eco-friendly technology that converts ambient mechanical energy (e.g., vibrations, noise) into chemical energy via piezoelectric materials, has emerged as a promising alternative to traditional catalysis for applications such as dye degradation, water splitting, medical therapy, and aquatic environment remediation. By generating highly reactive species for breaking down complex organic pollutants, piezocatalysts offer a sustainable, cost-effective solution to persistent contaminants like industrial dyes. The present work investigates $(Na_{0.8}K_{0.2})_{0.5}Bi_{0.5}TiO_3$ (NKBT) ceramic as a lead free piezocatalyst for sustainable wastewater treatment. NKBT powders were synthesized via solid state sintering (calcination at 800 °C for 6h and sintering at 1150 °C for 3 h) and confirmed by X ray diffraction to be a single phase perovskite with coexisting rhombohedral(R) and tetragonal(T) distortions at the morphotropic phase boundary. The SAED pattern of NKBT indicated the coexistence of R and T phase nanodomains in the ceramics, which is consistent with the XRD data. Piezocatalytic activity was assessed by degrading a $5 mgL^{-1}$ Rhodamine B solution using 100mg of NKBT dispersed in 50mL of dye solution. Ultrasonic treatment was conducted in a 53kHz, 100W bath with aliquots withdrawn every 15 min up to 90 min; dye concentrations were determined by UV–Vis spectroscopy at 554 nm. Under these conditions, NKBT achieved ~69 % decolorization within 90 min, following pseudo-first-order kinetics (k 0.013 min^{-1}). The performance was tempered by the use of micrometer-sized powders, partial depoling during pellet crushing, and the inability to remove catalyst particles after die degradation before recording the UV spectra. Further, the work is focusing on nanoscale NKBT synthesis, gentle poling methods, and catalyst separation techniques to fully realize its piezocatalytic potential. Piezocatalytic activity will also be evaluated using impact and attrition methods to enhance the understanding and significance of piezocatalysts in dye degradation processes. This study establishes NKBT as a promising candidate for mechanically driven advanced oxidation processes in real world wastewater treatment.

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NMSF-AFM-044

Plant-Mediated Synthesis of TiO_2 Nanoparticles Using Nephrolepisexaltata and their Therapeutic Potential against Prostate Cancer

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Abstract

This paper represents plant mediated Titanium dioxide nanoparticles (TiO_2 NPs) with their antibacterial, antioxidant, and anticancer properties. FT-IR spectrum showed peaks at 427 cm^{-1}, which correlate with the Ti-O (Metal-Oxide) bond. XRD spectra showed the crystalline TiO_2 NPs with a size of 18–30 nm. SEM analysis revealed that the synthesized nanoparticles were spherical. EDX analysis confirms the presence of Ti and O.The optical properties of TiO_2 NPs were confirmed by the UV–visible spectra, which have a wide absorption peak at 400 nm with a band gap energy of 3.0 eV. The antibacterial activity of TiO_2 NPs showed the maximum zone of inhibition observed against *E. coli* (0.8mm), followed by *P. aeruginosa* (0.8mm) and *K. pneumoniae* (0.7mm) at a 100 μg/mL concentration. DPPH analysis was used to measure the antioxidant activity. At a 100 μg/mL concentration, the DPPH assay of *Nephrolepisexaltata*-mediated TiO_2 NPs achieved 83% inhibition with an IC50 of 99.44 μg/mL. In the anticancer activity, TiO_2 NPs caused severe damage to the human prostate cancer cell line (PC3) with decreased cell viability at 100 μg/mL and an IC_{50} of 26.49 μg. *Nephrolepisexaltata*-mediated TiO_2

NPs can be used as new nano-medicine in near-future research analysis for therapeutic applications.

Keywords: *Nephrolepisexaltata, Titanium Dioxide, Antibacterial, Antioxidant, Anticancer-Prostate Cancer*

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NMSF-AFM-045

Fluence- Driven Evolution of Morphology and Optical Response in Krypton -Implanted Silicon Nitride

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Abstract

This work investigates the fluence-dependent modification of silicon nitride films (577 nm) under 30 keV Kr^+ ion implantation. Films deposited on Si(100) by RF magnetron sputtering were implanted at fluences ranging from 1×10^{16} to 1×10^{17} Kr^+cm^{-2}. These films were characterized using Raman spectroscopy, Atomic Force Microscopy (AFM), UV-visible spectroscopy and Spectroscopic Ellipsometry (SE). Raman analysis shows progressive peak broadening with increasing fluence, indicating amorphization due to ion-induced disorder, except at 5×10^{16} ions/cm^2 where reduced Full width at Half Maxima (FWHM) and enhanced intensity suggest partial crystallization. This indicates that at this fluence, sufficient energy is available for atomic rearrangement, leading to improved local ordering. This same behavior is consistently reflected in AFM results, where surface roughness and particle size exhibit non-linear variation, with FFT analysis confirming morphological reorganization at this fluence. Power spectral Density (PSD) analysis further confirms fluence-driven transitions in surface transport mechanisms, with the dominance of surface diffusion at 5×10^{16} ions/cm^2 leading to the formation of well-defined surface features. Optical measurements showed a similar trend of reflectance as that of roughness, while the optical energy gap decreases with fluence due to defect state formation, except at 5×10^{16} ions/cm^2 where partial crystallization leads to a slight increase. The refractive index also shows non-monotonic behavior with fluence. The correlated structural, morphological, and optical changes indicate that fluence-dependent Kr^+ ion implantation enables controlled tuning of silicon nitride film properties.

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NMSF-AFM-046

Eco-Friendly Polypyrrole–Biomass Carbon Composite for Antibacterial Applications

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Abstract

The study presents the facile synthesis of Polypyrrole (PPy) and orange-peel carbon black (OPC) composite for antibacterial applications. By utilizing orange peel an abundant agricultural waste as a carbon precursor, this approach successfully promotes waste valorisation and green material design. The PPy/OPC composite was fabricated via in-situ oxidative polymerization, yielding a highly porous structure with an expanded surface area and strong interfacial interactions between the PPy and OPC. Crucially, the composite demonstrated notable antibacterial efficacy against both Gram-negative Escherichia coli (MTCC − 7410) and Gram-positive Staphylococcus aureus (MTCC − 7443). This antibacterial performance is driven by a combination of bacterial membrane disruption, surface charge interactions, and induced oxidative stress. Ultimately, the use of biomass-derived carbon and a facile synthesis route position the PPy/OPC composite as a highly promising, sustainable material for advanced antimicrobial applications.

Keywords: *Insitu Oxidation, Polypyrrole, Orange Peel Carbon Black, E.Coli, S.Aureus*

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NMSF-AFM-048

Standardized Nanocellulose Extraction from Dendrocalamus Hamiltonii Shoot Sheath Waste Using Taguchi DOE

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Abstract

The present work extracts nanocellulose using the alkali-bleached-acid treatment. Herein, a novel resource was utilized i.e., waste of Dendrocalamus hamiltonii Shoot sheath, a bamboo species known for its delicious fermented bamboo shoot in the Northeastern region of India. During the preparation of soibum (fermented bamboo shoot), the outer bamboo shoot sheath (BSS), which encases the edible portion, is usually removed and discarded in substantial quantities, treated as food processing waste, and mostly burned, thereby increasing pollution. Initially, the alkali method was optimized using Taguchi L_{16} array design, resulting the optimum set as of 3M NaOH at 70 °C for 2h in 1:30 w/v ratio. Followed by using mild peroxide oxidation, recovering cellulose upto 77.27 ± 2.00% compared to raw BSS of 38.73 ± 0.78%. Nanocellulose synthesized using 40% and 50%(BAH_1 and BAH_2) treated with H_2SO_4 yields 71.99 ± 4.06% and 82.77 ± 1.17%, with average diameters of 37.44 ± 7.90 nm and 33.30 ± 6.45 nm, respectively. Fourier Transform Infrared spectroscopy (FTIR) spectra reveal the successful removal of hemicellulose and lignin. Zeta potential discloses stability of BAH_1 and BAH_2 exhibit zeta potentials of -31.38 ± 1.15 mV and -32.93 ± 0.34 mV. Thermogravimetric Analysis (TGA) and Derivative Thermogravimetry (DTG) confirmed the thermal stability. X-Ray Diffraction (XRD) curves were analyzed using two methods: Segal and peak deconvolution to determine the crystallinity of BAH1 (83.10%, 89.45%) and BAH2 (85.61%, 94.68%). By harnessing the potential of waste BSS, this research contributes to the development of green biomaterials, encouraging a shift towards environmentally responsible practices in material science.

Keywords: *Bamboo Shoot Sheath waste, Cellulose , Nanocellulose, Sustainability*

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NMSF-AFM-050

Performance Assessment of Mineral Oil and Ester-Based Insulating Fluids: A Comparative Physicochemical and Dielectric Investigation

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Abstract

The operational reliability and service life of power transformers are fundamentally determined by the dielectric integrity and physicochemical stability of the dielectric fluid utilized. In this work, a rigorous comparative evaluation of three classes of virgin insulating fluids—mineral oil (MIO), natural ester (NE), and synthetic ester (SE)—is undertaken to critically examine their performance under standardized testing conditions. A comprehensive suite of diagnostic parameters, including Breakdown voltage, moisture content, density and viscosity, is systematically analyzed in accordance with internationally recognized test methodologies.

The experimental findings reveal significant variations in both dielectric and physicochemical behaviour among the examined fluids, predominantly influenced by their intrinsic molecular structure and compositional characteristics. Ester-based fluids (NE and SE) exhibit enhanced moisture tolerance and inherent biodegradability; however, these advantages are accompanied by relatively elevated viscosity and dissipation characteristics. Conversely, mineral oil exhibits favourable dielectric performance and economic viability, but is constrained by lower environmental compatibility and higher susceptibility to moisture ingress.

Collectively, the outcomes of this study provide substantive insights into the performance and applicability of alternative insulating liquids for modern power transformer systems, particularly in the context of sustainability, fire safety, and enhanced operational reliability. Moreover, the results contribute to informed material selection and optimization strategies for the development of advanced and next-generation transformer insulation systems.

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NMSF-AFM-051

Green Photocatalytic Degradation of Crystal Violet and Eosin Y Dyes Using NiO/rGO Nanostructured Composites Under Sunlight

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Abstract

Rapid industrialization and urban growth have caused the release of many harmful pollutants into water bodies, leading to serious environmental and health problems. Among these pollutants, organic dyes from textile, paint, and pigment industries are considered highly dangerous because they are toxic, chemically stable, and difficult to break down naturally. Their presence in water not only reduces water quality but also blocks sunlight penetration, which negatively affects aquatic life and disturbs the natural balance of ecosystems. Photocatalysis is considered an effective, economical, and eco-friendly method for removing such pollutants because it helps convert harmful organic compounds into less toxic substances without producing secondary pollution. In this study, NiO/rGO nanocomposites were prepared using a hydrothermal method followed by calcination and were used for the photocatalytic degradation of methylene blue dye under sunlight. The prepared nanocomposites were characterized using X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Raman Spectroscopy, and Fourier Transform Infrared Spectroscopy (FTIR), while the surface area was measured using BET analysis. The photocatalytic results showed that NiO/rGO performed much better under sunlight than in dark conditions and achieved an excellent 92% degradation of crystal violet dye and 96% degradation of Eosin Y dye within 30 minutes. The effects of catalyst dosage, pH, and contact time on dye removal were also studied in detail. The results confirm that NiO/rGO nanocomposites have strong photocatalytic performance and can be considered a highly promising material for the fast and efficient removal of organic dyes from wastewater.

Keywords: *Photocatalysis, NiO/rGO nanocomposite, Sunlight Irradiation, Wastewater Treatment, Organic Dye Removal*

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NMSF-AFM-052

Structural and Electrical Characterization of High-Energy Ball-Milled Zinc-Substituted Manganese Nickel Ferrite

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Abstract

A series of zinc-substituted manganese nickel ferrites of the compositional formula $Zn_xNi_{0.25}Mn_{0.75-x}Fe_2O_4$ (x increasing in steps of 0.05 from 0.00 to 0.25) were synthesized via the ceramic technique using high-energy ball-milling. The structural and phase analysis from XRD spectra confirmed the FCC, cubic spinel structure. Calculations of the structural parameters, such as crystallite size and lattice constant of samples, were carried out using XRD data and studied for varying zinc content. FTIR shows two peaks centered around 416 cm^{-1} and 524 cm^{-1}. The SEM photograph depicts irregular grains with pores present. EDAX reveals the presence of the composition elements in the samples. The room-temperature measured electrical parameters exhibited dispersion behavior with varying frequencies. The electrical properties, like dielectric constant, dielectric loss, and ac conductivity, were investigated and reported, which find applications in electrical and electronic devices.

Keywords:

Manganese Nickel Ferrite, X-Ray Diffraction, EDAX, Dielectric, AC Conductivity

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NMSF-AFM-053

Thermal Influence on the Physicochemical Properties of Biomass-Derived Nanocellulose Polymer

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Abstract

Nanocellulose was successfully extracted via acid hydrolysis. The resulting suspension was subjected to drying at varying temperatures to investigate the influence of thermal conditions on its structural and chemical properties. Electron microscopy analysis provided valuable insights into the morphological characteristics of the dried nanocellulose, revealing notable temperature-dependent changes in surface structure and integrity. Infrared spectroscopy was further employed to assess the chemical functionality of the samples, where thermal exposure was found to influence the presence and intensity of key functional groups. Additionally, surface roughness analysis demonstrated considerable variations across samples dried under different temperature conditions. The findings collectively suggest that drying temperature plays a significant role in governing both the morphological stability and chemical functionality of nanocellulose. It was observed that lower drying temperatures are more favorable for preserving the structural and functional characteristics of nanocellulose. These outcomes highlight the importance of optimizing drying conditions during nanocellulose processing. The insights gained from this study are particularly relevant for applications in environmental remediation, where the surface chemistry and morphological integrity of nanomaterials are critical performance-determining factors.

Keywords: *Nanocellulose, Drying Temperature, Functionality, Morphology, Roughness*

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NMSF-AFM-054

Gadolinium-Doped ZnO Nanoparticles as High-Performance Photocatalysts for Efficient Antibiotic Degradation in Aqueous Media

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Abstract

The widespread contamination of aquatic ecosystems by antibiotic residues poses a critical threat to environmental integrity and public health, necessitating the development of efficient and sustainable remediation strategies. In this study, gadolinium (Gd^{3+})-doped zinc oxide (ZnO) nanoparticles were successfully synthesized via a facile wet chemical co-precipitation method and evaluated for their photocatalytic efficiency toward the degradation of ciprofloxacin and tetracycline antibiotics under UV/visible irradiation. The as-synthesized nanoparticles were comprehensively characterized using various spectroscopic techniques. X-ray diffraction analysis confirmed the wurtzite hexagonal crystal structure and phase purity of the fabricated nanoparticles, while Field Emission Scanning Electron Microscopy revealed the surface morphology and validated the successful incorporation of Gd^{3+} ions into the ZnO lattice. Elemental composition and dopant distribution were further corroborated by Energy-Dispersive X-ray Spectroscopy. The PVP capping agent effectively stabilized nanoparticle morphology by suppressing agglomeration, thereby preserving a high active surface area favorable for catalytic reactions. Photocatalytic performance studies demonstrated that Gd^{3+}-doped ZnO nanoparticles exhibited significantly superior degradation efficiency compared to their undoped counterparts, achieving notable removal of both ciprofloxacin and tetracycline in aqueous media under UV and visible irradiation. The enhanced photocatalytic activity is attributed to the synergistic effect of rare-earth doping, which narrows the bandgap and reduces electron–hole recombination, and polymer capping, which improves structural stability and dispersibility. Collectively, these findings establish Gd-doped ZnO nanoparticles as a promising, cost-effective, and scalable photocatalytic platform for the remediation of persistent pharmaceutical pollutants from wastewater.

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NMSF-AFM-055

Eco-Friendly Synthesis of Nitrogen-Doped Carbon Quantum Dots from Cow Urine & Coffee

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Abstract

Nitrogen-doped carbon quantum dots (N-CQDs) were synthesized via a green and cost-effective approach using coffee powder as the carbon source and cow urine as a natural nitrogen precursor. The synthesis was carried out in a domestic microwave oven for 300 s, offering a rapid and energy-efficient alternative to conventional methods without the need for additional chemical passivation. The obtained N-CQDs exhibited characteristic absorption in the UV-Vis range, attributed to π–π^* transitions of sp^2 carbon domains, and n–π^* transitions associated with surface functional groups. Photoluminescence (PL) spectra revealed pronounced excitation-dependent emission over the 300–400 nm excitation range, accompanied by a systematic red shift in emission maxima. The broad and overlapping emission profiles indicate that fluorescence is predominantly governed by surface defect states and nitrogen-induced functional groups rather than intrinsic band-edge transitions. X-ray diffraction (XRD) analysis displayed a broad diffraction peak centered around $\sim 40°$, corresponding to the (100) in-plane reflection of graphitic carbon, suggesting short-range ordering within an otherwise amorphous carbon framework. The combination of green synthesis and tunable properties highlights N-CQDs as next-generation sustainable nanomaterials. Findings demonstrate that microwave-synthesized N-CQDs possess tunable optical properties and hold strong potential for applications in bioimaging, sensing, photocatalysis, and optoelectronic devices.

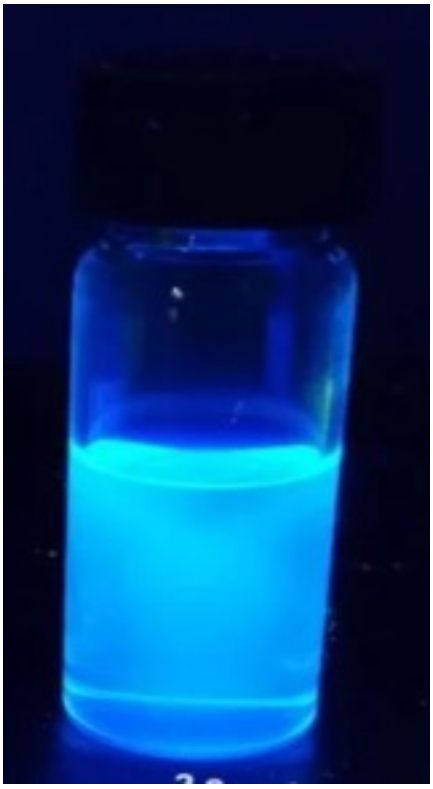

Figure: Blue emission N-CQDs under UV light

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NMSF-AFM-058

Preparation of CQDs By Green Precursor

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Abstract

Carbon quantum dots (CQDs) are zero-dimensional fluorescent nanomaterials exhibiting unique optical and physicochemical properties such as strong photoluminescence, high water solubility, chemical stability, and biocompatibility due to quantum confinement effects. In recent years, green synthesis approaches have gained significant attention for the sustainable fabrication of CQDs using natural precursors.

In the present work, nitrogen-doped carbon quantum dots (N-CQDs) are synthesized via a microwave-assisted bottom-up method using neem leaf aqueous extract and amla juice as carbon sources, while cow urine serves as a natural nitrogen-doping agent. The synthesis is carried out in a domestic microwave oven ,providing a rapid, energy-efficient, and eco-friendly route without the use of hazardous chemicals.

The primary objective of this study is to investigate the impact of precursor ratio on CQD formation. Different proportions of neem extract, amla juice, and cow urine are systematically varied to understand their influence on nucleation, growth, surface functionality, and optical behavior. The synthesized CQDs are characterized using XRD, UV–Vis, PL spectroscopy, and TEM. This study aims to establish precursor ratio as a key parameter for tuning CQD properties for advanced applications.

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NMSF-AFM-059

Nano-Enabled Therapeutics of Cissus Quadrangularis L.: A Review

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Abstract

The traditional uses of Cissus quadrangularis L in bone healing and fracture treatment as medicinal herb have gained interest among the scientist and due to its various phytochemical content. Chemical analysis methods have identified the predominant chemical constituents like titrepenoids, phenolic acids, flavonoids, stilbenes, essential minerals and phytosterols. The health benefits are numerous and these components helps in bone growth, act as anti-inflammatory, antidiabetic, antioxidants and anticancer agents. In addition to simply cataloguing the chemicals in the plant, scientists are also seeking to understand how the plant makes these chemicals and what controls their production. One area of research is into the role of the plant's micro biome the microorganisms living inside and around the plant in influencing the production of these secondary metabolites. At the same time, experiments are being conducted with new drug delivery methods, especially those based on nanoparticles, to improve the absorption, keep the drug stable for a longer time, and more accurately target the substances derived from C. quadrangularis. By combining molecular studies, microbiome, assisted biosynthesis, and advanced nano, based drug formulations, the research on Cissus quadrangularis of today is trying to find features that can help unlock a plant, based healing power and thus make traditional medicinal products work even better in today's health care system backed by scientific evidence.

Keywords: *Cissus quadrangularis L, Phytochemicals, Pharmacological Activities, Nanocarriers, Oestrogenic, Anticancer, Bioavailability*

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NMSF-AFM-060

Photocatalytic Degradation of Rhodamine B using $NiCoFe_2O_4$ Synthesized by Modified Combustion Method

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Abstract

The study reports the synthesis of ternary $Ni_{0.6}Co_{0.3}(Fe_2O_4)_{0.1}$ spinel oxide via a modified combustion method using citric acid as fuel, aimed at exploring its potential application as a photocatalyst for selective dye degradation. X-ray$_{0.3}$ diffraction (XRD) and Scanning electron microscopy (SEM) studies were conducted to study the crystalline phase and morphology of the sample. XRD study confirmed the formation of a cubic spinel structure. SEM revealed densely packed agglomerated particles with an average size of approximately 155 nm. Photocatalytic degradation of Rhodamine B was evaluated under varying pH, catalyst loading, and recycling conditions. The results of catalyst loading demonstrated a steady increase in degradation efficiency from 25.7% at 10 mg to a maximum of 56.5% at 30 mg. Kinetic analysis exhibited pseudo–first-order behavior, with rate constants (k) ranging from 1.78×10^{-3} to 4.35×10^{-3} min^{-1} and R^2 values between 0.94 and 0.99, confirming excellent linearity and photocatalytic activity of the $Ni_{0.6}Co_{0.3}(Fe_2O_4)_{0.1}$ catalyst. $Ni_{0.6}Co_{0.3}(Fe_2O_4)_{0.1}$ demonstrates a substitute material in removing organic pollutants from contaminated water, thereby enhancing water safety for ecological and human use.

Keywords: *Combustion Method, Spinel Structure, Photo Catalysis, Rhodamine B, Pseudo First Order*

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NMSF-AFM-061

Antibacterial Activity of $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ Spinel Oxide Synthesized via Modified Combustion Method

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Abstract

Spinel-structured transition metal oxides have attracted significant interest in recent years owing to their remarkable structural tunability, chemical stability, and multifunctional properties, including energy storage and antimicrobial activity. In this study, a ternary $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ spinel oxide was synthesized via a modified combustion method using citric acid as fuel. The structural and morphological characteristics of the synthesized material were investigated using X-ray diffraction (XRD) and scanning electron microscopy (SEM). XRD analysis confirmed the formation of a phase-pure cubic spinel structure, while SEM imaging revealed densely agglomerated particles with an average particle size of approximately 155 nm.The antibacterial potential of the synthesized $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ was evaluated against two clinically significant bacterial strains - gram-negative *Escherichia coli* (MTCC-7410) and gram-positive *Staphylococcus aureus*(MTCC-7443) - using the agar well diffusion method. Samples dissolved in DMSO at 20 mg/mL were tested at concentrations of 100, 200, and 300 μg, with kanamycin (30 μg) serving as the standard antibiotic. The inoculum was adjusted to approximately $5x10^5$ CFU/mL and incubated at 37 °C, after which zones of inhibition (mm) were measured.The results demonstrated a clear and consistent concentration-dependent increase in antibacterial activity for both bacterial strains. Against S. aureus, the maximum zone of inhibition of 17.66 ± 0.57 mm was recorded at 300 μg, while against *E. coli*, a maximum zone of 16.66 ± 0.57 mm was achieved at the same concentration. The material exhibited notably stronger activity against *S. aureus* at lower concentrations,

suggesting preferential interaction with gram-positive cell wall constituents. The activity, while lower than the kanamycin standard (~19–20 mm), remains promising for a purely inorganic oxide material with no surface functionalization.These findings highlight the inherent antibacterial nature of $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$, likely arising from the synergistic metal ion release and reactive oxygen species (ROS) generation from nickel, cobalt, and iron centres. Combined with its previously demonstrated electric double-layer capacitive (EDLC) behaviour for energy storage applications, $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ emerges as a versatile, multifunctional advanced material with potential in both biomedical and energy sectors.

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NMSF-AFM-062

Interdisciplinary Applications of Algebraic Structures in Science and Engineering Systems

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Abstract

Although algebraic structures provide the basis upon which multiple scientific and engineering fields build, their interdisciplinary applicability has been less explored in unified computational frameworks. In this research we investigate the role of algebraic systems to bridge numerous domains and propose an integrated analytical platform that connects algebraic properties to relevant real-world applications.

The study performs systematic analysis on finite algebraic systems and correlates structure-related property to domain requirements, of which physics, chemistry, computer science, economics and data science are just a few representative types.

The application of the framework considers the following algebraic properties such as associativity, commutativity, identity, and inevitability towards the validation of the suitable properties for application context. For example, associations of group structure with reversible transformations in cryptography are common, and associative operations provide computational economy in computer science.

Symmetry related properties are connected to physical and chemical systems, indicating algebra as an important mathematical tool for modelling natural phenomena. The dashboard interactive implementation allows automated classification and interdisciplinary mapping with a new level of understanding of how abstract mathematical constructs can be used to drive applied sciences innovation.

The findings illustrate that algebraic structures can act as an integration, for modelling, optimization as well as system design from different domains.

This research is a step toward interdisciplinary work, by providing a practical computational connection between abstract algebra and everyday purposes, in line with the trends of AI-led scientific research.

Keywords: *Algebraic Structures, Interdisciplinary Research, Computational Modelling, Applied Mathematics, Scientific Computing, System Design, Symmetry Analysis, Engineering Applications, AI Integration*

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NMSF-AFM-063

Effective Thermal Conductivity of Two-Phase System using Artificial Neural Network (ANN) Approach

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Abstract

This work investigates Optimizing the thermal performance of composite systems in engineering and construction applications requires precise estimation of effective thermal conductivity (ETC) in heterogeneous materials. ETC of a composite system made of steel fillers implanted in a concrete matrix is examined in this work. Because heat transfer in these composites is complicated and nonlinear, an Artificial Neural Network (ANN) technique is used to model and predict ETC accurately. The ANN is trained and validated using experimental data from different concrete-steel filler combinations, such as changes in filler volume fraction, distribution, and thermal boundary conditions. The model outperforms conventional empirical and analytical models in terms of prediction performance. The findings show that the ETC of the composite is highly influenced by the volume fraction and spatial distribution of steel fillers. When evaluating the thermal behaviour of two-phase materials, the ANN technique is a reliable and effective tool that provides important information for the design of thermally efficient composite structures.

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NMSF-AFM-064

CSRR-Based Metasurface RF Sensor for Glucose-Dependent Dielectric Sensing

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Abstract

Radio-frequency (RF) dielectric sensing has emerged as an effective approach for detecting variations in the electromagnetic properties of biologically relevant media. In this work, a compact complementary split-ring resonator (CSRR)-based metasurface is proposed for RF dielectric sensing of glucose variations. The designed structure enables strong electromagnetic field confinement within the CSRR split gaps, enhancing sensitivity to changes in the surrounding dielectric environment. The sensor is numerically investigated over the 1–20 G Hz frequency range using two low-loss substrates, namely PTFE and Rogers RT-Duroid 5880, to evaluate substrate-dependent sensing performance. Glucose variations are modelled by introducing a high-permittivity dielectric layer with relative permittivity ranging from 68 to 72 above the sensing region. The sensing mechanism is based on systematic shifts in resonance frequency induced by changes in effective permittivity. The results demonstrate stable and monotonic resonance shifts for both substrates, with Rogers RT-Duroid 5880 exhibiting deeper resonance characteristics and improved sensitivity compared to PTFE. The proposed compact metasurface structure offers stable RF response, repeatable sensing behavior, and enhanced field localization, making it a promising candidate for RF dielectric sensing applications involving glucose-related variations.

Keywords: *Metasurface, CSRR, RF Dielectric Sensing, Glucose Sensing, Dielectric Analysis, Biosensing*

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NMSF-CAM-016

Computer Modelling Approaches & Dielectric Spectroscopy in Herbal Bioactives: A Review

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Abstract

Herbal bioactives consist of quite a wide variety of phytochemicals whose behaviour is largely regulated by their intermolecular interactions, solvation dynamics, and the collective dipolar response. Isolated experimental or computational methods alone make it difficult to understand these phenomena at different scales. This review article, a narrative type, discusses an integrated approach that links dielectric spectroscopy with various molecular modelling methods, i.e., molecular dynamics (MD), quantum mechanical methods (DFT and QM/MM), and machine learning, thereby making it possible to draw predictive and mechanistic conclusions about phytochemical systems.

A comprehensive review of the literature (2000–2024) was done by the authors through major scientific databases with the objective of identifying research articles that merge experimental dielectric characterization with computational methods. Significant relationships have been discovered between dielectric measurements (dielectric constant, loss factor, and relaxation time) and molecular simulation outputs such as dipole moment distributions, hydrogen-bond lifetimes, diffusion coefficients, and interaction energies. The article also reveals the significance of data-driven modelling approaches, for example, support vector machines and ensemble learning techniques, in deriving quantitative structure, property relationships (QSPR) and therefore efficiently predicting interaction strength, bioactivity, and ADMET profiles of complex herbal systems.

The suggested framework, by linking large scale dielectric effects with detail molecular and electronic level explanations, makes it possible to gain a better understanding of the relationships between structure and interaction in natural products. This unified method not only improves the understanding of the subject but also helps in the logical design and enhancement of phytochemical formulations. The authors believe that the collaboration of experimental and computational paradigms can yield great improvements in predictive modelling and help in herbal drug discovery and formulation science.

Keywords: *Herbal Bioactives, Dielectric Spectroscopy, Molecular Dynamics, Quantum Chemical Modelling, Machine Learning, QSPR*

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NMSF-CAM-018

Explainable Artificial Intelligence and Machine Learning in Ferrite Materials Research: Emerging Paradigms in Predictive Design, Discovery, and Interpretability

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Abstract

Artificial intelligence (AI) and machine learning (ML) have evolved as revolutionary tools across science and technology, with materials science becoming one of the promising domains of application by enabling faster and more efficient materials discovery and design. In ferrite research, specifically in complex magnetic oxides, the traditional methods often are having limitations in capturing the nonlinear relationships and composition, crystal structure and functional properties. This has led to an inclination towards data- driven and interpretable computational approaches for prediction and optimization. Doped M-type hexaferrites such as $SrFe_{12}O_{19}$ benefit from these methods, and help in relating the compositional changes to magnetic and dielectric performance.

This review critically analyses the integration of AI, ML, and computational methods in ferrite and magnetic oxide research with a special focus on M-type hexaferrites. It explores the transition from first-principles, physics-based approaches to the data-driven frameworks for predicting materials design, highlighting the role of computational materials databases, ML models, and explainable AI tools such as LIME and SHAP in predicting the magnetic and dielectric properties.

This review summarises on AI-driven methodologies which show a potential for enhancing the prediction, optimization, and scientific understanding of M-type hexaferrites. The convergence of Ai, computational materials science, and ferrite physics has a scope of establishing new direction in materials research, with promising future opportunities in digital twins, autonomous materials design, and intelligent physics-informed discovery environments.

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NMSF-CAM-020

Ionic Qudit and Electronic Qubits Triple Entanglement in Single Step Double Photoionisation of N_2 Molecules

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Abstract

Quantum communications using multipartite and higher dimensional quantum computing systems (qudits) exhibit unusual characteristics, have greater ability and reduce distortion. Additionally, multipartite and qubit systems provide quantum computing more adaptability and effectiveness. In this study, we investigate ionic qudit and electronic qubits triple entanglement that develops from the double photoionisation of the N_2 without witnessing spin-orbit interaction (SOI) after it absorbs just one photon. When SOI is absent, Russell-Saunders (RS) coupling can be used.The electronic state of an ionic qudit determines its dimension. The interplay of the density matrix's components derived from the density matrix elements (DME) in double-photoionisation serves as a measure of the entanglement degree. For the double-photoionisation of N_2 molecules, a theoretical framework for entanglement has been developed. We show that the entanglement is dependent on the molecular spins in their doubly ionised states and on the spin quantisation and emission directions of photoelectrons.

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NMSF-CAM-026

Role of Quantum Capacitance and High-κ Dielectrics in Scaling Behavior of 2D Black Phosphorus

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Abstract

In this work, a physics-based analytical framework is developed to investigate the scaling behavior of black phosphorus MOSFETs, incorporating both quantum capacitance and short-channel electrostatics. The model explicitly captures key scaling effects, including threshold voltage roll-off, drain-induced barrier lowering, and subthreshold swing degradation, for channel lengths ranging from 20 nm to 5 nm. The influence of gate dielectric permittivity (SiO_2, HfO_2, and ZrO_2) is systematically analyzed through its impact on effective gate capacitance and electrostatic scaling length.

The results reveal that high-κ dielectrics enhance electrostatic control at moderate channel lengths; however, their effectiveness saturates in the ultra-short channel regime due to quantum capacitance limitations. This results in a non-linear dependence of device performance on dielectric constant, with diminishing returns beyond a critical κ value. Furthermore, black phosphorus devices exhibit improved ON/OFF current ratios and reduced short-channel effects compared to conventional bulk MOSFETs, highlighting the advantages of atomically thin channels. The proposed model is validated against reported experimental and theoretical studies, demonstrating consistent trends in subthreshold swing, ON/OFF ratio, and threshold voltage scaling.

This study provides deeper insight into dielectric channel coupling in 2D transistors and establishes design guidelines for optimizing high-κ dielectric and 2D material integration for future low-power nanoelectronic applications.

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NMSF-CAM-029

On Construction Secular Equation Determining Electronic Structure – All-Boron and Boron-Rich Materials

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Abstract

An updated semiclassical approach[1,2] to calculating the electronic structure of atoms and their bound systems allows for the construction of hydrogen-like atomic orbitals and, accordingly, integral representations of atomic and interatomic potentials in forms integrable into elementary functions. Based on the implementation[3,4] of such a program for boron, expressions will be derived for the matrix elements of the Hamiltonian and overlap integrals in the secular equation defining the electronic structure of all-boron and boron-rich materials, in particular, next-generation two-dimensional materials such as borophenes.

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NMSF-CAM-031

Electro-Optical, NLO, and Electronic Properties of NOBOW Bent-Core LC Molecule: A Comprehensive Study

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Abstract

In the present study, a bent-core LC namely NOBOW which possesses unique chiral smectic property, has been explored using DFT method with LC-BLYP functional along with 6–31G(d,p) basis set. The structural, electro-optical, nonlinear optical (NLO), and electronic properties of the NOBOW LC molecule have been computed using same method as discussed above. The thermotropic stability and phase tunability of NOBOW are demonstrated by its phase transition from the helical B4 phase to the smectic B2 phase at 142 °C and then to the isotropic phase at 170 °C. Because of its chiral layered arrangement, NOBOW has fast switching behaviour, high contrast ratios, and strong spontaneous polarization, according to electro-optical studies, making it appropriate for next-generation liquid crystal display (LCD) and photonic applications. Importantly, NOBOW exhibits promising nonlinear optical (NLO) properties, with significant first hyperpolarizability attributed to its asymmetric bent-core geometry and delocalized π-electron system. The HOMO, LUMO, HOMO–LUMO energy gap, and global descriptors that governs the optical and electronic response of NOBOW have also been studied in relation to its electronic structure. Thus, NOBOW is a good candidate for multifunctional LC-based technologies due to its advantageous electronic and NLO properties, anisotropic optical behaviour, and electro-optical performance.

Keywords: *NOBOW LC, Electro-optical, Optical, Anisotropy, NLO, Global Descriptors*

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NMSF-CAM-032

Shape-Dependent Structural, Electronic and Transport Properties of BP Nanowires for Next-Generation Nanoscale Interconnect

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Abstract

One-dimensional (1-D) nanowires have unique structural, electronic, and transport properties that come from being quantum confined and having fewer dimensions. This makes them good candidates for next-generation nanoelectronic devices. Among various low-dimensional systems, III-V compound nanowires have attracted considerable interest owing to their tunable electronic properties and applicability in device fabrication. In this research, we aim to systematically examine the impact of geometry on the structural stability, electronic band structure, and transport properties of boron-phosphide nanowires (BPNWs). Utilizing first-principles density functional theory, linear, zigzag, and triangular configurations are analyzed to elucidate geometry-induced transitions in stability and electronic behavior, yielding insights for the design of nanoscale electronic materials. We performed the geometry optimization using the generalized gradient approximation (GGA) functional with the Perdew- Burke-Ernzerhof (PBE) parameterization. We used plane wave functions with a cutoff energy of 70 Ry, and we did Brillouin zone integration with a k-point sampling of 1x1x50.

Depending upon the binding energy analysis, linear BPNWs are the most energetically stable configuration. Zigzag and triangular nanowires are still possible to make, even though they are not as stable. Calculations of electronic structure show that linear BPNWs are semi-metallic because the valence and conduction bands overlap at the Fermi level. On the other hand, zigzag and triangular geometries are metallic because the bands cross the Fermi level. An analysis of the density of states reinforces these conclusions further. The modulation of electronic behavior caused by geometry shows how important structural design is for customizing the properties of nanowires. These results give important information for the smart design of nanoscale electronic and transport devices that use boron and phosphide.

Keywords: *BPNWs, Band gap, Semi-Metallic, I-V Properties, Nano-Interconnect*

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NMSF-CAM-035

First-Principles Investigation of the Structural and Electronic Properties of Boron Arsenide Nanosheet and Nanoribbons

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Abstract

The emergence of graphene via mechanical exfoliation provided the experimental evidence of stable 2D matter, revolutionizing nanotechnology and driving the exploration of diverse layered materials. While graphene and hexagonal boron nitride (h-BN) are the most widely studied 2D systems, they face significant electronic limitations.

This study investigates the comparison of structural and electronic properties of monolayer of hexagonal boron arsenide (h-BAs) nanosheet and zigzag BAs nanoribbons (ZBAsNR), using first-principles density functional theory (DFT) calculations. The structural analysis reveals that h-BAs nanosheets are stable (with cohesive energy (Ec) = -5.62 eV) and possesses a direct band gap of 0.76 eV, thereby making it extremely appropriate for optoelectronics and photovoltaics. Additionally, the structural and electronic properties of zigzag BAs nanoribbons have also been examined. It has been observed that the ZBAsNR possess negative binding energy and exothermic behavior confirming the stability of the ribbon. The electronic band structure analysis reveals that bare nanoribbons exhibit metallic behavior. Furthermore, the passivated ones (H-ZBAsNR-H) for width (N_z) = 8 shows binding energy of (E_b) = -5.03 eV. The electronic band structure shows a semiconducting behavior with direct bandgap (E_g = 1.05 eV). Overall, the findings discussed above highlight the potential use of h-BAs nanosheets and nanoribbons in applications such as nanoelectronics, optoelectronics and photovoltaics.

Keywords: *Boron arsenide, Nanoribbon, Nanosheet, Density functional theory, Electronic band structure*

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NMSF-CAM-036

Effect of Strain on Electronic and Transport Properties of Inorganic Halide Perovskite Materials $AgCdX_3$ (X=F, Cl)

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Abstract

In the present work, we have studied the effect of mechanical strain (tensile or compressive) on the electronic properties of the inorganic halide perovskite materials $AgCdX_3$ (X=F,Cl). We have studied band structure, band gap and effective mass of charge carriers under varying strain conditions (+0. 5% & +1.0%) using first-principles calculations based on density functional theory (DFT). The results show that the band gap and effective mass can be tuned under applied strain conditions. Compressive strain causes a decrease in band gap whereas tensile strain causes an increase in band gap in both the materials. However, $AgCdCl_3$ has a larger band gap than $AgCdF_3$. The electron effective mass increases (decreases) in $AgCdF_3$ ($AgCdCl_3$) under tensile strain conditions. Our results show that the electronic properties of inorganic halide perovskite materials can be tuned by applying mechanical strain.

Keywords: *Halide Perovskite, Density Functional Theory, Strain, Effective Mass*

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NMSF-CAM-037

Electronic and Piezoelectric Properties of Janus GeOS Monolayer using Density Functional Theory

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Abstract

In this work, the Electronic, Structural and Piezoelectric Properties of GeOS janus monolayer were studied. All the calculations were carried out using the Density Function Theory (DFT) in Quantum ESPRESSO package. The PBE functionals were used with the PAW Pseudopotentials. The electronic properties of GeOS monolayer were calculated from the Band Structure, which shows that it has direct band gap with value 0.58 eV exhibiting the semiconducting nature of the monolayer. The strain was applied to monolayer in the range +2% to -2% for both biaxial and uniaxial directions to examine the tunability of band gap and effective mass with respect to strain conditions. The variation in bond angle, height and effective mass shows a consistent behaviour of GeOS monolayer throughout the strain values. We have also studied the piezoelectric and transport properties of this material and discussed the anisotropic nature of material w.r.t. transport. This work shows the tunability of the electronic and transport properties with respect to strain conditions.

Keywords: *Janus monolayer, Density Functional Theory, Quantum Espresso, Band Gap, PBE, Effective mass*

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NMSF-CAM-038

Structural, Optical and Electrical Investigations on Br Doped ZnS Thin Films Deposited via Spray Ultrasonic

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Abstract

In this study, we report the influence of Bromine (Br) doping levels on certain Zinc Sulphide (ZnS) thin films Thin films physical properties. Br doped ZnS films were deposited on glass substrates using ultrasonic spray method with a Zinc sulphide varied Br concentration from 0% to 2% to investigate its incorporation effect and identify the accurate doping Br doped ZnS amount. The obtained results indicated that low doping percentage has a crucial effect on the grown Br-ZnS Structural films. The structural, optical and electrical properties of the as prepared films were investigated by various techniques of characterization including X-ray diffraction (XRD), UV–Vis-NIR spectrophotometer as well as the electrical measurements via the four-probe technique. The XRD analysis pattern confirms that prepared films were polycrystalline with co-existence of cubic and hexagonal phases. Moreover, the films transparency exhibits a maximum value of 76% in the visible region, which decreases with increasing Br concentration in the material. The direct band gap values have been determined from the transmittance spectra, and these values increase in the optic band gap region (3.5–3.8 eV) with the increase of Br concentration. The electrical measurements reveal that films have a resistivity varying between 2.5×10^3 and 3.1×10^4 Ω.cm with increasing Br content. We concluded that 0.5% Br-doping ratio improves the ZnS physical properties and rends it suitable for optoelectronic devices fabrication.

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NMSF-CAM-039

Theoretical Study of Physical Properties of Co_2TiZ (Z= Si, Ge) and CoTiZ (Z= Si, Ge) Compounds Using First Priniciples Method

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Abstract

Using first principle approach, the structural, electrical, elastic, and magnetic characteristics of $L2_1$ structured Co_2TiZ (Z= Si, Ge) complete Heusler alloys with space group $Fm-3m$ and half-Heusler CoTiZ (Z= Si, Ge) compounds with space group $F-43\_m$ were examined. The full potential linearized augmented plane wave (FP-LAPW) approach, as implemented in WIEN$_2k$, is used here. Co_2TiSi exhibits zero band gaps in both the majority and minority spin channels, whereas Co_2TiGe exhibits a finite band gap of 0.568 eV in the minority spin channel and zero band gaps in the majority spin channel around the Fermi level implemented in the WIEN2k code, exhibiting 100% spin polarization. As a result, Co_2TiGe is discovered to be perfectly half-metallic ferromagnetic (HMF), whereas Co_2TiSi is metallic in nature. Indirect band gap decreases from Si to Ge due to lattice expansion and weaker hybridization. In both spin channels, CoTiZ (Z= Si, Ge) compounds exhibit no nmagnetic semiconducting behavior. Co_2TiZ (Z= Si, Ge) compounds have computed magnetic moments of 2.04 and 2.01 B, respectively, whereas CoTiZ (Z= Si, Ge) compounds have zero magnetic moment. Here, we see that the code's and Slater-Pauling rule's estimated results have good tuning. Pugh's ratio B/G values are more than 1.75 for all ductile compounds except CoTiGe having value 1.52, which is brittle in nature. Because a positive value of Cauchy pressure (CP = C_{12} - C_{44}) indicates ductile nature and a negative value indicates brittle nature, we can conclude that all compounds are ductile except CoTiGe, which is brittle. Pugh's ratio and Cauchy pressure both produce similar results.

Keywords: *Half-metallic ferromagnetic, Semiconducting, Band gap, Spintronics, Magnetic Moment*

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NMSF-CAM-042

Artificial Intelligence in the Development of Advanced Solar Materials: A Review

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Abstract

The increasing global demand for clean and sustainable energy has accelerated research into high-efficiency solar materials for advanced photovoltaic applications. Conventional silicon-based solar cells, although commercially dominant, are approaching their theoretical efficiency limits and face challenges related to cost and scalability. In response, significant efforts have been directed toward the exploration of emerging materials such as perovskites, organic semiconductors, quantum dots, and multi-junction architectures, which offer tunable electronic properties, superior light absorption, and enhanced charge transport mechanisms.

This review presents a comprehensive overview of recent advances in the design and optimization of high- efficiency solar materials, with a particular focus on the integration of machine learning (ML) and artificial intelligence (AI) techniques. Data-driven approaches have transformed traditional trial-and-error methodologies by enabling rapid prediction of key material properties such as band gap, carrier mobility, stability, and power conversion efficiency. Algorithms including Random Forest, Gradient Boosting and Artificial Neural Networks have been widely employed for accurate property prediction, while advanced deep learning models such as Convolutional Neural Networks and Graph Neural Networks have demonstrated significant potential in capturing complex structural and atomic-level interactions in materials.

Special attention is given to perovskite solar cells, which have achieved remarkable improvements in power conversion efficiency but still face challenges related to long-term stability and environmental concerns. Strategies including compositional engineering, defect passivation, and interface optimization are critically analyzed. Additionally, the role of nanostructuring and plasmonic effects in improving light harvesting is discussed.

This review highlights the transformative role of AI-driven methodologies in accelerating the discovery and optimization of high-efficiency solar materials. The synergy between computational modeling, data-driven techniques, and experimental validation is expected to drive future innovations, paving the way for cost-effective, stable, and highly efficient photovoltaic technologies that can meet global energy demands sustainably.

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NMSF-CAM-044

Development of Toxicity Prediction Tool using Machine Learning

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Abstract

Conventional in vivo toxicity testing is limited by ethical, financial, and time constraints, creating demand for fast and cost-effective computational alternatives. This study focuses on developing an integrated machine learning based tool for toxicity prediction, capable of classifying chemicals as toxic or non-toxic and estimating quantitative toxicity (LD_{50}). The results were obtained by a K-Nearest Neighbor classifier based on molecular descriptors (accuracy 0.71, ROC-AUC 0.78, PRC-AUC 0.75). For LD_{50} prediction, eight regression models were developed using Boruta-selected features and PCA components. KNN and Random Forest showed the strongest predictive ability with R^2 values of 0.80 and good test-set generalization, while a Decision Tree model overfitted despite perfect training R^2. Overall, the findings show that ML-based QSAR modelling can enhance early toxicity screening, aiding environmental risk assessment and safer chemical development.

Keywords: *Machine Learning, Toxicity Prediction, QSAR, LD_{50}, Boruta algorithm*

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NMSF-CAM-047

Electronic Structure and Bonding Mechanism of CO on Rh(100) Surface: A DFT Study

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Abstract

The adsorption and activation of CO on transition metal surfaces are crucial in heterogeneous catalysis. In this work, we perform a first-principles investigation of CO adsorption on a Rh(100) surface was carried out using density functional theory. The optimised geometry revealed that CO preferentially absorbed at top site, with the carbon atom bonded to the surface Rh atom. The molecule adopts a nearly vertical configuration.

Charge density difference analysis reveals a significant redistribution of electrons upon adsorption, characterised by charge accumulation at the CO–Rh interface and depletion near the carbon atom, indicating σ-donation from CO to the metal surface. Additionally, pronounced charge accumulation along the molecular axis confirms π-backdonation from Rh d-states into the antibonding orbitals of CO.

PDOS analysis showed strong hybridisation between C/O p-states and Rh d-states near the Fermi level. This supports the formation of bonding and antibonding states. LDOS and ILDOS analyses provide spatial and energy-resolved insights into the bonding mechanism. MOPDOS highlighted the orbital-level interaction between Rh d-states and CO π^* orbitals.

The combined results confirm that CO adsorption on Rh(100) is governed by a synergistic σ-donation and π-backdonation mechanism, resulting in the activation of the CO molecule. These findings provide valuable insights into the fundamental understanding of catalytic processes involving CO on Rh-based surfaces.

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NMSF-CAM-051

ML-Guided Prediction of Lattice Dynamics and Carrier Lifetime in $(CH_3NH_3)_2AgBiBr_6$ for Stable Solar Cells

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Abstract

Hybrid halide double perovskites have emerged as promising lead-free alternatives for next-generation photovoltaic applications due to their inherent stability and non-toxic composition. Among these, $(CH_3NH_3)_2AgBiBr_6$ exhibits excellent ambient stability and suitable optoelectronic properties; however, its power conversion efficiency remains limited by rapid carrier recombination and complex lattice dynamics. Understanding the interplay between phonon behavior and charge carrier lifetime is critical for enhancing device performance. In this work, we employ machine learning (ML) approaches combined with first-principles density functional theory (DFT) to predict lattice dynamics and carrier lifetimes in $(CH_3NH_3)_2AgBiBr_6$.We constructed a comprehensive dataset of phonon dispersion, Gruneisen parameters, and electron-phonon coupling matrices derived from DFT calculations. A neural network potential was trained to capture anharmonic lattice vibrations, enabling high-throughput prediction of thermal transport properties. Furthermore, a random forest regression model was developed to correlate specific phonon modes with non-radiative carrier recombination rates. Our ML models successfully identified low-frequency organic cation vibrations as primary contributors to carrier scattering, while predicting an optimal operating temperature window (280–320 K) where carrier lifetime exceeds 2.5 ns. The predicted lattice thermal conductivity (0.38 W/m · K) and carrier lifetime (2.8 ns at 300 K) align well with experimental reports, validating our ML approach. Importantly, our model enables rapid screening of chemical substitutions (e.g., A-site cation engineering) to further suppress phonon-mediated recombination. This study demonstrates that ML-guided prediction of lattice dynamics can accelerate the rational design of stable, high-efficiency hybrid halide double perovskites, contributing to sustainable photovoltaic technology.

Keywords: *Hybrid Halide Double Perovskites, $(CH_3NH_3)_2AgBiBr_6$, Machine Learning, Lattice Dynamics, Carrier Lifetime, Sustainable Photovoltaics*

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NMSF-CAM-054

Intelligent Optimization of Sustainable Materials for Precision Manufacturing Applications

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Abstract

The growing demand for sustainable and advanced materials in precision manufacturing has driven the need for smart optimization strategies. In this study, a holistic approach of integrated artificial intelligence (AI) techniques with sustainable material development, to improve the manufacturing processes and product quality. A range of sustainable materials, such as bio-derived nanomaterials and hybrid composites, are assessed for suitability in precision manufacturing process like wire electrical discharge machining (WEDM). The study utilizes hybrid AI methods such as Artificial Neural Networks (ANN), Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) to model, predict and optimize performance variables like surface finish, material removal rate and accuracy. Both experimental and simulation studies show that AI-driven optimization enhances process performance, leading to lower energy and material wastage.

The study underscores the promise of the use of sustainable materials combined with smart materials optimization for environmentally sustainable and high-precision manufacturing. The research is part of the next generation of manufacturing systems based on sustainability and Industry 4.0 paradigms.

Keywords: *Sustainable Materials, Precision Manufacturing, Artificial Intelligence, ANN-GA, ANN-PSO, Laser Cutting, WEDM, Optimization, Green Manufacturing, Micro/Nanomaterials*

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NMSF-CAM-056

Electronic, Magnetic and Optical Behaviour of Diluted Magnetic Semiconductors $CdMn_xGe_{1-x}P_2$

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Abstract

Spin-polarized density functional theory (DFT) employing the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method along with Tran-Blaha modified Becke-Johnson (TB-mBJ) functional was performed on Diluted Magnetic Semiconductor (DMS) $CdMn_xGe_{1-x}P_2$, within $0 \leq x \leq 0.5$ concentration range. Mn substitution at Ge sites preserves the chalcopyrite lattice symmetry (space group I42d) without inducing phase separation as confirmed by simulated X-ray diffraction (XRD) patterns. Structural properties remain intact across all given doping concentrations, though slight bond-length distortions in Cd–P and Ge–P bonds are observed with no axial anomalies. With increasing Mn concentration, narrow band gap noticed for the minority-spin while majority-spin channel retains its semiconducting band gap. Mn atoms d orbitals influenced by exchange interactions in the minority-spin state which shift the valence band upward. In contrast, the majority-spin channel exhibits degenerate semiconducting behaviour due to Mn-induced electron donation. Mn doping induces magnetic moments of approximately 3.5 μB/Mn atom, primarily due to Mn-d electrons, resulting in significant spin splitting and 100% spin polarization at E_F. The combined effect between Mn–P and Mn–Ge interactions allow tuning of the net magnetic moment from 0 to 0.38 μB/atom, depending on the doping level. Optical properties of the Mn doped materials are significantly modified and the dielectric function, particularly the real part $\epsilon_1(\omega)$, reveals distinct behaviour below 2 eV and exhibits a plasma resonance aligned with optical conductivity trends. Blue shifts in $\sigma(\omega)$ peaks indicate modified light–matter interactions due to Mn incorporation. Mn-doped $CdGeP_2$ illustrate tuneable half-metallicity, superior optical absorption, and thermodynamic stability, establishing it as a versatile material for advanced spintronic and optoelectronic devices.

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NMSF-CAM-057

Docking for Drug-Target Interactions Integrated Computational Insights into 1, 10-Phenanthroline: DFT Modelling, Preferential Solvation, and Molecular

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Abstract

This research delivers a thorough Density Functional Theory (DFT) analysis of 1,10-phenanthroline (1,10-Phen) to explore its electronic structure and chemical behavior while evaluating its stability. The study utilized the CPCM solvation model with water to replicate physiological conditions in its calculations. The molecule demonstrates stability alongside moderate polarity through its computed HOMO–LUMO energy gap of 4.753 eV and dipole moment of 5.18 D. NBO and NLO analyses demonstrate the molecule's electronic delocalization along with its optical properties. Thermodynamic parameters confirm its favorable energetic profile. Examination of solvation behavior in binary solvent mixtures showed that molecules preferentially associate with 1,4-dioxane (DXN) in their ground state but shift toward acetonitrile (ACN) when they are excited, which demonstrates how solvent environments affect molecular stability. The molecular docking analysis shows 1,10-Phen has the highest binding affinity for MAO-A with a score of –6.71 kcal/mol, while its binding to CA IX and GyrB scores –6.37 kcal/mol and –5.75 kcal/mol, respectively. The results demonstrate that 1,10-Phen shows significant promise as a therapeutic agent as a specific MAO-A inhibitor while remaining useful in materials science fields.

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NMSF-CAM-058

XAI-driven Seebeck Prediction in 2D Thermoelectric Materials

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Abstract

Explainable Artificial Intelligence (XAI) has become increasingly important in materials informatics, where understanding model predictions is essential for scientific reliability and meaningful interpretation. In this study, an XAI-driven machine learning framework is proposed for the prediction of the Seebeck coefficient in 2D thermoelectric materials. A descriptor-based dataset was employed to train and compare five regression models, namely Linear Regression, Decision Tree Regressor, Support Vector Regressor (SVR), Gradient Boosting Regressor, and Random Forest Regressor. The predictive performance of these models was evaluated using standard regression metrics, including the coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE), supported by actual-versus-predicted analysis. To improve model transparency and move beyond conventional black-box prediction, feature importance analysis, SHAP (Shapley Additive Explanations), LIME (Local Interpretable Model-agnostic Explanations), and partial dependence plots (PDP) were applied to identify the most influential descriptors governing Seebeck behavior. The proposed framework not only enables accurate prediction but also provides physically meaningful insight into descriptor–property relationships, thereby bridging the gap between predictive modeling and scientific understanding. Overall, this study demonstrates that the integration of machine learning with XAI offers a transparent and effective strategy for accelerated screening and design of thermoelectric materials.

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NMSF-CAM-060

Analysis of Intensities of X-Ray Diffraction Data for Full-Heusler Alloys

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Abstract

Abstract- Magnetic properties of the Heusler alloys have been tuned through the elemental substitution and spontaneous swapping between the elements. In order to scale the magnetic property of the Heusler alloys, we would have to ensure the exact atomic position of the elements in their ground state structure. Here, we reveal the associated X-Ray diffraction (XRD) pattern of different Heusler alloys such as Co_2-based, Mn_2-based, Fe_2-based and Ni_2-based full-Heusler alloys using Vesta software. This software enables us to fill the position of the atoms with desirable occupancy. This will help to extract the corresponding XRD pattern. In order to obtain the atomic positions, we can observe the intensity pattern of each peak of these full-Heusler alloys. Since, we have found a significant change in the first two peaks which is known as super-reflection peaks (111 and 200). Therefore, we have taken the ratio of these peaks and plotted the results and discussed the results with the scattering factors of the individual atoms.

Keywords: *Full-Heusler Alloys, Super-Reflection Peaks, X-Ray Diffraction, Rietveld Refinement, Swapping etc*

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NMSF-CAM-061

Hybrid Predictive and Optimization Framework for Failure Analysis using NTXFD and Data-Driven Intelligence

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Abstract

In modern engineering and material systems, the ability to accurately predict failure behaviour and optimize system reliability is crucial for enhancing performance, reducing downtime, and enabling intelligent decision-making.

This paper presents a hybrid predictive and optimization framework that integrates the Novel Transmuted Exponential Failure Distribution (NTXFD) with data-driven intelligence techniques to model and analyse failure dynamics in complex systems. The proposed approach leverages maximum likelihood estimation for robust parameter identification and employs statistical validation metrics such as Akanke Information Criterion (AIC) and Bayesian Information Criterion (BIC) to benchmark NTXFD against conventional reliability models.

The framework extends beyond traditional statistical modelling by incorporating predictive machine learning techniques to establish relationships between system variables such as load, stress, and operational time. A regression-based learning model is utilized to forecast system behaviour, while anomaly detection mechanisms are implemented to identify irregular patterns that may indicate early-stage failures.

Additionally, Monte Carlo simulation is employed to generate probabilistic forecasts, enabling uncertainty quantification and risk assessment under varying operational conditions.

A key contribution of this study is the integration of optimization strategies aimed at maximizing Mean Time to Failure (MTTF), providing a systematic approach for enhancing system reliability through parameter tuning. The developed dashboard-based system facilitates real-time analysis, visualization, and automated reporting, making it a powerful tool for researchers and industry practitioners. The proposed hybrid framework demonstrates significant potential in advancing predictive maintenance, smart materials analysis, and AI-driven reliability engineering.

Keywords: *Failure Prediction, NTXFD Model, Predictive Analytics, Reliability Optimization, Machine Learning, Monte Carlo Simulation, Anomaly Detection, MTTF, Smart Systems, Data-Driven Engineering*

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NMSF-CAM-062

A Computational Framework for Reliability and Survival Analysis using NTXFD Model with Machine Learning Integration

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Abstract

With accurate modelling of failure behaviour as key to performance optimization and risk reduction, reliability and survival analysis are at the heart of engineering system modelling, material science, and predictive maintenance. The proposed computational framework utilizes the Novel Transmuted Exponential Failure Distribution (NTXFD) along with machine learning methods for the improvement of reliability assessment.

The method employs maximum likelihood estimation (MLE) for accurate parameter estimation, and statistical models are compared based on Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC) to check the best choice from established classical distributions like Weibull, Gamma, Lognormal, and Exponential.

The proposed system is deployed as an interactive dashboard, allowing real-time data ingestion using automation while automatically processing and visualizing the probability density, survival, and hazard functions in the data by adding it dynamically.

Monte Carlo simulations are also applied to predict failure probabilities as well as to estimate the reliability of a system in uncertainty. This work integrates machine learning models in a critical way, including linear regression models to perform forecasting, and Isolation Forest models to detect anomaly, which can improve the analysis of abnormal patterns and predictive accuracy of the system.

More importantly, the framework uses optimization methods to maximize Mean Time to Failure (MTTF) and offers practical feedback for optimizing system design and maintenance decisions. This statistical modelling, synthetic simulation and AI analytics combine to provide a full-fledged tool for the interrelationship of various fields, in engineering, materials science and data-driven reliability analysis, with various cross-discipline utility.

This project illustrates how both types of computational approaches can be applied in order to integrate well-established reliability theory with 21st-century intelligent systems and can be used in a hybrid computational manner.

Keywords: *Reliability Analysis, Survival Analysis, NTXFD Distribution, Maximum Likelihood Estimation, AIC BIC, Machine Learning, Monte Carlo Simulation, Anomaly Detection, Predictive Modelling, MTTF Optimization*

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NMSF-CAM-063

Algebraic Structure Identification Using Computational Intelligence and Entropy-Based Analysis

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Abstract

Computational techniques are making progress so the identification of complex mathematical structures can be automated at a rapid pace and plays a very important role in modern scientific and engineering applications.

Therein, we introduce an intelligent algebraic analysis framework based on binary operations over finite sets that classifies elementary algebraic structures like magmas, semigroups, monoids, groups, and Abelian groups. The system presented is guided by algorithmic validation of key properties such as closure, associativity, identity, inevitability, and commutativity while requiring rigorous validation of internal structure.

In particular value in this work is to measure Shannon entropy as a measure of statistical complexity and distribution characteristics in algebraic systems. Leveraging deterministic algebraic rules and entropy-based insights, the framework presents a dual-layer assessment tool that is interpretable and insightful.

In addition, the system is developed as an interactive computational dashboard and allows performing real-time data input, automatic proof creation, and structured reporting on data. In areas like cryptography, data science, and computational modelling, algebraic consistency and structural predictability is one of the core objectives of computational modelling.

In the end, it connects the dots between the realm of abstract algebra and intelligent computational systems, contributing to AI-driven mathematical analysis tools.

Keywords: *Algebraic Structures, Computational Intelligence, Shannon Entropy, Group Theory, Automated Verification, Binary Operations, AI in Mathematics, Data Analysis, Mathematical Modelling*

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NMSF-ENM-001

2D Nanostructure for PV Application: Pathway Towards Sustainable Future

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Abstract

Nanotechnology paved the path for fastest-growing and most promising fields in sustainable energy development. Modern energy - harvesting research focuses on specially engineered 2D nanostructures and device configurations. Morphology engineering, shape, sizes are essential for improving the efficiency of photovoltaic application.

In this regard the scientist searching new materials where CZTS shows good candidature for future photovoltaic (PV) and Photoelectrochemical (PEC) application. Recent studies shows that novel nanostructured quaternary chalcogenide Cu_2ZnSnS_4 (CZTS), P-type semiconductor due to multicomponent nature, attracted significant attention & promising material for the development of low-cost, high-performance photovoltaic devices. Its high absorption coefficient ($\sim 10^{-4} cm^{-1}$), optimal band gap (~1.4–1.5 eV) in the visible range, it has been considered an alternative absorber layer for the fabrication of solar cells, non-toxic, naturally abundant constituent elements provide several advantages over most thin-film absorber materials. CZTS bearing optical and electrical properties shows excellent energy-related properties, such as high power conversion efficiency, eco-friendly, and long operational lifetime. The use of nanostructures strategies and dopants promotes better charge separation, reduces recombination losses, and leads to improved power conversion efficiency. A low-cost, conservational, and facile hydrothermal method employed for the synthesis of keseterite phase for CZTS nanoparticles. These include improving long term stability, achieving uniform large growth area, further enhancing photovoltaic efficiency, and extending device service life.

Keywords: *2D nanostructure, CZTS, PEC, Sustainable Energy, Power Conversion Efficiency*

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NMSF-ENM-002

Defect-Engineered N and Co (Mono- and Co-doped) Anatase TiO_2 Nanoparticles with Enhanced Electrical Properties for Energy-Efficient Applications

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Abstract

The growing demand for sustainable and energy-efficient materials for next-generation electronic systems has driven extensive research on functional metal oxides. Titanium dioxide (TiO_2), due to its excellent chemical stability, non-toxicity, and low-cost synthesis, has emerged as a key material for environmentally sustainable technologies. However, its limited electrical response necessitates strategic modification. In this work, defect engineered nitrogen and cobalt doped anatase TiO_2 nanoparticles are systematically investigated to enhance their dielectric and conduction properties. Pure, N-doped (0.7 mol %), Co-doped (1 mol %), and N-Co co-doped TiO_2 nanoparticles were synthesized via a cost-effective sol-gel route and sintered at 450 °C. The temperature and frequency dependent electrical properties were analysed using complex impedance spectroscopy over a wide frequency (20 Hz - 2 M Hz) and temperature range (30–40 °C). A significant enhancement in dielectric response is observed in doped samples, particularly in $N-TiO_2$, attributed to defect-induced space charge polarization and improved dipolar contributions. The ac conductivity exhibits a dispersive behaviour with frequency, following a hopping conduction mechanism governed by localized charge carriers. Temperature dependent behaviour indicates defect-mediate transport, suggesting tunable conduction pathways via control doping. The impedance spectra reveal a single semicircular arc across all temperatures, confirming dominant bulk-controlled conduction with non-Debye type relaxation. The synergistic effect of nitrogen and cobalt co-doping plays a crucial role in tailoring the electrical response through band structure modulation and defect state engineering. From an application perspective, the enhanced dielectric and conduction characteristic pose these materials as promising candidates for energy storage devices, high dielectric constant materials, and smart sensor technologies. Importantly, the use of low-temperature synthesis and eco-friendly materials aligns with the principles of sustainable material development. This study not only provides deeper insight into polarization and charge transport mechanisms but also establishes a pathway

for designing next-generation functional materials for green electronics, energy systems, and environmental applications.

Keywords: *AC conductivity, Anatase* TiO_2*, Complex impedance spectroscopy, Hopping conduction, Non-Debye relaxation, Space charge polarization*

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NMSF-ENM-004

Electrochemical Analysis of Lithium-Incorporated PVA/Graphite Solid Polymer Composites

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Abstract

Lithium-modified polyvinyl alcohol (PVA)/graphite solid polymer composites were prepared using a shear exfoliation technique, and their structural and electrochemical properties were systematically investigated. Powder X-ray diffraction (PXRD) analysis, through comparison between PVA/graphite and PVA/graphite/lithium composites, confirmed the successful incorporation of lithium into the polymer matrix without altering the inherent structural features of PVA and graphite. This observation was further supported by Fourier-transform infrared (FTIR) spectroscopy. Scanning electron microscopy (SEM) revealed ellipsoid-shaped clustered morphologies, indicating the presence of abundant electrochemically active sites. Energy-dispersive spectroscopy (EDS) verified the elemental purity and homogeneous distribution of the constituents within the polymer matrix.

Thermal analysis indicated a reduction in glass transition temperature (Tg), suggesting enhanced polymer chain flexibility and improved ion transport. Electrochemical performance was evaluated using a three-electrode configuration with 1 M H_2SO_4 as the electrolyte. Galvanostatic charge–discharge (GCD) measurements at a current density of 0.003 A g^{-1} yielded a specific capacitance of 1381 mF g^{-1}, an energy density of 192 mWh kg^{-1}, and a power density of 1670 mW kg^{-1}. Notably, the composite exhibited excellent cyclic stability, retaining 100% of its initial capacitance after 5000 charge–discharge cycles, indicating outstanding electrochemical durability.

The combined structural, thermal, and electrochemical results demonstrate that the developed PVA-based composite solid polymer electrolyte exhibits moderate ionic conductivity and promising capacitive performance, making it a suitable candidate for solid-state electrochemical energy storage applications.

Keywords: *Polyvinyl Alcohol (PVA), Shear Exfoliation, Solid Polymer Electrolyte, Electrochemical Performance, Cyclic Stability*

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NMSF-ENM-007

Synergistic Role of Zn^{2+} Substitution in Tailoring the Electrochemical and Antibacterial Performance of $MgFe_2O_4$ Quantum Dots

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Abstract

Spinel ferrite quantum dots (QDs) are promising multifunctional materials for energy storage and biomedical applications due to their tunable optical and electronic properties. In this study, pure and Zn^{2+}-doped $MgFe_2O_4$ QDs were synthesized via a facile co-precipitation method. Structural and morphological studies confirmed a single-phase cubic spinel structure with ultra-fine particles (~6.23 nm), while XPS verified effective Zn^{2+} substitution and electronic structure modulation. Band gap tuning observed from UV–visible studies indicates altered charge carrier dynamics. Electrochemical measurements demonstrate that Zn incorporation significantly enhances specific capacitance, rate capability, and cycling stability by improving charge transport kinetics and reducing interfacial resistance. Additionally, Zn-doped QDs exhibit superior antibacterial activity against *Staphylococcus aureus* (Zone of inhibition = 15 mm). These findings highlight Zn-engineered $MgFe_2O_4$ QDs as efficient multifunctional nanomaterials for advanced supercapacitor and biomedical applications.

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NMSF-ENM-010

MoS^2 Nanomaterial-Integrated Optical Fibre Sensors for Smart Energy and Gas Monitoring

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Abstract

Incorporating MoS^2 nanomaterials in Optical fibre sensors have gotten a lot of attention for monitoring energy and gas as they have better light-matter interaction and higher surface reactivity. This review provides an extensive examination of sensing mechanisms predicated on evanescent field modulation, refractive index variation, and optical absorption alterations resulting from gas adsorption. Sensitivity and response of different types of fibre sensors are, such as tapered, D-shaped, and fibre Bragg grating sensors have been checked. The incorporation of these sensors into biogas, hydrogen, and solar photothermal systems is examined, showcasing their ability for real-time monitoring and process enhancement. The photothermal properties of MoS_2 also make it possible to combine sensing and energy functions. Key challenges like environmental stability, cross-sensitivity, and fabrication reproducibility are looked at in depth, giving ideas for future research.

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NMSF-ENM-011

Hydrogen Production by Steam Reforming of Ethanol in the Presence of Ni-Mo Catalysts on Al_2O_3-CeO_2 Supports in a Fixed Bed Reactor

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Abstract

Hydrogen is being considered increasingly as one of the more important energy bearers of the future, mainly due to its potential and capability of allowing a transition towards cleaner energy systems. This paper considers the experimental investigation of steam reforming of ethanol over a Ni-Mo/Al_2O_3-CeO_2 catalyst in a fixed-bed reactor under different operating conditions: temperature range 453–673 K, LHSV = 2 mL min^{-1}, and steam/ethanol molar ratio equal to 3, 6, and 8. The idea is to find the optimal conditions that give the maximum production of hydrogen. The catalysts were prepared by the excess solution impregnation method and then characterized with different techniques such as SEM, ICP-OES, BET, FTIR, and TGA. The results showed that, as compared to commercial Al_2O_3-CeO_2 supported catalysts, the Ni-Mo bimetallic catalyst supported on Al_2O_3-CeO_2 exhibited better catalytic performance with improved resistance to coking at an intermediate temperature of 553 K. This catalytic performance enhancement, especially in ESR, is attributed to the role of Mo-La promoters that enable the interaction between Ni-Mo nanoparticles and support materials of Al_2O_3-CeO_2. This stronger interaction can prevent Ni nanoparticles from agglomeration and hence improve dispersion of nanoparticles, which inhibits the sintering of the nanoparticles. Consequently, it can improve both effectiveness and longevity of the catalyst. The Ni-Mo/Al_2O_3-CeO_2 catalyst gave the best catalytic results in the study, where ethanol conversion of 88.6% and hydrogen selectivity of 68% were achieved. These results were maintained up until about 48 hours of continuous operation. After 90 hours, it showed a slight decline of up to 93%, thus proving the efficiency and durability of the catalyst for a longer period of time.

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NMSF-ENM-012

Optimization of Surface Roughness and Thickness for Enhancing Electrochemical Storage Properties of Ni-Mg Alloy

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Abstract

The Ni-Mg alloy-based supercapacitors are considered promising ones because of their high specific energy and specific power density. Nickel-based material has gained interest because of its exceptionally high theoretical capacitance value and several other advantages, such as low cost and eco-friendly nature. To deal with the problem of lower conductivity, the Ni-Mg alloy has been used, as it reacts with the hydroxyl ion and creates an additional active pore for the faradic reaction, and hence improves the kinetics. The present study involves the surface roughness and thickness optimization of prepared films for enhancing their Supercapacitive applications. The thermal evaporation deposition technique is used to prepare the binder-free thin films. The present study clearly demonstrates the fall in the specific capacitance with the increase in the electrode thickness and decrease in the surface roughness. The prepared binder-free Ni-Mg film unveiled a maximum specific capacitance of 2634.93 F g^{-1} at a lower scan rate of 10 mVs^{-1}, as it exhibits the optimized surface roughness of 95.09 nm and thickness of 877.26 nm. The GCD results also confirm the same trends and show the maximum specific capacitance of 990 F g-1 at a current density of 4.5 Ag^{-1} for the NM^{-1} film. The highest obtained specific energy and specific power are 88 $WhKg^{-1}$ and 1800 WKg^{-1}, respectively. The structural properties of the films have been analyzed using XRD, FT-IR, and Raman spectroscopy, which reveal the reorientation of crystallite growth direction during deposition. The Rietveld refinement has been performed for the quantitative analysis of the multiphases present in the ball-milled material. The crystal structure was also constructed based on the refined parameters using the Vesta software. The prepared film's surface roughness and thickness can be measured using AFM imaging and cross-sectional FESEM analysis. The electrochemical analysis results clearly prove the electrode material as a promising one for high-energy storage applications, such as a grid-like system or in hybrid electric vehicles that require both high energy and power.

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NMSF-ENM-013

Structural, optical and photocatalytic properties of La-doped SnSe/SnO_2 nanocomposites

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Abstract

Highly efficient photocatalysts accelerate the redox reactions of breaking harmful long chain organic molecules to harmless products CO_2 and H_2O, in the presence of UV-visible light. Photocatalysts are generally semiconducting material which generates electron-hole pairs in presence of visible light that further produces free radicals to completely oxidize the desired organic dye pollutant. Nanocomposites photocatalyst made up of two semiconductors whose band schemes gets matched in such a way that quantum efficiency increases and photo-generated electron-hole pair recombination decreases to increase the photocatalytic efficiency, are of great research interest. Pristine, 1% and 2% lanthanum (La) doped SnSe/SnO_2 nanocomposites are prepared by chemical co-precipitation method [1]. Structural, optical and photocatalytic properties of the nanocomposites are studied. XRD results confirm the growth of cubic SnSe and tetragonal SnO_2 nanoparticles in all the samples. It has been observed that the Lanthanum (La) doping has decreased the photocatalytic efficiency of SnSe/SnO_2 nanocomposites, although La doping is expected to improve optical bandgap making it suitable for light harvesting and inhibit of grain growth improves the surface area thereby increasing its catalytic property. This could be attributed to higher concentration of La ions that created a high density of defects in the crystal lattice. These defect sites act trapping sites for both electrons and holes, thereby increasing the probability of recombination significantly.

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NMSF-ENM-015

Engineering Microwave-Synthesized ZnO-CuO Microflower Heterostructure Composites as a Bifunctional Electrocatalyst for OER and HER

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Abstract

Bifunctional electrocatalysts that efficiently drive both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are essential for enabling cost-effective, scalable alkaline water electrolysis to produce green hydrogen. Here, we report the rapid synthesis of ZnO-CuO microflower-like heterostructured nanocomposites via a microwave-assisted method (200 W) in a monowave reactor, employing 1-butyl-3-methylimidazolium bromide ([BMIM][Br]) ionic liquid as the reaction medium. The resulting materials were thoroughly characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), field-emission scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HRTEM), and X-ray photoelectron spectroscopy (XPS), revealing well-defined hierarchical morphologies, intimate ZnO-CuO nanointerfaces, and phase-pure heterojunction formation. Electrochemical evaluation in 1 M KOH demonstrated the nanocomposite's superior bifunctional performance. For HER, an overpotential of 229 mV versus the reversible hydrogen electrode (RHE) was required to achieve a current density of 10 mA cm^{-2}, with a Tafel slope of 101.04 mV dec^{-1}, reflecting favorable kinetics likely arising from optimized hydrogen adsorption/desorption at the heterojunction. For OER, the material delivered 50 mA cm^{-2} at a remarkably low overpotential of 157 mV versus RHE, accompanied by a Tafel slope of 128 mV dec^{-1}. These metrics, combined with extended chronoamperometric stability, highlight the synergistic electronic modulation and enhanced active site exposure provided by the ZnO-CuO p-n heterostructure. The microwave-assisted ionic liquid route offers a fast, energy-efficient, and scalable approach to engineer such transition metal oxide heterostructures. This work underscores the

promise of ZnO-CuO nanocomposites as earth-abundant, high-performance bifunctional electrocatalysts for advancing sustainable alkaline water splitting and renewable hydrogen production technologies.

Keywords: *Microwave-Assisted Method, Electrocatalyst, Oxygen Evolution Reaction, Hydrogen Evolution Reaction, Ionic Liquids*

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NMSF-ENM-018

Synergistic Effects of MWCNT and Al_2O_3 Nanoparticles on Paraffin-Based Phase Change Materials for Energy Storage

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Abstract

This work investigates the synthesis and thermal characterization of nano-enhanced paraffin-based phase change materials (PCMs) for solar thermal energy storage applications. The inherently low thermal conductivity, supercooling, and limited thermal reliability of paraffin restrict its practical use. To address these limitations, multiwalled carbon nanotubes (MWCNTs), Al_2O_3 nanoparticles, and their hybrid combinations were dispersed into paraffin. The incorporation of nano-additives resulted in a notable enhancement in thermal conductivity compared to pure paraffin. Differential scanning calorimetry and thermal cycling analyses indicate improved latent heat storage and enhanced thermal stability of the nano-enhanced PCMs. Among the samples, hybrid MWCNT–Al_2O_3 composites exhibited superior performance, attributed to synergistic effects in heat transfer enhancement. However, nanoparticle agglomeration and increased viscosity were observed, which may influence long-term dispersion stability and processability. Overall, the developed nano-enhanced PCMs demonstrate improved thermophysical properties, making them promising candidates for efficient and reliable solar thermal energy storage systems.

Keywords: *Phase Change Materials, Nano-Enhanced PCM, MWCNT,* Al_2O_3*, Hybrid Nanoparticles, Solar Thermal Energy Storage*

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Indoor Light Energy Harvesting Using Organic and Perovskite Solar Cells: A Comparative Study for IoT Applications

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Abstract

This work presents a critical analysis of advanced photovoltaic technologies tailored for indoor light energy harvesting, an emerging solution driven by the rapid expansion of Internet of Things (IoT) devices. Unlike conventional solar energy systems optimized for AM1.5G illumination, indoor environments are characterized by low-intensity (100–1000 lux) and narrow-spectrum artificial light sources such as light-emitting diodes and fluorescent lamps, necessitating fundamentally different design strategies.

The study systematically evaluates two leading material platforms organic solar cells (OSCs) and perovskite solar cells (PSCs) from a device physics perspective. Organic solar cells are analyzed in terms of their tunable bandgap and high absorption coefficients, enabling efficient spectral alig nment with indoor light sources. In contrast, perovskite solar cells are examined for their superior power conversion efficiencies under low illumination, while addressing limitations associated with trap-assisted recombination and operational stability.

Furthermore, this review highlights the critical role of spectral matching, charge transport dynamics, and recombination mechanisms in determining device performance under indoor conditions. By identifying key material and device-level optimization pathways, the work provides a framework for the development of efficient, battery-free energy solutions for next-generation smart sensors and portable electronics.

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Tuning Hydrogen Storage Performance of Rippled Si_9C_{15} Monolayer via Lithium Functionalization: A Computational Study

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Abstract

A recently synthesized rippled Si_9C_{15} monolayer has been reported to exhibit a direct band gap and excellent environmental stability. In this study, first-principles density functional theory (DFT) calculations are employed to investigate Li-functionalized Si_9C_{15} (2Li@ Si_9C_{15}) as a potential hydrogen storage medium for reversible and onboard storage in lightweight fuel cell vehicles (FCVs). We systematically examine the electronic, thermal, and mechanical properties of the pristine Si_9C_{15} monolayer. The adsorption energy of an H_2 molecule on pristine surface (-0.124 eV) is insufficient to meet the U.S. Department of Energy (DOE) criterion for practical storage. To enhance the interaction strength and hydrogen uptake, lithium doping is introduced. A Li adatom binds strongly to the Si_9C_{15} surface with a binding energy of -1.23 eV and transfers a charge of 0.98e, ensuring structural stability up to 500 K as verified by ab-initio molecular dynamics simulation. Li diffusion is restricted by a substantial migration barrier (~0.98 eV), preventing clustering of the surface. The 2Li@Si_9C_{15} system accommodates 16 H_2 molecules per unit cell, achieving a gravimetric capacity of 6.68%, surpassing the DOE 2025 target. The average adsorption energy of -0.20 eV/ H_2 lies within the optimal thermodynamic window for reversible storage, with desorption estimated to occur in the range 291–444 K at 5–12 bar. Non-covalent interaction (NCI) and pCOHP analyses elucidate the weak physisorption nature between the H_2 molecules and the 2Li@Si_9C_{15} surface. Overall, Li-decorated Si_9C_{15} emerges as a robust, high-capacity, and kinetically viable reversible hydrogen storage material for next-generation practical application in clean energy technologies.

Keywords: *First-Principles Calculations, Ab Initio Molecular Dynamics (AIMD), Reversible Hydrogen Storage, Thermodynamic Stability*

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NMSF-ENM-022

Solvent and Annealing Effect on the Characteristics of Sprayed SnO_2 Thin Films and Their Utility as Heterojunction Solar Cells

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Abstract

The impact of solvent and air annealing on the different characteristics of SnO_2 thin films produced on pre-cleaned substrates using an economical spray pyrolysis method is investigated in this study. For spray pyrolysis, the $SnCl_{4.5}H_2O$ precursor solution was prepared using two distinct solvents: double-distilled water (DDW) and deionized water (DIW). XRD-Raman-FTIR, SEM, EDS, UV-VIS-IR spectroscopy, and Hall effect measurement studies are used to examine the consequences of these solvents and air annealing on the structure of the crystal, surface morphology, stoichiometry, optical, and electrical characteristics of the deposited films. Higher crystallinity, O: Sn ratio, FTIR transmission, Raman shift, extinction coefficient, mobility, and charge concentration were found in DIW-prepared SnO_2 thin films; nevertheless, the crystal size, crystallinity, grain size, and the sheet resistance were found to be negligible. It turned out that SnO_2 thin films made with DDW had greater transmission. Hall-effect experiments revealed that SnO_2 thin films based on DDW and DIW both converted from n-type to p-type conductivity on air annealing. SnO_2/p-Si heterojunction solar cells developed using DIW-based SnO_2 thin films, found to have reduced series resistance, ideality factor, and open circuit voltage. It had been found that DIW-based SnO_2/p-Si heterojunction solar cells had improved light sensitivity and decreased interface states. Industrial feasible approach for producing inexpensive portable heterojunction solar cells in bulk is spray pyrolysis.

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NMSF-ENM-023

Evaluating Electrochemical Performance of Electrospun Polyindole Nanofibers for Supercapacitor Application

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Abstract

Developing efficient electrode materials are essential for next-generation supercapacitors. Herein, electrospun polyindole (PIn) nanofibers were fabricated using PVA as a sacrificial carrier polymer to ensure continuous fiber formation and structural integrity. The interconnected non-woven architecture exhibited uniform morphology and enlarged surface area, offering abundant electroactive sites and fast ion diffusion pathways. Electrochemical evaluation in a three-electrode system with 3 M KOH revealed dominant pseudocapacitive behavior arising from reversible redox reactions of the PIn backbone. The optimized electrode delivered a high specific capacitance of 387 F g^{-1} at 5 mV s^{-1}, highlighting its promise for next-generation supercapacitor applications.

Keywords: *Electrospinning, Polyindole, Nanofiber, CV, Supercapacitance, Supercapacitor*

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NMSF-ENM-024

Comparative Study of Dopant-Modified ZnO and CuO Nanocrystalline Thin Films: Conventional Thermal Versus Microwave Annealing for Photovoltaic Applications

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Abstract

Increased interest in functional metal oxide thin films has been added by the development of efficient, stable and low-cost photovoltaic materials. Nanocrystalline thin films of zinc oxide (ZnO) and copper oxide (CuO) were prepared in this paper through a solution-based deposition route, the, then the dopants engineered and finally annealed using standard thermal and microwave methods. Dopants were added in order to adjust the electronic and defect properties of the films and the impact of annealing route on the structural, optical, and electrical properties was also compared relatively. The phase-pure wurtzite ZnO and monoclinic CuO structures were confirmed by the X-ray diffraction analysis, and the films annealed by microwave radiation showed a higher degree of crystallinity and higher crystallites size than the traditionally annealed samples. During morphological studies, denser grain packing and less surface roughness was observed with microwave annealing. The optical analysis revealed that the band-edge sharpness was improved and that the number of defects was lowered in films doped by the method of microwaves whereas the electrical analysis revealed that the resistivity was smaller and carrier concentration was also higher especially in the samples that were optimally doped. This was shown to be advantageous by comparative analysis since the microwave annealing offers quick defect recovery and excellence in property enhancement at low thermal budgets. The transparency and conductivity of ZnO films are better indicating that it is well suited as electron transport layer and the enhanced absorption and charge transport in CuO films emphasize their potential as absorber or hole transport layer. On the whole, this paper has demonstrated that microwave annealing is a promising and energy-saving post-deposition annealing method of doped ZnO and CuO thin films with potential applications in the future in scalable photovoltaic systems.

Keywords: *ZnO Thin Films, CuO Thin Films, Dopant Engineering, Microwave Annealing, Conventional Annealing, Photovoltaic Materials*

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NMSF-ENM-025

Effect of Phyllanthus Emblica Biomass on the Structural and Electrochemical Properties of $MnFe_2O_4$

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Abstract

In this work, Phyllanthus emblica (Amla) leaf extract was used to synthesise $MnFe_2O_4$ nanostructures via a green, biomass-assisted method. Using plant biomass offers a straightforward, economical, and eco-friendly approach to modifying the surface and structural characteristics of spinel ferrites. X-ray diffraction (XRD) confirmed the phase purity and crystalline structure of the materials, demonstrating the formation of single-phase spinel $MnFe_2O_4$. Morphological investigation using FESEM and TEM revealed agglomerated nanoparticles with discernible changes in surface texture upon biomass incorporation. X-ray photoelectron spectroscopy (XPS) analysis verified surface oxygen species and mixed oxidation states of Mn and Fe ions, indicating potential defect development. Raman spectroscopy provided additional evidence for the structural stability of the spinel phase. Cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) were used to examine the electrochemical performance of the materials. The results, with moderate specific capacitance, indicate pseudocapacitive behaviour. Impedance studies show that biomass-assisted synthesis affects surface properties and charge-transfer characteristics, despite the comparatively modest capacitance. Particle agglomeration, a limited electroactive surface area, and structural characteristics together produce the observed electrochemical activity. Overall, this study offers insights into structure–property interactions for sustainable electrochemical energy storage applications and emphasises the importance of Phyllanthus emblica leaf biomass in modifying $MnFe_2O_4$ nanostructures.

Keywords: *Phyllanthus Emblica,* $MnFe_2O_4$*, Spinel Ferrites, Electrochemical Performance*

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NMSF-ENM-026

Binder Free Cobalt MOF for Supercapacitor Application

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Abstract

According to the International Energy Agency (IEA), global demand for energy increased by 2.2 % in 2025 than 2024, and the majority of the energy was supplied by renewable energy sources like solar, wind and tidal energy. The development of renewable energy sources is quite welcoming, still, there is a challenge in storing it as they are seasonal and depend on the climate. For storing energy, supercapacitors are more beneficial than batteries because of their fast charging and discharging, and cyclic stability. In supercapacitors, an emerging field is MOF based supercapacitors as they have a large surface area and tuneable properties which leads to high specific capacitance compared to other materials. Among these, cobalt MOF has greater conductivity and electrochemical properties since they have enhanced redox reactions due to their multiple oxidation states. This work reports a facile solvothermal synthesis of cobalt MOF using benzene dicarboxylic acid as the organic ligand. The synthesis was carried out at 160 degree Celsius for 6 hours in a sealed autoclave. The structural and morphological properties of the synthesised sample were studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR), confirming the formation of a crystalline material.Electrochemical performance of cobalt MOF was analysed using a three-electrode system with the help of Cyclic voltammetry(CV), Galvanostatic charge discharge cycle(GCD),and electrochemical impedance spectroscopy(EIS) in aqueous potassium hydroxide. The material exhibited a high specific capacitance of 1126.3 F/g at a current density of 4 A/g, demonstrating excellent charge storage capability. The low internal resistance obtained from the Nyquist plot shows its viability as an electrode material. Overall, the synthesised Co-MOF demonstrates significant promise for energy storage devices, offering a combination of high capacitance, stability, and conductivity.

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NMSF-ENM-027

Electrospun Derived Sn/SnO_2-CNF Composites as Anode Material for Sodium ion Battery

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Abstract

Developing high-capacity anodes remains challenging for next-generation Sodium-ion batteries. In this wok. Tin based carbon nanofibers (Sn/SnO_2-CNFs) are fabricated by electrospinning method followed by thermal treatment. X-ray diffraction analysis and Raman results confirms the presence of Sn/SnO_2 - CNFs. The high resolution scanning electron microscopy result shows fiber like structure with diameter of 200 nm and length of 2 μm. Sn/SnO_2-CNFs versus Na^+ cells delivers the initial discharge capacity of 634 mAh g^{-1}. The unique one- dimensional fibrous architecture provides continuous electron transport pathways and short Na^+ diffusion lengths, while the carbon matrix accommodates the volume expansion of Sn-based active species during alloying/dealloying processes. Additionally, the synergistic combination of metallic Sn and SnO_2 contributes to enhanced sodium storage through both alloying and conversion reactions, improving overall capacity.

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NMSF-ENM-029

Advanced Transport Layer Integration of SnO_2 and NiO for High-Efficiency Double Perovskite Solar Cells

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Abstract

This research employs the halide double perovskite (FA)2BiCuI6 as a light-harvesting layer for the device structure NiO/$(FA)_2BiCuI_6$/SnO_2/FTO. With a fill factor (FF) of 86.25% and a power conversion efficiency (PCE) of 20%, the device exhibits ideal photovoltaic performance. NiO/$(FA)_2BiCuI_6$/SnO_2/FTO double perovskite solar cell (DPSC) structure is further modelled for optimal absorber layer input specifications. The optimized thickness for the absorber layer and the defect density for the $(FA)_2BiCuI_6$ layer are 1.1µm and 1.0x10^{14} cm^{-3} respectively. It has been observed that solar cell performance is enhanced at temperatures between 250 K and 350 K. The SCAPS-1D tool is utilized to calculate the ideal device input parameters. The device structure is optimised. The findings highlight that the DPSC performance is much superior compared to the previously reported works.

Keywords: *Fill Factor, Power Conversion Efficiency, DPSC, Photovoltaics*

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NMSF-ENM-030

Thermal Treatment Driven Enhancement in Thermoelectric Properties of α-GeTe Thin Films at Room Temperature

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Abstract

Germanium telluride (GeTe) is a widely studied phase-change material (PCM) that exhibits reversible transformation between amorphous and crystalline phases. This phase transition leads to significant modifications in crystallite dimensions, defect distribution, and charge carrier transport, thereby influencing the thermoelectric (TE) performance of the thin films. In the present work, as-deposited amorphous films were crystallized into polycrystalline phases via post-deposition thermal annealing up to 473 K. The α-GeTe thin films were deposited on glass substrates using thermal evaporation technique, followed by annealing at 383 K, 403 K, 423 K, and 473 K to induce phase transformation. The thermoelectric properties, including electrical conductivity (σ), Seebeck coefficient (S), and power factor (PF), were evaluated at room temperature (RT) 303 K. Maximum electrical conductivity of 45.64×10^3 Sm^{-1} was obtained for the film annealed at 473 K, while a significantly lower value of 0.01×10^3 Sm^{-1} was observed for the amorphous film annealed at 383 K. The transition from the amorphous to polycrystalline phase resulted in increased crystallite size and reduced lattice strain, which enhanced the charge carrier mean free path and consequently improved electrical conductivity. Highest Seebeck coefficient and power factor values of 800 μVK$\hat{}-1$ and 1139 $\mu Wm^{-1}K^{-2}$ respectively, were achieved at room temperature for film annealed at 423 K. Reduction in the Seebeck coefficient is attributed to the enhanced contribution of low-energy charge carriers induced by the phase transformation. The structural characteristics of the thin films were analysed using X-ray diffraction (XRD) and Raman spectroscopy.

Keywords: *α-GeTe Thin Films, Crystallization, Thermal Evaporation, Amorphous*

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NMSF-ENM-031

Defect-Induced Enhancement in Power Factor of $AgSbTe_2$ Thin Films

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Abstract

Defect engineering has emerged as an effective strategy to enhance thermoelectric performance by modulating carrier transport. In this work, a significant improvement in the Seebeck coefficient (S) and power factor (PF) of $AgSbTe_2$ thin films is achieved through a controlled chemical etching approach. $AgSbTe_2$ was synthesized via the melt–quench method, and thin films were deposited using thermal evaporation. Defects in films were introduced via wet chemical etching in a dilute HNO_3 solution for different etching durations, followed by thermal annealing at 363 K. The thermoelectric properties were subsequently measured at 303 K. Films etched for 5 min exhibited a maximum power factor of 1391.83 $\mu Wm^{-1}K^{-2}$, corresponding to an enhancement of 160 % compared to without etched sample along with a high Seebeck coefficient of 215 μVK^{-1}. Highest electrical conductivity of 3.56×10^4 Sm^{-1} was achieved for sample etched for 1 min. The enhancement in thermoelectric performance is attributed to defects-induced energy filtering and enhanced carrier scattering at defects interfaces. UV–Vis spectroscopy indicated a gradual increase in the optical band gap with increasing etching duration, indicating the presence of quantum confinement effects. Structural and morphological investigations carried out using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and atomic force microscopy (AFM) revealed enhanced porosity, increased defect density, and significant modifications in surface roughness after etching. These results indicate that controlled chemical etching is an effective route for defect engineering, enabling enhanced thermoelectric performance in $AgSbTe_2$ thin films.

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NMSF-ENM-032

Multifold Enhancement in Thermoelectric Power Factor of β-Zn_4Sb_3 Thin Films via Surface Roughness Tuning.

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Abstract

Surface roughness–induced resistivity and surface scattering are key factors in optimizing charge carrier transport in thin-film surfaces. In this study, the influence of surface roughness on thermoelectric (TE) parameters—namely the Seebeck coefficient (S), electrical conductivity (σ), and power factor (PF)—was examined. Thin films with thicknesses ranging from 69 nm to 363 nm were fabricated using thermal evaporation, leading to a variation in surface roughness from 6.94 nm to 37.51 nm. The highest values of S (227 μVK^{-1}) and PF (814 $\mu Wm^{-1}K^{-2}$) at room temperature were observed for the film with a roughness of 28.94 nm, representing enhancements of 3.05 and 41.84 times, respectively, compared to the film with 6.94 nm roughness. The increase in S with roughness is attributed to surface energy filtering effects. The maximum electrical conductivity (2.25×10^4 Sm^{-1}) was obtained for a film with a roughness of 21.75 nm. Initially, σ increased due to a longer carrier mean free path associated with larger crystallite sizes; however, at higher roughness, σ decreased due to increased resistivity, enhanced surface scattering, and carrier trapping. Structural properties were analyzed using X-ray diffraction (XRD) and Raman spectroscopy, while morphological, topographical, and optical characteristics were studied through FESEM, AFM, and UV–Vis spectroscopy, respectively.

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NMSF-ENM-033

Robust Hydrogen Storage in Ti_2N Under Small Mechanical Strain: A DFT Study

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Abstract

Strain engineering is often seen as a subtle yet powerful way to tune the behavior of two-dimensional (2D) materials. By gently stretching or compressing the lattice, one can alter bond lengths, angles, and symmetry, changes that usually translate directly into modified electronic properties. In many hydrogen storage systems, e.g. in conventional hydrides such as MgH_2, applying mechanical strain can reduce hydrogen storage capacity and lower the decomposition temperature by destabilizing the crystal structure. Compressive strain may improve reaction kinetics by weakening metal-hydrogen bonds, but it often does so at the expense of storage capacity, making the material more susceptible to instability and hydrogen-induced degradation.

Two-dimensional MXenes have emerged as promising alternatives for hydrogen storage. Among them, Ti_2N stands out due to its relatively high hydrogen storage capacity (~4.2%) and favorable surface chemistry. In this work, we use first-principles density functional theory (DFT) calculations to explore how Ti_2N MXene responds to externally applied uniaxial and biaxial strains, both compressive and tensile, with particular attention to hydrogen adsorption behavior. We systematically analyze strain-induced changes in the electronic structure, including band renormalization, orbital-resolved density of states (DOS), and shifts in the d-band center, a key descriptor of surface reactivity. Interestingly, our results reveal that, unlike many conventional hydrogen storage materials, Ti_2N exhibits remarkable resilience to mechanical deformation. Even under applied strain, the DOS, d-band center, and overall electronic structure remain largely unchanged.

This robustness suggests that the hydrogen storage characteristics of Ti_2N MXene are intrinsically robust against mechanical strain. Such stability under strain is important, especially for real-world applications where materials often experience mechanical stress. Overall, these findings provide useful insight into the design of durable, high-performance 2D materials for next-generation hydrogen energy systems.

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NMSF-ENM-034

Interfacial Engineering of MXene-MOF Hybrid Photoanodes for Enhancing the Performance of Dye-Sensitized Solar Cells

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Abstract

Dye-sensitized solar cells (DSSCs) have attracted significant attention as sustainable and low-cost photovoltaic devices, however, their performance is often constrained by inefficient charge transport and limited light absorption within the mesoporous TiO_2 nanoparticles (NPs) matrix in the photoanode. In this direction, doping the m-TiO_2 layer with nanostructures with diameter comparable to wavelength of visible light can effectively provide improved light scattering and high charge transport network. To this, MXene and metal organic framework, $ZIF-67$, have been incorporated as dopants to the mesoporous TiO_2 layer in the photoanode and the as-fabricated DSSC device exhibited enhanced power conversion efficiency (PCE) as compared to pristine TiO_2 NPs based DSSC. This enhanced performance is attributed to the combined effect of efficient light scattering augmented from Mie scattering theory and faster electron transport confirmed through electrochemical impedance spectroscopy. The synergistic integration of MXene and $ZIF-67$ within the TiO_2 matrix leads to improved electrical conductivity and rapid charge transfer pathways provided by MXene nanosheets, while the high surface area and tunable porous architecture of $ZIF-67$ facilitates increased dye adsorption and efficient light scattering resulting in extended light interaction within the active layer. This leads to increased generation of excitons, thereby increasing the short circuit current density (JSC) and overall power conversion efficiency compared to pristine TiO_2-based DSSCs devices. This study highlights the potential of integrating multifunctional nanomaterials to engineer advanced photoanodes, offering a sustainable and scalable pathway for the development of high-performance DSSCs.

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NMSF-ENM-035

Comparative Study of ZIF-67αGO Electrodes on Nickel Foam and Carbon Paper: Effects of KOH Concentration on Supercapacitor Performance

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Abstract

The growing demand for efficient energy storage devices has driven the development of advanced composite materials with enhanced electrochemical performance. In this study, a porous ZIF − 67@GO nanocomposite was synthesized using a simple stirring method and investigated as an electrode material on two substrates: nickel foam (NF) and carbon paper (CP). The influence of electrolyte concentration was evaluated using KOH solutions at 2 M, 4 M, and 6 M. The ZIF − 67@GO/NF electrode demonstrated a high specific capacitance of 231 F/g at a scan rate of 10 mV/s within a potential window of -0.1 to 0.5 V in 6 M KOH, significantly outperforming the native ZIF − 67/NF (167 F/g in 0 to 0.5 V). In contrast, the ZIF − 67/CP and native ZIF − 67@GO/CP electrodes exhibited lower performance, achieving 18 F/g and 20 F/g, respectively, under the same conditions. Electrochemical impedance spectroscopy revealed reduced internal and charge transfer resistance in the composite electrode. Despite a capacitance retention of 53% after 500 charge-discharge cycles, the composite shows promising stability. The incorporation of GO nanosheets onto ZIF − 67 enhances conductivity, surface area, and overall electrochemical properties, making the ZIF − 67@GO composite a strong candidate for high-performance supercapacitor applications.

Keywords: ZIF-*67@GO Composite, Supercapacitor, Nickel Foam, Carbon Paper, KOH Concentration, Electrochemical Performance, Specific Capacitance, Electrochemical Impedance Spectroscopy (EIS), Graphene Oxide, Energy Storage*

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Biowaste-Derived Carbon Allotropes for Next Generation Clean Energy Applications

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Abstract

Research into renewable and sustainable energy technologies has accelerated due to the pressing need to mitigate climate change and minimize reliance on fossil fuels. This urgency has driven the demand for high- performing, reasonably priced, and ecologically friendly materials. Among these, the carbon allotropes such as graphene, graphene oxide (GO) and reduced graphene oxide (rGO) have emerged as highly versatile carbon- based no nmaterials. Owing to their unique physiochemical properties, including high electrical conductivity, large specific surface area, excellent mechanical strength and tuneable surface chemistry resulting from residual oxygen functional groups and structural defects, these materials hold significant potential for addressing contemporary energy and environment challenges.

The present study is focused on the sustainable synthesis of carbon allotropes from lignocellulosic biomass wastes, namely, pine cones, walnut shells and coconut shells along with the investigation of their physiochemical properties. The X-ray diffraction (XRD) signifies the formation of rGO as one of the carbon allotropes from these bio wastes. The dielectric/electrical properties such as dielectric constant, dielectric loss, ac impedance, ac conductivity were measured using dielectric spectroscopy. As a highly versatile no nmaterial, rGO exhibits properties advantageous for diverse technological applications. These include environmental remediation, gas sensing, energy storage devices, flexible electrodes, supercapacitors, lithium-ion batteries, sodium-ion batteries and new flexible storage devices. Furthermore, rGO based composites containing nanostructured metals and transition metal oxides show better durability, decreased over-potentials and significantly increased catalytic activity in both fuel cells and electro-catalytic systems.

Keywords: *Coconut Shell, Dielectric Spectroscopy, Pine Cone, Reduced Graphene Oxide, Walnut Shell, XRD*

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NMSF-ENM-037

Renewable and Sustainable Energy Materials

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Abstract

Sustainable and renewable energy materials are an important part of addressing the growing challenges of finding suitable energy solutions amid environmental degradation and the limited supply of fossil fuels. This abstract describes the current state of research on the development, characterization, and implementation of innovative materials capable of effectively harvesting, storing, and transforming energy derived from renewable sources such as solar, wind, and bioenergy. The emphasis in this paper is on the use of environmentally friendly, abundant, and inexpensive materials for sustainable energy solutions. Some of these include nanomaterials, bio-composites, and hybrid materials. The sustainability of these materials is achieved through a lifecycle assessment, and their end-of-life management through the principle of a circular economy. The main problems and challenges in achieving sustainable energy with these materials are explored, with solutions from computational simulations and high-throughput screening highlighted.

Keywords: *Renewable Energy, Sustainable Materials, Nanomaterials, Energy Storage, Photovoltaics, Lifecycle Assessment, Circular Economy, Energy Conversion*

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Chloride-Based Additive Engineering for Efficient Perovskite Solar Cells

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Abstract Additive engineering is a widely adopted strategy for depositing high-quality perovskite films in photovoltaic research. In this study, we investigate the influence of chloride-based additives, specifically methylammonium chloride (MACl) and lead chloride ($PbCl_2$), on the performance of mixed-halide perovskite solar cells, with an emphasis on site-specific modification strategies. Two material systems are examined: double-cation, double-halide perovskites ($FA_{1-x}MA_xPb(I_{1-y}Bry)_3$) and triple-cation, double-halide perovskites ($Cs_x(FA_{1-y}MA_y)_{1-x}Pb(I_{1-z}Br_z)_3$). Mixed-cation, mixed-halide perovskite thin films.

Thin films were systematically prepared on fluorine-doped tin oxide (FTO)-coated glass substrates. The precursor solution, consisting of PbI_2, $PbBr_2$, FAI, MABr, and CsI in a mixed solvent system of DMF and DMSO, was first deposited via spin-coating. To promote controlled crystallization, chlorobenzene was dispensed during the spin-coating process. Following deposition, the films were thermally annealed to complete the perovskite crystal formation. The influence of MACl and of $PbCl_2$ with different percentages on film formation and device performance was investigated. After optimizing the perovskite layer, full photovoltaic devices were fabricated. The device architecture consisted of the FTO substrate as the transparent electrode, followed by a compact electron transport layer (ETL), the perovskite active layer, a hole transport layer (HTL) of Spiro-OMeTAD, and finally a metallic top silver electrode Each layer was sequentially deposited under controlled conditions to ensure reproducibility and performance. The complete devices were then characterized for their photovoltaic performance under simulated solar illumination. We explain a method whereby different percentages of MACl and $PbCl_2$ are used to form highly efficient perovskite solar cells. Structural, compositional, showed that optimized additive concentrations significantly enhance crystallinity, improves uniform morphology, and reduce defect densities. We perceive that, MACl appears to modulate crystal growth kinetics, while $PbCl_2$ contributes to defect passivation and improved interfacial contact. As a result, perovskite solar cells fabricated with optimal MACl and $PbCl_2$ percentages achieved higher power conversion efficiencies (PCEs) compared to control devices.

Keywords: *Perovskite Solar Cells, Additive Engineering, MACl, $PbCl_2$, Defect Passivation, Crystal Growth, Power Conversion Efficiency*

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Physicochemical Characterization of Biomass Feedstocks for Suitability Assessment for Better Quality Pelletization Towards Energy Sustainability

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Abstract

The need of renewable and sustainable energy sources has led to the development of alternative forms of biomasses/ agro-residues for production of better fuel through pelletization. Using thorough physicochemical characterization, this study assesses the suitability of two readily available raw agro-residues in Punjab, India: rice straw (RS) and pods of Vigna radiata (L.) R. Wilczek (PVRW) as feedstocks for the production of high-quality pellets as good energy sources. As per proximate analysis, RS and PVRW collected from fields of Punjab, India had moisture contents of 6.0% and 7.88% respectively, volatile matter of 63.0% and 61.21% respectively, ash contents of 12.0% and 11.04% respectively, and fixed carbon contents of 18.91% and 19.87% respectively. These factors have a big impact on the pellets' energy yield, handling qualities, and combustion efficiency. A blended feedstock consisting of RS and PVRW in a 50:50 ratio had shown the significant calorific value (13.65 MJ kg^{-1}), suggesting that co-pelletization has a synergistic effect on energy performance. In addition, important engineering characteristics were evaluated to ascertain the behavior of pelletization, the appropriateness of storage and mechanical strength. Behavior of RS and PVRW for pelletization have been studied through the bulk densities and corresponding tapped densities, angle of repose, porosity with reduction in particle size, FESEM for surface morphology, XRD to reveal crystalline phase composition and structural changes. Overall, the findings demonstrate that RS and PVRW, either individually or in blended form, possess desirable physicochemical and engineering properties, supporting their potential as sustainable feedstocks for efficient pellet fuel production.

Keywords: *Pelletization, Agro-Residues, Physicochemical Properties, Biomass Characterization, Renewable Energy Source, Sustainability*

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Valorisation of Waste: Modification of Granite Stone as Renewable Heterogeneous Catalyst for Waste Cooking Oil Biodiesel Synthesis

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Abstract

The present study valorises the granite stone by modifying to an environmentally friendly heterogeneous catalyst for transesterification of waste cooking oil to biodiesel. The characterization of the catalyst is done by FT-IR, XRD, BET, and SEM-EDX techniques. The raw granite stone powder and modified granite stone powder are utilized as catalyst in the transesterification of waste cooking oil. Due to the presence of good amount of potassium and other active metals, the catalyst possesses high catalytic activity. The optimum reaction conditions for the transesterification catalysed by the prepared catalyst are found to be 12:1 methanol to oil ratio, 7 wt.% of catalyst and 65 of reaction temperature, resulting in 97.63% of biodiesel yield in a short reaction time of 30–40 minutes. The activation energy of the catalyst is found to be 37.95 kJ mol^{-1}. The FT-IR and GC-MS characterization of the produced biodiesel reveals the complete conversion of the oil to biodiesel. The present catalyst is non-toxic, environmentally friendly, and green. The catalyst is cost effective as the raw material is available with no cost. The generation of catalyst from waste granite as well as production of biodiesel from waste cooking oil gives a value addition to the waste and the catalyst could contribute in reduction of overall biodiesel cost.

Keywords: *Waste Granite Stone, Transesterification, Green Catalyst, Biodiesel, Waste Cooking Oil*

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NMSF-ENM-042

A Review- $BiFeO_3$-Based Nanomaterials for Next-Generation Energy and Sensing Applications

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Abstract

Due to the simultaneous presence of two or more characteristics, such as ferroelectricity, ferromagnetism, and ferroelasticity, multiferroic nanomaterials have garnered a lot of attention and have the potential to be widely used in low-power, environmentally friendly, multifunctional devices. At ambient temperature, bismuth ferrite ($BiFeO_3$, BFO) displays both ferroelectric and (anti)ferromagnetic characteristics. As a result, its significance in multiferroic systems has grown. The advancements of BFO nanoparticles, including their shape, structures, characteristics, and possible uses in multiferroic devices with unique functions, Photo-catalysis, spintronics, data storage (Memory Devices), Microwave and RF Devices, Multiferroic Tunnel Junctions (MTJ), Energy storage- electrodes as for super-capacitors, photovoltaic for converting solar energy to electricity, biomedical applications will be methodically covered in this review. All of the opportunities and difficulties will be examined and condensed. We hope that this review will serve as an update and motivate other researchers to continue developing BFO nanomaterials in the future.

Keywords: *Bismuth Ferrite, Multiferroic Devices, Photocatalysis, Data Storage, Energy Storage, Nanomaterials*

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NMSF-ENM-043

Hydrothermally Synthesized Porous MoS_2 Nanosheets for High-Performance Supercapacitors

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Abstract

Global energy crisis has emerged as one of the major and burning issues and establishment of sustainable and efficient energy storage technology should take place. A lot of interest has been received by the supercapacitors and other energy storage systems due to their high charge/discharge, cyclic stability and high-power density. In this study, the hydrothermal method was used for the preparation of molybdenum disulfide (MoS_2) with the calcination time of 18h. The comprehensive characterization methods were used for studying structural, morphological and compositional characteristics. The X-ray diffraction (XRD) was performed for calculating the crystallite size, and it gave the average crystallite size of 63.90 nm. The scanning electron microscopy (SEM) was used for displaying nanosheet-like morphology with porous structure, and this type of structure is favorable in electrochemical use. The energy-dispersive X-ray spectroscopy (EDX) displayed the elemental composition of the synthesized MoS_2. Good charge-discharge capacity was revealed by the electrochemical performance; it displayed a specific capacitance of 563.57 μFcm^{-1} at a scan rate of 1 mVs^{-1}, there was high cyclic stability, and the rate performance was also good. In addition to this, a maximum power density of 6240 W kg^{-1} at the energy density of 0.52 $Whkg^{-1}$ was found after performing the galvanostatic charge-discharge (GCD) experiment. All these findings shows that synthesized material has a bright future as a material for supercapacitors. Thus, the ready-made nanosheets of MoS_2 exhibit a great future as a high-quality and inexpensive electrode material in next generation supercapacitor-based energy storage devices.

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Li-Doped Praseodymium Perovskite HECs for Room-Temperature Water Splitting and Power Generation

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Abstract

The hydroelectric cell (HEC) presents an innovative and sustainable approach for clean energy generation through room-temperature water dissociation, eliminating the need for UV irradiation, electrolytes, or external bias. In this study, defect-engineered praseodymium-based perovskite oxides are explored as efficient and eco-friendly materials for electrolyte-free water splitting. The developed HEC utilizes oxygen vacancies and nanoporous structures within $Pr_{0.8}Na_{0.2}-xLiAlO_3$ (x = 0.00, 0.01 and 0.03) perovskite to facilitate spontaneous water dissociation, enabling direct electricity generation at ambient conditions. The ceramic samples were synthesized via a conventional solid-state method and characterized to investigate structure–property correlations. X-ray diffraction (XRD) analysis confirmed phase purity and lattice distortion due to Li^+ substitution, while field emission scanning electron microscopy (FESEM) revealed enhanced nanoporosity and defect formation. Lithium incorporation was found to increase oxygen vacancy concentration, promoting efficient ionic transport. Among the studied compositions, $Pr_{0.8}Na_{0.17}Li_{0.03}AlO_3$ exhibited the highest performance, producing an open-circuit voltage (Ocv) of 0.96 V and a short-circuit current (Scc) of 6.1 mA, corresponding to a maximum output power of 5.85 mW at room temperature using only distilled water. These findings highlight the potential of defect-engineered perovskite oxides as promising candidates for sustainable, self-powered energy devices.

Keywords: *Hydroelectric Cell, Perovskite, Nanopores, Vacancy, Electrolyte*

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Thermoelectric and Vibration-Harvesting Materials for Self-Powered Telemetry Systems in Next-Generation Aerodynamic Platforms: A Review

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Abstract

The rapid expansion of unmanned aerial systems and high-speed aerospace platforms has created a growing need for lightweight, maintenance-free, and energy-efficient sensor systems capable of operating in harsh thermal and mechanical environments. Traditional battery-powered systems impose limitations such as added weight, frequent replacement, and environmental concerns related to disposal. In this context, energy harvesting from ambient sources especially mechanical vibrations and thermal gradients naturally present in aerospace structures offers a promising solution for developing self-powered telemetry systems that support sustainable engineering practices. This review provides a detailed overview of thermoelectric and piezoelectric materials used for energy harvesting in advanced aerodynamic platforms. In thermoelectric systems, widely used Bi_2Te_3-based materials are discussed alongside emerging alternatives such as half-Heusler alloys and oxide-based thermoelectrics. The role of material engineering approaches, including nanoscale structuring, grain boundary control, and enhanced phonon scattering, is highlighted for their ability to significantly improve efficiency, with reported increases in thermoelectric performance exceeding 30% compared to bulk materials.

For vibration-based energy harvesting, the review focuses on piezoelectric materials such as PZT ceramics, PVDF polymer films, and $BaTiO_3$-based nanocomposites. These materials are evaluated based on their ability to convert mechanical vibrations into electrical energy, considering parameters such as coupling efficiency, power output, and adaptability to varying vibration conditions typically encountered in aerospace environments. Their suitability for integration into aircraft structures and unmanned aerial vehicles is also examined. The study further explores material design strategies aimed at ensuring durability under extreme conditions. This includes the development of thermoelectric modules capable of operating at high temperatures, flexible piezoelectric devices for seamless structural integration, and environmentally friendly materials that support recyclable and sustainable manufacturing processes. Key challenges

in system integration are also addressed, including efficient power management, impedance matching, miniaturization of electronic circuits, and long-term reliability under continuous mechanical stress. Overcoming these issues is essential for the practical implementation of self-powered systems in real-world aerospace applications. The review emphasizes current progress and future directions in the development of self-powered, high-performance telemetry systems, supporting the advancement of greener and more efficient aerospace technologies.

Keywords: *Energy Harvesting, Thermoelectric Materials, Piezoelectric Sensors, Aerospace Applications*

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Wide Bandgap Semiconductor Materials for Power Device Applications: A Schematic Review

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Abstract

The accelerating demand for compact, high-efficiency, and high-reliability power electronics in applications such as electric vehicles, renewable energy systems, aerospace, and industrial automation has driven a paradigm shift from conventional silicon (Si) to wide bandgap (WBG) and ultra-wide bandgap (UWBG) semiconductor materials. This review synthesizes the current state of knowledge on key WBG materials—including silicon carbide (SiC), gallium nitride (GaN), gallium oxide (β-Ga_2O_3), diamond, aluminum nitride (AlN), and boron nitride (BN)—covering their intrinsic properties, growth and fabrication technologies, device architectures, reliability considerations, and emerging application trends. Special emphasis is placed on schematic comparisons of critical material parameters—bandgap, breakdown field, electron mobility, thermal conductivity, and saturation velocity—highlighting the performance trade-offs that guide device selection for specific applications. The review identifies SiC and GaN as commercially mature technologies for high-voltage, high-frequency power devices, while UWBG materials such as β-Ga_2O_3, diamond, and AlN offer unprecedented breakdown strengths and operating temperatures, albeit with significant challenges in doping control, thermal management, and large-area substrate availability. Future research directions include quantum-enabled device concepts, high-entropy semiconductor systems, and hybrid integration strategies that combine the maturity of Si with the superior performance of WBG/UWBG materials. This work provides a comprehensive and visually structured reference for researchers, engineers, and industry practitioners, serving both as a state-of-the-art resource and as a roadmap for advancing next-generation power electronics.

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Study of Electrolyte's Effect on the Energy Storage Performance of WS_2 Electrodes

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Abstract

The growing global demand for energy, along with the ongoing energy crisis, has increased the urgency for developing efficient and sustainable energy storage solutions. Among different electrochemical storage systems, supercapacitors have gained considerable interest due to their high power density, fast charge–discharge rates, and long cycle life. Despite these advantages, improving their energy density without compromising power performance remains a major challenge. A key factor influencing the overall performance of supercapacitors is the interaction between electrode materials and electrolytes. In particular, the physicochemical properties of the electrolyte play a vital role in ion transport, charge storage mechanisms, and interfacial charge transfer. In this study, the electrochemical performance of symmetric supercapacitors using WS_2 nanosheets as electrodes was systematically examined in three aqueous electrolytes: alkaline (1 M KOH), acidic (1 M H_2SO_4), and neutral (1 M Na_2SO_4). The results show that electrolyte type has a significant impact on capacitive performance. At a current density of 1 A g^{-1}, the specific capacitance follows the order: KOH > H_2SO_4 > Na_2SO_4. A similar trend is observed for energy density at a constant power density, with the alkaline electrolyte delivering the highest values, followed by the acidic and neutral media. Among the electrolytes studied, the alkaline solution provides the best electrochemical performance, likely due to its higher ionic conductivity and more effective electrode–electrolyte interactions. In addition, the WS_2-based supercapacitor demonstrates excellent cycling stability, maintaining 100% of its initial capacitance even after 6,000 charge–discharge cycles in KOH. These results emphasize the critical role of electrolyte selection in enhancing the performance of WS_2-based supercapacitors for advanced energy storage applications.

Keywords: *Supercapacitors, Electrolyte Effect, Electrochemical Energy Storage, Cycling Stability*

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Recombination Reduction and Defect Thermodynamics in Co-doped CdTe Solar Cells with Arsenic and Phosphorus.

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Abstract

Cadmium telluride (CdTe) is a leading thin-film photovoltaic material, yet its efficiency is hindered by deep-level defects, defect compensation, and an open-circuit voltage deficit due to unstable p-type doping. This study explores arsenic–phosphorus co-doping as a thermodynamic method to enhance dopant activation, reduce deep recombination centers, and stabilize the Fermi level within CdTe. A comprehensive framework integrating defect thermodynamics, recombination physics, and experimental characterization highlights the microscopic mechanisms affecting carrier lifetime and device performance. Thermodynamic analysis reveals that co-doping elevates the formation energy of compensating donor defects, boosting the energy of cadmium interstitials from approximately 1.2 eV in single-dopant systems to 1.8 eV in co-doped CdTe, which mitigates donor formation and defect compensation. The interaction between arsenic and phosphorus fosters the creation of a stable neutral defect complex with about 0.35 eV binding energy, stabilizing acceptor configurations and lowering deep-level trap density. Time-resolved photoluminescence studies show a significant increase in minority carrier lifetime, rising from 0.8 ns in undoped CdTe to 5.8 ns in co-doped films, indicating reduced non-radiative recombination. Additionally, Kelvin probe force microscopy indicates improved electrostatic homogeneity, with surface potential fluctuations declining from ~75 mV to ~28 mV, representing a ~60% reduction in potential inhomogeneity. These advancements correlate with device performance enhancements, as open-circuit voltage rises from 0.78 V to 0.86 V alongside better fill factor and power conversion efficiency. The findings confirm that cooperative defect engineering through arsenic–phosphorus co-doping offers a viable Cu-free approach to diminish recombination losses and boost the performance and stability of CdTe solar cells.

Keywords: *Cadmium Telluride (CdTe) Solar Cells, Arsenic–Phosphorus Co-Doping, Defect Thermodynamics, Non-Radiative Recombination Suppression, Carrier Lifetime Enhancement, Open-Circuit Voltage Improvement*

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Study of Latent Heat Retention and Thermal Stability of Phase Change Material via SEBS and Graphene Oxide Incorporation

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Abstract

This paper aims to develop a phase change material (PCM) with shape stabilization using Paraffin/SEBS embedded with Graphene Oxide (GO) to use in the storage of thermal energy. Differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and X-ray diffraction (XRD) were used to determine the thermal and structural properties of the composite. The XRD shows that the typical crystalline peaks of paraffin are maintained in the composite, which means that the PCM maintains its crystalline structure in the SEBS matrix. The peak intensity is reduced, indicating the partial inhibition of crystallinity through the encapsulation effect of the polymer and the existence of GO. The lack of other peaks suggests that GO is not precipitated physically, but rather dispersed in the form of a physical entity that does not change the chemical structure of the composite. Next, the DSC indicate that the latent heat of fusion of the Paraffin/SEBS/GO composite is in the range of about 150–160 J/g, which is a moderate decrease with the addition of the matrix and filler. Although this reduction is made, the composite still has a large energy storage capacity and fixed phase change behavior. Further, the TGA analysis indicates that the thermal stability is improved and the temperature of the onset degradation elevates to about 245–250 °C, compared to the original Paraffin/SEBS system. This is achieved by the barrier effect of GO and interaction with the polymer matrix, which retards thermal degradation.

In general, the Paraffin/SEBS/GO composite prepared in the present study exhibits excellent thermal reliability, improved thermal stability, and high latent heat storage capacity, which makes it potential materials to be used in efficient and long-term thermal energy storage processes.

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Interface-Engineered MoS_2–ZIF-Derived Carbon Nanocomposite for Enhanced Hydrogen Evolution Reaction

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Abstract

The design of efficient and stable electrocatalysts for the hydrogen evolution reaction (HER) is essential for sustainable hydrogen production. In this work, a MoS_2–ZIF–Carbon hybrid nanocomposite was developed to enhance catalytic activity through interfacial engineering and improved charge transport. The composite was synthesized via a controlled approach that integrates MoS_2 with a conductive carbon matrix derived from a ZIF precursor. Structural analysis using X-ray diffraction confirmed the successful formation of the hybrid phase, while UV–Vis spectroscopy provided insight into its electronic structure. High-resolution transmission electron microscopy revealed a well-dispersed MoS_2 phase embedded within the porous carbon framework, establishing intimate interfacial contact. Electrochemical measurements demonstrate that the MoS_2–ZIF–Carbon composite exhibits enhanced HER activity compared to its individual components, delivering a lower overpotential at a current density of 10 mA cm^{-2} and an improved Tafel slope, indicative of favourable reaction kinetics. The enhanced performance is attributed to the synergistic interaction between MoS_2 active sites and the conductive carbon network, which facilitates rapid electron transfer and increases the availability of catalytic sites. Furthermore, the porous architecture derived from the ZIF precursor contributes to improved electrolyte accessibility and mass transport. The improved electrocatalytic behaviour is associated with efficient charge transfer, increased electrochemically active surface area, and the presence of defect-rich active sites. These findings demonstrate that ZIF-derived carbon-based hybrids are promising candidates for high-performance HER electrocatalysis.

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NMSF-ENM-052

Dynamic Scaling Theory in Semiconductor Thin Films: Insights and Advances

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Abstract

Thin films play an important role for the advancement of semiconductor technologies toward miniaturization and high-performance devices. The surface morphology on the nanoscale is known to strongly influence electronic, optical and mechanical properties; thus, growth dynamics dictates the morphology. Dynamic Scaling Theory (DST) describes the evolution of roughness on deposited surfaces in terms of system size and growth time. In this review, I focus on kinetic roughening in thin films, with particular emphasis on deposition parameters such as growth rate and film thickness. Competing behaviors have emerged from a variety of experimental methods (e.g., Atomic Force Microscopy (AFM), roughness analysis), such as anomalous scaling that encodes the multi-scale character of the growth process. It starts with the Family–Vicsek (FV) model, a minimal model with rapid predictions about certain kinds of roughening evolution and the link between smoothing mechanisms and fluctuations. However, electrodeposited films have been less studied up until now due to the fact that they were generally made by vacuum-based methods like evaporation and sputtering. Ion transport, electric fields and surface diffusion, these not only have a quantitative effect on electrodeposition (in particular its rate, growth state), but it also really determines the film's final form. It is crucial to expand research on electrodeposited films now in order to tailor current morphologies to meet those demanded of modern semiconductors.

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NMSF-ENM-053

Thickness Optimization and Simulation Study of a MAPI Perovskite Solar Cell

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Abstract

Perovskites emerged as one of the most promising materials for next-generation photovoltaic technology, due to their exceptional optical absorption and tunable bandgap. Power conversion efficiency (PCE), and hence the device performance is influenced by individual layer thicknesses specially the active layer or the perovskite layer.

In this study, we present a simulation-based investigation of thickness optimization in a planar MAPI (methyl ammonium lead iodide) perovskite solar cell using Oghmanano software (formerly known as gpvdm). The device architecture consists of FTO/TiO_2 (ETL)/MAPI (absorber)/Spiro (HTL)/Au (back contact layer). Layer thickness variations were performed for the perovskite absorber layer in the range of 200 to 600 nm, and photovoltaic parameters — open-circuit voltage (Voc), short-circuit current density (J_{sc}), fill factor (FF), and PCE — were extracted and analyzed.

Simulation results indicate that absorber layer thickness significantly influenced PCE, which ranges from 15.84 to 24.46%. The simulation study is a cost effective way to achieve the high performance configuration before fabrication.

Keywords: *Perovskite Solar Cell, MAPI, Oghmanano, Thickness Optimization, Power Conversion Efficiency*

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Oblique Ar^+ Irradiation Induced Structural, Morphological and Optical Modifications in ZnTe Films

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Abstract

ZnTe thin films deposited on Si (100) substrates were irradiated with 95 keV Ar^+ ions at a fixed fluence of 7×10^{17} Ar^+ cm^{-2} under varying angles (0°, 30°, 45°, 55°, 65°). The effect of irradiation angle on structural, morphological and optical properties was investigated. X-ray diffraction results show a reduction in peak intensity with increasing angle, indicating decreased crystallinity and ion-induced disorder, along with changes in crystallite size, micro strain, and dislocation density. The emergence of the Si (100) peak suggests sputtering-induced thinning of the ZnTe layer. Atomic force microscopy reveals a transition from smooth surfaces to ripple morphology at higher angles (55°and 65°), attributed to curvature-dependent sputtering. Diffuse reflectance measurements indicate a significant increase in reflectance in the shorter wavelength region after ion-irradiation, along with a variation in optical band gap, as estimated from Kubelka-Munk analysis, indicating defect-induced modification of the electronic structure. These findings highlight the potential of ion beam engineering for tailoring ZnTe thin films for applications in optoelectronic devices, surface patterning, and nanoscale photonic structures.

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NMSF-ENM-055

Biosynthesized Mn_2O_3 Nanoparticles for Enhanced Sunlight-Driven Photocatalytic, Antibacterial, and Antioxidant Activities

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Abstract

Organic pollutants in wastewater pose a major threat to the environment and human health, making it important to develop effective removal techniques. Photocatalysis is an effective, cost-effective and environmentally friendly method for the elimination of pollutants with low secondary waste production. In this regard, biosynthesis has emerged as an eco-friendly and sustainable approach to produce photocatalysts, as it doesn't require high energy, it's non-toxic and it enhances the surface properties of the catalyst, leading to enhanced activity. In this study, Mn_2O_3 nanoparticles were synthesized via a green co-precipitation approach utilizing *Allahabad Safeda* extract as a natural reducing and stabilizing agent. The as-prepared nanoparticles were systematically characterized to evaluate their structural, morphological, compositional, thermal, and optical properties. Techniques including X-ray diffraction (XRD), transmission electron microscopy (TEM), energy-dispersive X-ray analysis (EDAX), thermogravimetric and differential scanning calorimetry (TGA-DSC), and UV-Visible spectroscopy. Structural and morphological analyses confirmed that the synthesized nanoparticles possess a cubic bixbyite-type crystal structure with predominantly spherical morphology and an average crystallite size of approximately 11.2 nm. Optical analysis indicated that the biosynthesized Mn_2O_3 nanoparticles exhibit strong absorption in the visible region, with an estimated band gap of 2.94 eV. Photocatalytic investigations revealed that the biosynthesized nanoparticles achieved approximately 90% degradation of RhB dye within 60 min under irradiation. Furthermore, antibacterial and antioxidant assays demonstrated notable biological activity of the prepared nanoparticles. Overall, the results indicate that Allahabad Safeda-mediated Mn_2O_3 nanoparticles exhibit enhanced photocatalytic efficiency along with significant antibacterial and antioxidant properties, highlighting their potential for sustainable environmental and biomedical applications.

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NMSF-ENM-056

Exploration of Structural Phase Stability and Mechanical Response of Transition Metal Carbides at High Pressure

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Abstract

We have investigated the structural stability and elastic properties of four transition-metal carbides (TMCs), namely TiC, NbC, HfC, and TaC, using a temperature-dependent realistic interaction potential (RIP) formalism. These compounds exhibit a pressure-induced structural phase transition from the NaCl-type (B1) structure to the CsCl-type (B2) structure at relatively higher pressures compared to many other binary systems. The transition pressures, corresponding volume collapses, and elastic parameters were evaluated under ambient conditions and show good agreement with available experimental data and previous theoretical studies. In order to validate the reliability of the RIP approach, electronic structure calculations based on density functional theory (DFT) were computed which includes the analyses of the band structure and density of states, carried out using the Quantum ESPRESSO package.

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NMSF-ENM-058

Eco-Friendly Carbon Dots from Ipomoea aquatica as Sustainable Electrode Material for Supercapacitor Applications

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Abstract

Carbon dots (CDs) were successfully prepared from Ipomoea aquatica (Water Spinach) employing a green, chemical-free hydrothermal process. The CDs prepared were comprehensively characterized by UV–Vis absorption, PL emission, FTIR, XRD, DLS, and zeta potential. The UV–Vis spectrum demonstrated a characteristic peak at around 268 nm, whereas the PL spectra showed prominent blue fluorescence under UV light excitation. FTIR spectra indicated rich surface functional groups like hydroxyl, carboxyl, and carbonyl, which are responsible for increased hydrophilicity and electrochemical activity. XRD patterns demonstrated amorphous carbon morphology, and DLS indicated particle sizes in the 6–10 nm range. The zeta potential value of –31mV revealed excellent colloidal stability. Electrochemical performance was assessed through a CRO-based cyclic voltammetry (CV) system, and the CDs showed close to rectangular CV curves at varying scan rates, verifying electric double-layer capacitive (EDLC) characteristics. The results indicate the promise of Ipomoea aquatica-derived carbon dots as eco-friendly, low-cost electrode materials for energy storage in supercapacitor devices.

Keywords: *Carbon dots, Ipomoea Aquatica, Green Synthesis, Supercapacitor, Energy Storage, CV Analysis*

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NMSF-ENM-059

Hydrothermal Synthesis of Carbon Dots from Mixed Aquatic Plant Biomass: Optical and Structural Characterization

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Abstract

Carbon dots (CDs) are an emerging class of fluorescent carbon-based nanomaterials known for their superior photostability, biocompatibility, and environmentally friendly synthesis routes. In this work, CDs were synthesized via a green hydrothermal process using a mixed aquatic plant biomass composed of Eichhornia crassipes [EC] and Ipomoea aquatic [IA] in a 1:1 ratio. The use of mixed biomass precursors aims to exploit the synergistic interaction of different phytochemical compositions to enhance the optical and structural characteristics of the resulting CDs. The synthesis involved direct hydrothermal treatment of the blended plant material without addition of toxic passivation or doping agents, thereby maintaining the eco-friendly nature of the process. The prepared mixed biomass-derived CDs (Blend-CDs) were comprehensively characterized using SEM-EDX, UV–Visible (UV–Vis) spectroscopy, photoluminescence (PL) spectroscopy, Fourier-transform infrared (FT-IR) spectroscopy, and X-ray diffraction (XRD) analysis, TGA and electrochemical studies. The SEM-EDX analysis confirmed the nanoscale morphology and carbon-rich composition with homogeneously UV–Vis spectrum exhibited characteristic absorption bands attributed to n–π^* transitions of C=O groups, along with a weak broad shoulder in the visible range associated with surface defect states. PL spectrum revealed strong excitation-dependent emission behaviour, with maximum emission observed in the blue and cyan regions, arising from radiative recombination at surface defect states and functional groups. FTIR spectrum confirmed the presence of hydrophilic functional groups such as –OH, –CO, indicating good aqueous dispersibility and potential for surface-mediated interactions. XRD analysis indicated a predominantly amorphous carbon phase with a broad peak around $2\theta \approx 28°$, along with minor crystalline features likely arising from residual mineral components in the biomass. The TGA analysis indicated high thermal

stability with a substantial amount of carbon residue at higher temperatures. The electrochemical analysis revealed high stability, reversibility, and a combination of EDLC and pseudocapacitive properties, confirming the high suitability of the biomass-derived carbon dots as efficient electrodes for supercapacitors. The results highlighted that using a mixed aquatic plant precursor not only offers a sustainable pathway for CD production but also enables tuning of their physicochemical properties through precursor composition. This approach opens new possibilities for developing cost-effective, environmentally benign nanomaterial for the applications in photocatalysis, sensors and water purification.

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NMSF-ENM-060

Life Cycle Assessment of Waste Biomass-Derived Biopolymeric Films: Environmental Impact Evaluation

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Abstract

Life Cycle Assessment (LCA) is a systematic and scientifically grounded methodology used to evaluate the environmental impacts associated with a product, process, or system across its entire life cycle. In the context of bioplastic production, LCA plays a critical role in assessing sustainability by considering all stages, from raw material cultivation and biopolymer synthesis to processing, usage, and end-of-life disposal or recycling. Unlike conventional assessment approaches that focus on isolated stages, LCA adopts a comprehensive "cradle-to-grave" perspective, enabling the identification of hidden environmental burdens such as upstream agricultural inputs, energy consumption, and downstream waste generation. Standardized under ISO 14040/44 guidelines, LCA comprises four key phases: goal and scope definition, life cycle inventory (LCI), life cycle impact assessment (LCIA), and interpretation. These stages collectively facilitate the quantification of resource inputs (e.g., biomass, water, and energy) and outputs (e.g., emissions, effluents, and solid waste), and translate them into environmental impact categories such as global warming potential, eutrophication, acidification, and resource depletion. In bioplastic systems, LCA is particularly valuable for comparing environmental performance against conventional petroleum-based plastics. It helps determine whether bioplastics genuinely reduce greenhouse gas emissions and fossil resource dependency when factors such as land use, fertilizer application, and processing energy are accounted for. Additionally, LCA highlights critical hotspots, including feedstock cultivation and end-of-life management, thereby guiding improvements in process efficiency, material selection, and waste handling strategies. Overall, LCA serves as a robust decision-support tool in advancing sustainable material development. By integrating environmental metrics with technological innovation, it supports the transition toward a circular economy and promotes environmentally responsible production practices. The application of LCA in bioplastic production thus contributes significantly to achieving global sustainability and climate goals.

Keywords: *Life Cycle Assessment, Biopolymers, Sustainability, Environmental Impact, Circular Economy*

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NMSF-ENM-061

Structural, Morphological, and Electrochemical Analysis of $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ Spinel Oxide for Supercapacitor Electrodes

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Abstract

This study investigates the structural and electrochemical properties of ternary $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ spinel oxides synthesized through a modified combustion method using citric acid fuel for supercapacitor applications. X-ray diffraction (XRD) analysis confirmed the successful formation of a cubic spinel phase, while Scanning Electron Microscopy (SEM) revealed a morphology characterized by densely packed, agglomerated particles with an average size of approximately 155 nm. The electrochemical characteristics of the $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ electrode, deposited on a carbon substrate, were evaluated via Cyclic Voltammetry (CV) in a 1 M KOH electrolyte within a potential window of –0.1 V to 0.4 V. The resulting CV profiles exhibited a near-rectangular geometry, indicative of electric double-layer capacitive (EDLC) behaviour. Notably, the incorporation of Ketjen Black (KB) as a conductive additive enhanced the current density to approximately 0.03 mA/cm^2, suggesting significantly improved electron mobility and charge transfer kinetics. These results demonstrate that $Ni_{0.6}Co_{0.3}Fe_{0.1}O_4$ serves as a highly effective and promising electrode material for the development of advanced energy storage systems.

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NMSF-ENM-062

Urea-Mediated Seawater Electrolysis Enabled by Durable Fe-doped NiTe Nanowire Electrocatalysts

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Abstract

Direct saltwater electrolysis is suggested as a possible low-cost method of producing green hydrogen by utilising the abundance of seawater and the extensive use of offshore renewable energy. To address the sluggish kinetics of the oxygen evolution reaction (OER), urea oxidation reaction (UOR) is employed, offering a low-energy alternative to conventional water electrolysis and significantly reducing energy input. Nonetheless, creating effective, naturally occurring electrocatalysts that can withstand severe corrosive environments for an extended period of time remains a formidable technical obstacle. Herein, we report the successful fabrication of Fe-doped NiTe nanowire electrode via one pot hydrothermal method approach. The proposed electrocatalyst exhibits remarkable activity and durability for HER, OER and UOR in alkaline seawater, with overpotentials of 250 mV vs RHE for HER, 1.70 V vs RHE for OER and 1.39 V vs RHE for UOR at 100 mA cm^{-2} current density, and stability of over 100 h. The Fe-doped NiTe also exhibits good bifunctional catalytic performance for water and urea electrolysis. The bifunctional Fe-NiTe electrode pair can efficiently catalyze the overall water electrolysis at a potential of 2.01 V and urea-mediated alkaline-saline water electrolysis under 1.78 V at 100 mA cm^{-2} for 100 h without notable performance degradation, demonstrating its strong potential for scalable, energy-efficient, and sustainable hydrogen production.

Keywords: *Alkaline Seawater Electrolysis; Urea Oxidation Reaction, Hydrogen Production*

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NMSF-ENM-063

Role of Cerium Oxide on Physical, Structural and Optical Characteristics of Boro-Phosphate Glasses

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Abstract

Two boro-phosphate glass samples, one without cerium oxide (CeO_2) and other with 1.0 % content in mole percent of CeO_2, were synthesized using the conventional melt-quenching technique to investigate the effect of CeO_2 on their physical and optical properties. The physical parameters of the prepared glasses were evaluated through density measurements using the Archimedes principle, and the corresponding molar volume values were calculated. The experimental results reveal an increase in density accompanied by a decrease in molar volume with incorporation to CeO_2 content, indicating enhanced structural compactness of the glass network. Optical absorption spectra were recorded in the ultraviolet–visible region in the wavelength range 300–900 nm to analyze the optical response of the glass system. Distinct absorption features related to cerium ions were observed, confirming the incorporation of CeO_2 into the glass matrix. The absorption band observed in the ultraviolet region between 300–380 nm is attributed to the allowed $4f^1 \rightarrow 5d^1$ electronic transition of Ce^{3+} ions. The optical band gap values are determined from Tauc's plots. Other optical parameters, viz. refractive index, polarizability etc were also calculated. The experimental findings demonstrate that cerium oxide has modifying the physical, structure and optical characteristics of boro-phosphate glasses, highlighting their potential applicability in optical and photonic devices.

Keywords: *Boro-Phosphate Glasses, Cerium Oxide, Density, Optical Band Gap, Refractive Index, Optical Properties*

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NMSF-EPM-001

Electrical Switching Properties of Chemically Synthesized Ag:CdS-PVK Nanocomposite

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Abstract

Memristive devices have shown a promising potential for next generation computing systems as they offer high density, nonvolatility, low power consumption and multiple memory capacity. Recently, polymer nanocomposites exhibit functionalities which can closely resemble with biological synapses. Extending our earlier work, the present work focuses on the electrical switching properties of the two-terminal device with Ag doped CdSe-PVK nanocomposite as an active layer. Ag doped CdSe-PVK nanocomposite was synthesized by using ex-situ chemical technique. XRD spectra reveals the cubic zinc blende structure of the polymer nanocomposite with diffraction peaks corresponding to (111), (220) and (311) planes. UV-Vis absorption data also shows the successful synthesis of polymer nanocomposite. The value of optical band gap calculated by using Tauc relation is 2.12 eV. The pinched hysteretic behavior in the Current-voltage characteristics confirms the memristive behavior of the fabricated device. Electrical switching is due to the charge storage and tunneling through the CdSe and PVK matrix, respectively. The present outcomes can be useful for optimizing the performance of these devices for future computing applications.

Keywords: *Polymer Nanocomposite, Doping, Electrical Switching, Hysteresis*

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NMSF-EPM-002

Development and Characterization of Lead-Free $BaTiO_3$-$Na_{0.5}Bi_{0.5}TiO_3$ Perovskite Ceramics for Electronic Applications

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Abstract

The increasing demand for environmentally safe and high-performance electronic materials has driven significant research toward lead-free perovskite ceramics. In this study, lead-free ceramics based on the 1-x ($(Na_{0.5}Bi_{0.5}TiO_3)_{1-x}(BaTiO_3)_x$) system (x = 0.0, 0.1, 0.2, 0.4) were synthesized using the conventional solid-state reaction method. The prepared ceramics were systematically investigated through structural, dielectric, and impedance analyses to evaluate their functional properties and application potential. X-ray diffraction (XRD) confirmed the formation of perovskite phase structures and revealed a composition-dependent structural transition from rhombohedral to tetragonal symmetry. Dielectric studies exhibited strong frequency and temperature dependence of permittivity along with relaxor ferroelectric behavior, indicating suitability for capacitor and actuator applications. Impedance spectroscopy showed negative temperature coefficient resistance (NTCR) behavior and identified distinct contributions from grains and grain boundaries through Nyquist and electric modulus analyses. The electrical behavior was further explained using the Havriliak–Negami model and Arrhenius-type conduction mechanism, suggesting thermally activated charge transport. The results demonstrate that compositional variation significantly influences the structural and electrical properties of the material, making these lead-free ceramics promising candidates for sustainable electronic devices.

Keywords: *Lead-Free Pervoskite Ceramics, BNT-BT System, Dielectric Properties, Impedance Spectroscopy, Sustainable Electronics*

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NMSF-EPM-003

Temperature Dependent Electrical Transport of NiO Thin Films Grown by RF Magnetron Sputtering

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Abstract

Nickel oxide (NiO) thin films are of great interest as p-type wide band gap semiconductor for electronic and optoelectronic device applications. In this work, we have grown NiO thin films on single crystal (001) sapphire substrates at room temperature by rf magnetron sputtering. Structural, optical, morphological and temperature dependent electrical resistivity measurements were performed on NiO thin films of variable thickness ~ 40 – 100 nm. The optical band gap of as grown thin films was found to be in the range of ~3.3 eV to ~3.5 eV. Grazing incidence X-ray diffraction pattern revealed that NiO films were polycrystalline in nature having a cubic phase and the observed diffraction peaks were assigned to be at (111), (200) and (220) planes. It is found that the film crystallinity improves with increasing thickness as evident from the increase in peak height and decrease in peak broadening. Surface morphology measurements were performed using scanning electron microscopy. The surface of thinner films was found to be relatively smooth as compared to thicker films which indicates the presence of more compact and well-defined grainular structure in thicker films. Temperature dependent electrical resistivity measurements revealed semiconducting behaviour, with resistivity values decreasing monotonically with increasing temperature. Electrical transport data were analysed over the entire temperature range based on various conduction models. In the high-temperature region, the conduction follows a small polaron hopping mechanism, indicating thermally activated transport of localized carriers. In contrast, at lower temperatures, the resistivity data were well described by Mott's variable range hopping model, suggesting carrier transport through localized states over variable distances. Results of these studies will be systematically presented and discussed at the conference.

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NMSF-EPM-004

Optical Properties of Mn^{4+} Activated $CaSrAl_2SiO_7$ Phosphors

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Abstract

A series of novel deep red lighting emitting $CaSrAl_2SiO_7$:xMnˆ4+ phosphors were synthesized in air atmosphere by using conventional high temperature solid state reaction process. Synthesis of as prepared phosphor was checked by X-ray diffraction (XRD) analysis. Concentration dependent thermoluminescence (TL) and photoluminescence (PL) were systematically investigated. TL investigation of synthesized phosphor was done after exposure time of UV radiation of 254 nm. Concentration quenching was observed in TL investigation. Optimum TL glow curve was deconvoluted and TL parameters were estimated for all the deconvoluted peaks. PL excitation spectra consist of an intense peak at around 440 nm and PL emission spectra have an intense peak at near 663 nm and a less intense peak at around 690 nm which belongs to deep red region. PL analysis results that $CaSrAl_2SiO_7$: Mn^{4+} phosphor may be applicable for red LEDs useful for growth of the plant, driving photosynthesis and energy creation, stimulating flowering, budding and stem/leaf development.

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NMSF-EPM-005

"Spectator Exciton" Effects on Quantum Confined Nanocrystals

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Abstract

Quantum-confined $CsPbBr_3$ nanocrystals exhibit unique photophysical properties, including particle size-dependent brightness of the lowest-lying exciton state and appearance of unusual photoinduced absorption bands in relaxed mono-exciton transient absorption. Given recent studies that contest this, similar samples are revisited here by comparing time-resolved fluorescence and wavelength-dependent three-pulse "spectator exciton" experiments. Results clarify the long-term debate regarding bi-exciton interaction, which is indeed strongly attractive. Hot exciton cooling following recombination of several excitons is found to be prolonged from less than one to several picoseconds, slower even than bi-exciton recombination itself. Using the 3-pulse "spectator exciton" method, we have determined the cross-section for stimulated emission from the relaxed single excitons in quantum-confined perovskite nanocrystals, even in overlapping continued absorption at the band edge [1]. In the second part, I will present the results of "spin-blockades" phenomena in CdTe-based QDs. Spin orientation conflicts between hot and cold electrons in the same doubly excited nanocrystal were shown to block the former from relaxing to the band edge [2]. This blockage was ultimately overcome by phonon-assisted flipping of the hot carrier's spin, allowing it to pair with its band edge counterpart within tens of picoseconds.

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NMSF-EPM-007

Synthesis & Characterization of Magnetite & Cobalt Ferrite Magnetic Nanoparticles for Removal of Heavy Metal Ions from Wastewater using Co-Precipitation Technique.

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Abstract

Urbanization and human activities near water bodies are the primary contributors of heavy metal discharge into the water. The ecosystem and human health have been negatively affected when drinking water sources are contaminated with heavy metals. Copper (Cu), arsenic (As), lead (Pb), zinc (Zn), cadmium (Cd), mercury (Hg), chromium (Cr), etc. are some of the heavy metals that are typically utilized. Humans, plants, and animals are all at risk from the heavy metal ions since they are readily absorbed by living organisms through water and disperse throughout the food chain. There are numerous ways to remove heavy metals from water, including chemical precipitation and coagulation, electrochemical techniques, photocatalytic degradation, membrane filtration, ion exchange, bioremediation, and adsorption. In this work, Magnetite (Fe_3O_4) and Cobalt Ferrite ($CoFe_2O_4$) was synthesized using Co-precipitation method. XRD, SEM, EDS techniques were used to characterize the shape, structure, and chemical analysis of the nanoparticles. To study the surface and functional characteristics, FTIR & BET surface area characterization was carried out. Finally, using Langmuir Isotherm model, the adsorption and performance studies was carried out. Various factors influencing the adsorption of metal ions, e.g., pH, temperature, and contacting time were investigated to optimize the operating condition for the use of Magnetite (Fe_3O_4) and Cobalt Ferrite ($CoFe_2O_4$) nanoparticles as adsorbent. The experimental results indicated that the adsorption is strongly influenced by pH and temperature, the effect depending on the different metal ion considered.

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NMSF-EPM-008

Multiexciton Generation and Electron Transfer in Semiconductor Quantum Dots-Molecule Hybrid

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Abstract

Metastable multi-excitonic states (MES) of semiconductor quantum dots can be involved in multi-electron transfer reaction, which opens new perspectives in nanomaterials-based opto-electronic applications. Here, we will discuss the generation of MES in $CsPbBr_3$ perovskite quantum dots (PQD) and its dissociation dynamics through multiple electrons transfer to molecular electron acceptors, anthraquinones (AQs), bound to the PQD surface by carboxylic anchor. As many as 14 excitons are produced at excitation density of roughly 220 μJ cm$^{\check{}2}$ without detectable PQD degradation. Addition of AQ results in formation of PQD-AQ hybrids with excess of AQs (PQD : AQ $\approx$ 1 : 20), which opens the possibility of multi-electron transfer acts from MES to AQs. It was found that the electron transfer saturates after roughly five transfer acts and the first ET time constant as short as 1 ps. However, each ET increases Coulomb potential barrier for the next ET, which decreases the rate of ET resulting saturation after five ETs.

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NMSF-EPM-009

Ferrimagnetic Ordering in the V-Cr Prussian Blue Analogue

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Abstract

Prussian blue analogues (PBA) represent a versatile family of molecule-based magnets whose transition temperatures and magnetic properties can be systematically tuned by judicious choice of transition metal ions and their oxidation states within a robust cyanide-bridged framework. Structural and magnetic properties are reported for PBA $VO[Cr(CN)_6]_{2/3} \cdot 1.7H_2O$, synthesized via a coprecipitation method. This compound possessed a face-centered cubic structure (space group $Fm\bar{3}m$ with a lattice parameter of 10.48(8) Å, as confirmed by Rietveld refinement of x-ray diffraction data. Infrared spectroscopy reveals a characteristic CN stretching frequency at 2177 cm^{-1}, consistent with bridging $V^{4+}-CN-Cr^{3+}$ linkages. DC magnetization measurements indicate a ferrimagnetic ordering below $T_C \approx 102$ K, arising from antiparallel superexchange coupling between V^{4+} ($S = 12$) and Cr^{3+} ($S = 32$) ions mediated through the cyanide $2p_\pi$ molecular orbitals. The experimentally observed effective paramagnetic moment ($\mu_{\text{eff}} = 3.6\,\mu_B$ formula unit) and maximum magnetization ($M_{\max} = 0.98\,\mu_B$/formula unit at at temperature 5 K and 11.5 Tesla) are in excellent agreement with the theoretically expected spin-only values of $3.61\,\mu_B$/formula unit and $1\,\mu_B$/formula unit, respectively, confirming the V^{4+} oxidation state. The compound exhibits a low coercive field of 62 Oe. A comparative analysis with other V–Cr based PBAs demonstrates that the transition temperature is strongly sensitive to the oxidation state of the vanadium ion, with V^{2+} and V^{3+} variants yielding significantly higher T_C values, in some cases exceeding room temperature. The present study highlights the role of metal ion oxidation state as a key tunable parameter in designing PBAs for molecular electronics applications.

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NMSF-EPM-010

A Comparative Analysis of Transparent Conducting Thin Films (Sn-Doped ZnO) for Future Optoelectronics Applications

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Abstract

In this study, Sn-doped Zinc Oxide (ZnO) thin films were synthesized on glass substrates using thermal evaporation, followed by annealing at 400 °C for one hour. Doping concentrations 6% of tin (Sn) were introduced to investigate the impact on the film's structural, morphological, optical and electrical properties.The polycrystalline hexagonal wurtzite structure was validated by X-ray diffraction (XRD) analysis. Field Emission Scanning Electron Microscopy (FESEM) provided detailed surface morphology, revealing uniform grain distribution and reduced particle size with increasing Sn content presence, which was further validated by Energy Dispersive X-ray Spectroscopy (EDAX) analysis.According to optical analysis, the direct band gap decreased somewhat (from 3.22 eV for pure ZnO to 3.18 eV for doped films), indicating that the optical properties of the film might be tuned. Electrical measurements revealed a significant enhancement in conductivity, ranging from 0.2994 to 1.3698 ($10^{-6}\,\Omega^{-1}\,\mathrm{cm}^{-1}$) as Sn concentration increased. For use in next-generation optoelectronic devices such light-emitting diodes (LEDs), transparent thin-film transistors (TFTs) and photovoltaic systems, these findings show that Sn-doped ZnO thin films have intriguing properties.

Keywords: *Thermal Evaporation Technique,* ZnO : Sn *Thin Films, Electrical Conductivity, Optical Band Gap, Transmittance*

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NMSF-EPM-011

Study on Synthesis and Characterization of Nanocrystalline CuS Film by Slurry Coating Method

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Abstract

CuS film was deposited via the slurry coating method using commercially available CuS powder. XRD and Raman study indicated the evolution of pure covellite hexagonal phase of CuS. SEM study of the film revealed the voids between the particles. From EDX study, the individual at % of Cu and S in the film was estimated. The optical band gap ascertained from the diffuse reflectance spectrum study conveyed that the film has direct band gap of 2.24 eV. The D.C. resistivity variation with reciprocal of temperature for the film communicated that resistivity drops with temperature substantiating the semiconducting behavior of the film. The Hall effect study at room temperature conveyed the p-type conductivity for the film.

Keywords: *Thin films, Slurry coating, DC resistivity, Hall Effect*

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Spin Dynamics of $Fe(phen)_2(NCS)_2$ Spin Crossover Complex in Ethylene Glycol Matrix Probed by Electron Paramagnetic Resonance

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Abstract

Spin-crossover (SCO) materials exhibiting reversible switching between high-spin (HS) and low-spin (LS) states are of considerable interest for spin-based electronic applications. In this work, spin-state bistability and spin-transition behavior of the SCO complex $Fe(phen)_2(NCS)_2$ embedded in an ethylene glycol (EG) matrix were investigated. The composite was synthesized using a wet chemical method. Spin transitions were probed through electrical and magnetic measurements. Current–voltage (I–V) characteristics measured at 300 K and 90 K reveal thermally driven HS $\leftrightarrow$ LS switching accompanied by a pronounced hysteresis loop. At 90 K, the complex stabilizes in the LS state and exhibits higher electrical conductivity, whereas at 300 K it remains in the HS state with reduced conductivity. Time-dependent current (I–t) measurements under dark and illuminated conditions at both temperatures show an enhanced photoinduced response at lower temperature. Due to reversible, stimulus-induced transitions, these systems undergo switching between distinct magnetic states, such as low-spin/high-spin or diamagnetic/paramagnetic configurations. Therefore, Electron paramagnetic resonance (EPR) provides direct, spin-state sensitive insights into the behavior of unpaired electrons and their local environments. Variable-temperature EPR spectra show clear spin-state switching with distinct differences between the SCO and EG-embedded SCO systems. The embedded sample exhibits suppression of some high-spin features and a reduced spin state transition temperature, indicating matrix-induced stabilization of the low-spin state. These results highlight the role of the ethylene glycol matrix in modulating spin dynamics and intermolecular interactions.

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Keywords: *Spin crossover, Electron paramagnetic resonance, spin state switching*

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NMSF-EPM-013

Systematic Analysis of Chitosan Coated MFe_2O_4 (M=Co, Ni, Zn) Quantum Dots/Nanocomposites Prepared by Co-Precipitation Route

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Abstract

The chitosan (Chi) coated MFe_2O_4 (M=Co, Ni, Zn) (Chi@CoF, Chi@NiF, and Chi@ZnF) quantum dots (QDs) /nanocomposites (NCs) were synthesized by the co-precipitation route. X-ray diffraction (XRD) patterns of the MFe_2O_4 NCs confirm phase analysis with cubic structure. Increased lattice parameters of the cubic structure of the prepared MFe_2O_4 NPs indicating the expansion of the lattice. The average crystallite size of 15.9±0.2, 2.6±0.06, and 3.3±0.08 nm was evaluated for highest intensity peak (311) of the XRD patterns of the MFe_2O_4 NPs. The highest value of lattice strain (139.4), and dislocation density (647.8 nm-2) was estimated from the XRD pattern for Chi@NiF NPs. The mean particle size of 15.3±0.3, 3.32 ±0.02, and 3.47±0.06 nm was evaluated for Chi@CoF, Chi@NiF, and Chi@ZnF NPs, respectively with the spherical shape morphology. X-ray photoelectron spectroscopy (XPS) was used to observe the oxidation states of Fe, Ni, Co and O present in the prepared NCs samples. The saturation magnetization (58.80, 6.55, 9.04 emu/g), coercive field (823,15.5,18.08 Oe), and remanance (18.72, 0.0022, 0.0037 emu/g) were reported for Chi@CoF, Chi@NiF, and Chi@ZnF NPs, respectively. The prepared MFe_2O_4 NPs were employed on MCF -7, and MDA − MB − 231 cell lines of the Breast cancer (BC).

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Interface-Driven Phase Tailoring of PVDF/Fe_3O_4 Nanocomposites for Sustainable Low-Frequency Energy Harvesting

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Abstract

Piezoelectric nanogenerators are emerging as sustainable energy solutions for harvesting ambient mechanical energy. This study enhances energy conversion efficiency through interfacial mechanisms and controlled phase transition. Structural and morphological analyses confirmed a significant transformation from the nonpolar α-phase to the electroactive β-phase upon adding Fe_3O_4 nanoparticles at optimal loading conditions. FTIR studies revealed that the composites contain 81% β-phase. The enhanced dielectric response of the composite is attributed to interfacial polarization, which improves charge storage and transfer. This study demonstrates the coupling between magnetic nanoparticle-induced phase evolution and enhanced output from piezoelectric nanogenerators (PENGs). The direct correlation between nanoparticle-induced phase evolution and improved PENG performance highlights an emerging strategy for polymer-based energy-harvesting systems. Compared to pure PVDF films, the fabricated composites exhibited a higher electrical output under low-frequency excitation. The PENG generated an output voltage of 6V, capable of powering various LEDs. This study presents a scalable pathway for designing multifunctional materials for real-world, low-frequency energy-harvesting applications.

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NMSF-EPM-016

Electrical Characterization of Junction Device Fabricated on GaSb Substrate

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Abstract

Device grade III-V direct band gap semiconductor Gallium Antimonide, p-GaSb was developed by the vertical directional solidification (VDS) technique. Once required crystalline, electrical, optical and morphological characterization of the substrate was accomplished, it was subjected to Tellurium implantation for the type conversion of u nmasked area. Some of the substrates were irradiated with 200 K eV Lithum ions that created ion-traps and optimized the carrier concentration prior to the implantation. Both irradiated and as grown substrates were implanted by Tellurium at 100 and 50 KeV energies and multiple particle flux of 1.8×10^{14} and 2×10^{15} ion/cm^2. The as-implanted and annealed samples were characterized for electrical transport at room temperature. I-V As well as C-V profiling exhibited rectification characteristics in all the cases. Optimum ideality factor was obtained for the p-n devices that were irradiated-then-implanted with higher flux 2×10^{15} ion/cm^2 and later annealed.

Keywords: *Vertical Directional Solidification, GaSb, I-V Characteristics*

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NMSF-EPM-017

Negative Differential Resistance in Single Molecular Transistor: The Role of Nonlinear Electron-Phonon Coupling and Rashba Spin-Orbit Interaction

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Abstract

We theoretically study the effects of the non-linear electron-phonon interactions and Rashba spin orbit interaction on the negative differential resistance (NDR) in single molecular transistor (SMT) device using the Keldysh non-equilibrium green function technique in the sequential tunnelling regime. We have employed the Anderson-Holstein (AH) model to describe the SMT device in which a molecular quantum dot with a single energy level with both linear and non-linear electron-phonon interactions and Rashba spin-orbit interaction, symmetrically coupled to two leads. We study the spectral function and differential conductance as a function of bias voltage for different values of non-linear electron-phonon interaction and Rashba spin-orbit interaction comparing to the system without any of these interactions.

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NMSF-EPM-018

Two-Step Spin Crossover with Asymmetric Cooperativity in the Cyanide-Bridged $Fe(py)_2[Ag(CN)_2]_2$ Polymer

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Abstract

Multistep spin-crossover (SCO) materials are promising candidates for high-density molecular memory and switching devices due to their ability to access multiple stable spin states. In this work, we investigate a thermally induced two-step spin transition in the cyanide-bridged coordination polymer $Fe(py)_2[Ag(CN)_2]_2$ using variable-temperature optical absorption spectroscopy and SQUID magnetometry, complemented by Slichter–Drickamer thermodynamic analysis. The optical spectra exhibit four ligand-field absorption bands in the 443–576 nm range, whose temperature-dependent evolution reflects redistribution of spin populations between low-spin (LS) and high-spin (HS) states via an intermediate spin state (IS). The persistence of LS-associated features throughout the transition region provides direct spectroscopic evidence for LS–HS coexistence in the IS state. Magnetic measurements reveal a two-step transition with asymmetric cooperativity: the first step occurs at ~104 K (heating) and ~88 K (cooling) with a hysteresis of ~15 K, while the second step occurs ~145 K with negligible hysteresis. The two-step Slichter–Drickamer model reproduces the experimental behavior and indicates stronger cooperativity at lower temperatures. These results demonstrate the role of lattice-mediated interactions in stabilizing intermediate spin states and highlight the potential of cyanide-bridged SCO materials for multistable molecular switching and information storage applications.

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Keywords: *Two-Step Spin Crossover, Cyanide-Bridged Coordination Polymer, Optical Absorption Spectroscopy, Slichter–Drickamer Model*

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NMSF-EPM-019

Anisotropic Magneto-Chemiresistive Effect: From High-Performance Gas Sensing to Magnetoreception

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Abstract

Magnetic fields can effectively regulate the sensitivity of chemiresistive gas sensors, a phenomenon we term the magneto-chemiresistive effect [1]. Unlike conventional approaches dependent on complex material synthesis, this strategy offers a simple, non-destructive route to high-performance sensing. To investigate this systematically, we developed a custom sensor module integrated with an electromagnet, enabling sensing experiments under precisely controlled magnetic fields [2]. Application of a 1 mT magnetic field enables parts-per-billion (ppb) level detection of nitrogen dioxide (NO_2) by a Fe-doped In_2O_3 sensor that shows no detectable response in the absence of a magnetic field. Under an optimized field of 0.5 mT, the sensor also exhibits a fivefold enhancement in response toward 20 ppm NO_2. We attribute this enhancement to magnetic-field-induced modulation of charge transport and surface adsorption processes, involving spin alignment and modified oxygen species interactions. Validation across diverse sensing materials confirms this as a general strategy for enhancing sensor performance. Building on this concept, we further establish that the magneto-chemiresistive property of magnetite (Fe_3O_4) is anisotropic in nature[3]. We show that the magneto-chemiresistive responses of magnetite towards different analytes vary anisotropically with respect to the strength, direction and inclination of the applied magnetic field, with a magnitude comparable to that of the Earth's field. Our work suggests that biological species that possess magnetite nanocrystals may navigate during migration by effectively 'smelling' the geomagnetic field. This work simultaneously advances gas sensor technology and offers a materials-science framework that may help resolve the long-standing biological mystery of magnetite-based magnetoreception in migratory species.

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NMSF-EPM-021

Competing Interactions and Spin Glass Phenomena in Frustrated Magnetic Oxides

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Abstract

Magnetically frustrated oxides have emerged as a fascinating class of materials owing to their ability to host unconventional magnetic ground states arising from competing interactions and structural complexity. Among these, double perovskites with the general formula A_2BBO_6 constitute an important class, where the ordered or partially disordered arrangement of B-site cations plays a vital role in governing the magnetic ground state. In such systems, the coexistence of ferromagnetic and antiferromagnetic exchange interactions, often mediated through superexchange interactions, hinders the formation of long-range magnetic ordering and instead favors disordered spin configurations. In this work, we study the origin of spin glass phenomena in various nanoparticles and thin films of double perovskite based systems such as Nd_2NiMnO_6 and Dy_2CoMnO_6. Spin glass behavior arises from magnetic frustration induced by competing interactions, cation disorder, epitaxial strain and lattice distortions, leading to a non-equilibrium state characterized by randomly frozen spins below a characteristic freezing temperature. The presence of antisite disorder in double perovskites further enhances the competition between exchange interactions, thereby strengthening the glassy magnetic response. Experimental identification of spin glass behavior is carried out through detailed magnetic measurements, including temperature-dependent magnetization, frequency-dependent AC susceptibility, and time-dependent relaxation studies. Unequivocal signatures such as the bifurcation between zero-field-cooled and field-cooled magnetization curves, the shift in the AC susceptibility peak, and slow magnetic relaxation confirm the existence of metastable spin states. Furthermore, the correlation between structural parameters and magnetic properties is analyzed to understand the microscopic origin of magnetic frustration in these materials. The findings demonstrate that subtle variations in cation ordering, strain and lattice distortions can effectively tune the balance of competing interactions. This study provides valuable insights into glassy magnetism in double perovskites and frustrated oxides, offering potential pathways for designing materials with tailored magnetic disorder for advanced technological applications.

Keywords: *Double Perovskites, Spin Glass, Magnetic Frustration, Cation Disorder, Magnetic Relaxation*

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NMSF-EPM-022

Magnetoelastic Waves in Hexagonal Multiferroic Media

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Abstract

In this work, we study the magnetoelastic waves and hybrid excitations arising from the coupling between magnetic and elastic degrees of freedom in a hexagonal multiferroic system. We develop a complete theoretical framework combining the Landau-Lifshitz-Gilbert (LLG) equation for magnetization dynamics, elastic waves represented via Lagrange equations for lattice deformations and a modified Landau-Khalatnikov (LK) equation for polarization dynamics through free energy functionals incorporating magnetoelastic, magnetoelectric, and elastic interactions. The analysis of dispersion relations reveals strong magnon–phonon coupling and mode hybridization, confirming the presence of magnetoelastic polarons and coherent energy transfer between spin and lattice subsystems. The system is found to be strongly sensitive to the magnetoelastic coupling and it is found that the magnonic branches can be tuned without significantly affecting phononic modes. The results further illustrate the spatial and temporal evolution of displacement, magnetization, and polarization fields under varying coupling strengths, bias fields, and damping parameters. It reveals wave behaviors ranging from harmonic oscillations to localized and nonlinear patterns, including interference and field-induced modulation effects. Phase-space analysis indicates transitions from regular to chaotic dynamics, emphasizing the roles of nonlinearity, anisotropy, and damping in governing wave stability and coherence. Our results provide a comprehensive description of magnetoelastic wave propagation in hexagonal multiferroics and highlight their potential for applications in spintronics, magnonics, and multifunctional device engineering.

Keywords: *Magnetoelastic Waves, Multiferroics, Magnon–Phonon Coupling, Nonlinear Dynamics, Spintronics*

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NMSF-EPM-024

A Theoretical and Experimental Approach Towards the Universal Constants μ_0 and ϵ_0

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Abstract

At the macroscopic scale, electricity and magnetism manifests itself in many a familiar phenomenon that give the force its name. Rather remarkably, a full description of the force of electromagnetism is contained in a rather simple yet elegant set of four relations; called the Maxwell's Equations. These four vector equations encompass all the phenomenon relating to electricity and magnetism as well as what connects them. And yet, the Maxwell's Equations remain incomplete without the presence of seemingly arbitrary physical constants μ_0 and ϵ_0. Thus, there occurs a necessity to study the presence of these constants in order to better understand Maxwell's Equations and hence; and hence it is of significance that we classically derive Maxwell's Equations that tells us the existence of these constants and prove their existence empirically.

The Theoretical Value for Magnetic Permeability for Free Space is $\mu_0 = 1.25663706127 \times 10^{-6}$ T $\cdot$ m/A. The Magnetic Permeability for Free Space at Constant Current Component is $\mu_0 = 1.25614441596219 \times 10^{-6}$ T $\cdot$ m/A.

The Magnetic Permeability for Free Space at Constant Length Component is $\mu_0 = 1.25007861700157 \times 10^{-6}$ T $\cdot$ m/A. The Theoretical Value for Dielectric Permittivity for Free Space is $\varepsilon_0 = 8.8541878188 \times 10^{-12}$ F/m. The Dielectric Permittivity for Free Space at Constant Area Component is; $\varepsilon_0 = 8.89205026122884 \times 10^{-12}$ F/m. The Dielectric Permittivity for Free Space at Constant Distance Component is;$\varepsilon_0 = 8.8764880952381 \times 10^{-12}$ F/m.

This paper aims to theoretically obtain Maxwell's Equations as well as to experimentally obtain the values of universal constants; the vacuum magnetic permeability constant (μ_0) and the vacuum dielectric permittivity constant (ϵ_0) up to a significant degree of accuracy as a means to verify the equations.

$\mu_0 = 1.25663706127 \times 10^{-6}$ T $\cdot$ m/A *and* $\varepsilon_0 = 8.85418781881 \times 10^{-12}$ F/m.

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NMSF-EPM-025

Comparative Study on the Effect of Frequency Response on The DC Resistance of Chromium and Tin Thin Films

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Abstract

Nowadays, thin film technology gives bulk materials' surfaces certain physical and chemical characteristics in almost every industrial industry. This is because improvements in vacuum technology and electric power facilities have increased the technology's range of uses. We have used thermal evaporation in vacuum approach to study the a.c. electrical characteristics of thermally evaporated thin films of tin and chromium. This study covers a frequency range between 30 Hz - 10 MHz at room temperatures of 22 °C, for chromium and tin films of thicknesses 60 nm and 100 nm, respectively. It has been noticed that the effective d.c. resistance as a function of frequency increases with the increase in a.c. source signal voltages for both the metal films.

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NMSF-EPM-026

Giant Electronic Structure Modulation in P-Type $Pb_{1-x-y}Sn_xMn_yTe$ and Ensuring WSM Window at Cryogenic Temperatures

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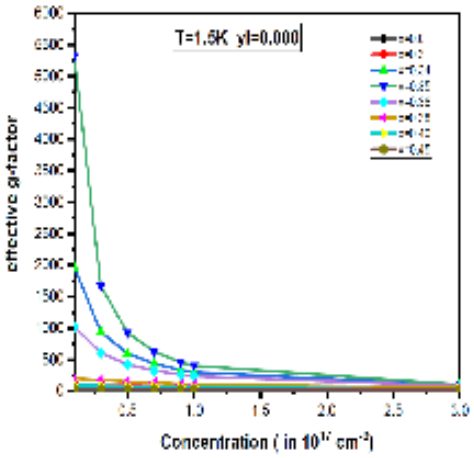
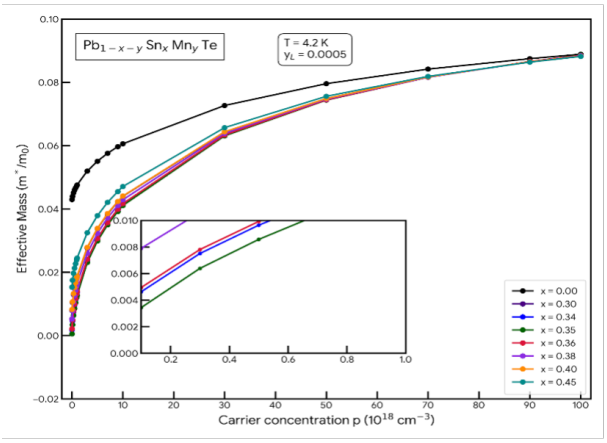
Abstract

The variation in the fundamental threshold is an important band parameter in determining the properties of a semiconductor. The fundamental band gap is a function of impurity concentration, temperature and strain. In this communication, we explored exotic electronic structure modulations of $Pb_{1-x-y}Sn_xMn_yTe$ near band-inversion regions by tuning the fundamental threshold from 1.5K to 12K at cryogenic temperatures. We considered Green's function expansion method by incorporating spin-orbit and p-hybridisation in the presence of a magnetic field. We measured an anisotropic huge effective g factor, specifically g_{eff} = 2713.4, g_{eff}=4255.6, g_{eff}= 3270 and low effective masses; m= 0.00339m_0, m= 0.00331m_0, m= 0.00340m_0 at x = 0.356, x = 0.353, x = 0.351, respectively, within the concentration range of 10^{17} cm^3 to 1018cm^3.Within the temperature range, the values of these electronic parameters are approximately constant with respect to changes in temperature. These values underscore the Weyl Semimetal (WSM) character and are approximately constant over the cryogenic temperature range. The persistence of the WSM state over a wide temperature range establishes the WSM window in this strongly spin-orbit-interacting system and qualifies it for use in temperature-tuned spintronic devices.

Keywords: *$\vec{k}.\vec{\pi}$-method-method method, Spin-orbit Interaction, p-f Hybridisation, Green's Function, Effective g-Factor, Effective Mass*





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NMSF-EPM-027

Interplay of Spin and Charge Density Waves under Magnetic Fields in Iron Pnictide Superconductors

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Abstract

Iron pnictide superconductors, exhibiting transition temperatures up to ~55 K [1], provide a platform for exploring unconventional superconductivity and correlated electronic phases. In contrast to cuprates, their parent compounds display itinerant spin-density-wave (SDW) metallic states associated with stripe-type antiferromagnetism. Understanding the coexistence and competition of electronic orders is crucial for elucidating their superconducting mechanism [2]. In this work, we employ a BCS-type mean-field Hamiltonian model to investigate the influence of an external magnetic field on spin-density-wave (SDW) and charge-density-wave (CDW) orders in underdoped iron pnictides within the normal state regime [3]. The model is treated using Zubarev single-particle Green's functions [4], enabling the derivation of correlation functions and self-consistent determination of temperature-dependent order parameters.

Our results show that SDW and CDW orders can coexist in the underdoped regime, with stability governed by coupling strengths. The associated energy gaps and critical temperatures depend systematically on these interactions. A magnetic field progressively suppresses both orders, indicating sensitivity to external perturbations. The electronic density of states exhibits Zeeman splitting, producing spin-resolved quasiparticle spectra and redistribution of spectral weight near the Fermi level. The field also induces spin dependent band shifts and weakens density-wave-driven band reconstruction. These findings highlight the interplay between magnetic field effects and coupled density-wave orders, showing qualitative agreement with experimental observations [5] and relevance to superconducting and spintronic material applications.

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Keywords: *Iron-Based Superconductors, Spin-Density Wave, Charge-Density Wave, Magnetic Field Effects, Green's Function Formalism*

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NMSF-EPM-028

Cobalt Iron Oxide for a Next-Generation Sustainable Future

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Abstract

Cobalt iron oxide ($CoFe_2O_4$) is a promising candidate for a sustainable next-generation future because of its exceptional thermal, optical, mechanical, chemical, and electrical properties. Additionally, $CoFe_2O_4$ exhibits high coercivity, moderate saturation magnetisation, good corrosion resistance, and good magnetostrictive behaviour. These properties make $CoFe_2O_4$ suitable for next-generation devices for a sustainable future. Emerging technologies, namely nanotechnology, biotechnology, and nanoelectronics, have further amplified their applications through the controlled synthesis of thin films, nanocomposites, nanoparticles, and doped structures. These developments in the synthesis of $CoFe_2O_4$ have opened new opportunities for the manufacturing of high-density data storage devices, gas sensors, supercapacitors, electromagnetic interface shielding, batteries, photocatalysis, and biomedical devices, including targeted drug delivery and magnetic hyperthermia. This review article elaborates on the extraordinary properties of $CoFe_2O_4$, its fabrication techniques, and its applications across diverse fields of emerging technologies.

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NMSF-EPM-030

Functional Magnetic Properties of $YFeO_3$ Single Crystals for Spintronics

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Abstract

Yttrium orthoferrite ($YFeO_3$) with an orthorhombic perovskite structure was synthesized via a conventional solid-state reaction route with stringent control to suppress secondary garnet phase formation, and high-quality single crystals were subsequently grown using the optical floating zone technique. Magnetic characterization revealed a Neel transition (TN) at ~630 K, marking the transformation from long-range antiferromagnetic (AFM) order to a paramagnetic state. In the 300–20 K temperature window, magnetization measurements under zero-field-cooled (ZFC) and field-cooled (FC) protocols exhibited a field-induced metamagnetic transition, with pronounced magnetic anisotropy and enhanced susceptibility under applied fields, indicative of spin canting and weak ferromagnetism inherent to the orthoferrite structure. Below 91 K, well-defined hysteresis loops were observed, confirming stable magnetic domain behavior, whereas at elevated temperatures the loops became constricted and distorted due to thermally driven spin reorientation transitions of Fe_{3+} sublattices. An additional magnetic anomaly near ~600 K suggests the emergence of spin-glass-like dynamics, likely associated with competing exchange interactions and local spin disorder. The temperature dependence of spontaneous magnetization follows Bloch's $T_3/2$ law with a spin-wave parameter B 3.4×10–5 K − 3/2, consistent with magnon excitation behavior. Furthermore, coercivity (HC) exhibited a non-monotonic, wave-like variation with temperature and decreased significantly above ~550 K, attributed to the weakening of AFM domain wall pinning in the presence of weak ferromagnetic interactions, defining a characteristic blocking regime. The overall reduction in saturation magnetization (MS) with increasing temperature is governed by the progressive spin reorientation of canted Fe_{3+} moments, underscoring the suitability of $YFeO_3$ single crystals for advanced spintronic and magneto-functional device applications.

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Synthesis of Magnetic Bio Composites for Efficacious Adsorption of Cr(VI) ions

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Abstract

Release of toxicants from multiple industrial sectors into water streams cause adverse enviornmental effects. Amongst various pollutants, heavy metal (Cr, Zn, Pb, Hg, Ni, Cu & Fe) contamination create numerous health hazards and also affect surface water quality. Magnetic particles are gaining prominence for sorbing toxic materials. This is driven by their expansive surface area and exceptional magnetic properties. This study is focussed on the synthesis of magnetite composite using co-precipitation technique, employing acid / base treated Magnolia champacca Barks (TMCB) and Attapulgite Clay powder (TACP) as precursors to confiscate Cr(VI) ions from aqueous environs. Sequestering ability of these magnetite composites (TMCB@MC and TACP@MC) were juxtaposed against the treated counterparts (TMCB and TACP). Batch Equilibration experimental verification performed for TMCB@MC and TACP@MC – Cr(VI) systems revealed the influence of parameters viz., particle sizes, sorbent dose, initial Cr(VI) concentration, time interval, pH and temperature, optimized for enhanced sorption effectiveness. Composite sorbents when subjected to FT-IR, SEM / EDAX, TG-DTA, VSM and XRD analyses, exposed their nature, targeting the role of functional groups, morphological variations, elemental contribution, temperature withstanding ability and magnetic property. Initial and residual Cr(VI) concentrations in the sorbate solutions were determined using Atomic Absorption Spectrophotometer (Shimadzu AA 6200). From the recorded observations and made comparisons, it is apparent that 97% and 98.6% Cr(VI) removal show augmented sorption capacities of TMCB@MC and TACP@MC which is due to the homogenizing the native materials with the prepared magnetite, effectively showcasing the superior performance of the magnetic composites.

Keywords: *Cr(VI), Magnetite, Precursor, Batch, Parameters*

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Synthesis–Structure–PLQE Correlation in Gd^{3+}-Doped Phosphor Systems

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Abstract

This work presents a systematic investigation of the relationship between synthesis methods, structural characteristics, and photoluminescence quantum efficiency (PLQE) in Gd^{3+}-doped phosphor systems. Phosphor materials based on different host lattices were synthesized using solid-state reaction, combustion, co-precipitation, and hydrothermal routes. X-ray diffraction analysis confirmed the formation of crystalline phases, while variations in crystallinity, crystallite size, and lattice strain were observed depending on the synthesis technique. Complementary FTIR and SEM studies revealed the presence of characteristic functional groups and distinct morphological features, including particle size variation and agglomeration.

Photoluminescence studies exhibited the characteristic ultraviolet emission of Gd^{3+} ions , along with possible host-mediated energy transfer mechanisms. The PLQE was evaluated using integrating sphere measurements and relative spectral analysis. A strong dependence of PLQE on structural quality was observed, where improved crystallinity and reduced defect density led to enhanced emission efficiency. Among the synthesis routes, solid-state and optimized combustion methods showed comparatively higher PLQE values.

The results demonstrate a clear synthesis–structure–PLQE correlation and highlight the importance of controlled synthesis in optimizing luminescent performance. This study provides useful insights for the development of efficient Gd^{3+}-doped phosphors for ultraviolet and photonic applications.

Keywords: *Gd^{3+}-Doped Phosphors; Photoluminescence (PL); Photoluminescence Quantum Efficiency (PLQE); Synthesis methods; XRD; Luminescent Materials; Rare-Earth Ions; Energy Transfer*

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Tailoring the Optical and Structural Properties of SnS Thin Films via Cu- and In- Doping for Sensing Applications

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Abstract

Nanocrystalline pure and Cu-/In-doped SnS thin films were synthesized using the chemical spray pyrolysis technique with controlled dopant concentrations of 3%, 5%, 7%, and 9%. The incorporation of copper and indium was achieved without altering the fundamental chemical composition and crystal structure of SnS. Comprehensive characterization of the deposited films was carried out using X-ray diffraction (XRD), field-emission scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (FESEM–EDX), atomic force microscopy (AFM), transmission electron microscopy (TEM), and ultraviolet–visible (UV–Vis) spectroscopy. XRD analysis confirmed that both undoped and doped SnS thin films crystallize in an orthorhombic phase with a preferred orientation along the (111) plane. However, the incorporation of Cu and In dopants led to a gradual deterioration in this preferential orientation. Crystallite size and lattice strain were evaluated using Scherrer's formula and Williamson–Hall (W–H) analysis, with results showing good agreement with TEM observations. TEM images revealed predominantly spherical nanocrystals for both undoped and doped samples. Surface morphology studies using AFM demonstrated notable modifications in surface topography upon doping, with a consistent reduction in surface roughness as dopant concentration increased. Compositional analysis via EDX confirmed the successful incorporation of Cu and In into the SnS lattice, with their atomic percentages increasing proportionally with doping levels. Optical studies indicated enhanced absorption characteristics in doped films. The optical band gap (E_g), estimated from UV–Vis spectroscopy, exhibited a systematic decrease with increasing dopant concentration, attributed to the formation of defect states within the SnS lattice. These defect-induced modifications in band structure, along with improved surface and structural properties, suggest that Cu- and In-doped SnS thin films are promising candidates for applications in humidity and gas sensing technologies, owing to their tunable optical and electronic properties.

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NMSF-EPM-040

Enhanced Solar-Driven Photocatalytic Dye Degradation and Antioxidant Activity of TMs-Doped (TMs=Zr, Mg) LSMO Perovskite Magnetic Nanoparticles

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Abstract

Pollution of water bodies with organic pollutants and synthetic dyes, such as crystal violet (CV), is a major problem. Traditional methods are often inefficient in removing such persistent contaminants. In this regard, photocatalysis has emerged as a green and sustainable approach for water treatment. In the present study, $La_{0.76-x}TM_xSr_{0.24}MnO_3$ (TMs=Zr, Mg; x=0 and 0.01), labeled as LT1-LT3 MNPs, were successfully synthesized via a simple citrate gel route and investigated for photocatalytic and antioxidant applications. Detailed characterization employing XRD (with Rietveld refinement), TEM, XPS, and UV-Vis spectroscopy was performed. Structural and morphological analyses confirmed successful dopant incorporation and the formation of a single-phase rhombohedral perovskite structure (R-3c), comprising predominantly spherical nanoparticles with an average crystallite size of approximately 17 nm. XPS results verified the coexistence of La^{3+}, Sr^{2+}, Mn^{3+}/Mn^{4+}, and Mg^{2+} species in Mg-substituted LSMO MNPs, while La^{3+}, Sr^{2+}, Mn^{3+}/Mn^{4+}, and Zr^{4+} were identified in Zr-substituted samples. Furthermore, the introduction of Mg and Zr dopants was found to reduce the band gap of the LSMO MNPs. The Zr-substituted LSMO sample exhibited superior photocatalytic efficiency, achieving nearly 99% removal of crystal violet within 90 minutes under natural sunlight. Radical trapping experiments revealed that superoxide and hydroxyl species play key roles in the degradation pathway. Furthermore, the recyclability of the catalyst and a plausible degradation mechanism were comprehensively evaluated. In addition, both Zr- and Mg-doped LSMO MNPs exhibited superior antioxidant activity. These findings demonstrate that Zr-doped LSMO magnetic nanoparticles serve as a promising multifunctional material platform, combining efficient sunlight-driven photocatalytic performance with notable antioxidant activity, making them suitable for environmental remediation and potential biomedical applications.

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Role of Substrate in Tailoring the Structural, Morphological, Optical and Electrical Properties of Molybdenum Thin Film

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Abstract

Molybdenum (Mo) is widely employed as a back-contact material in thin-film solar cells such as CZTS, CIGS, and CdTe due to its excellent thermal stability, high melting point, chemical inertness, and low resistivity. These attributes also make it suitable for applications in microheaters, gas sensors, energy storage, and optoelectronic devices. In the present work, a systematic comparative study of Mo thin films deposited on crystalline Si (100) and amorphous quartz substrates having different thickness of 150, 200, 250, and 300 nm using RF sputtering at room temperature.

The influence of substrate type and film thickness on structural, morphological, optical, and electrical properties is investigated in detail. Grazing incidence X-ray diffraction (GXRD) analysis reveals enhanced peak intensity and increased crystallite size with increasing thickness, accompanied by a reduction in microstrain and dislocation density for films on both substrates. However, these improvements are more pronounced for Mo films on Si (100). Atomic Force Microscopy (AFM) studies show a systematic increase in particle size and RMS surface roughness with thickness, with comparatively higher values observed using substrates of silicon than on quartz. Optical characterization using spectroscopic ellipsometry indicates that absorbance, reflectance, and refractive index increase with film thickness, with more significant changes in films deposited on Si (100). Electrical measurements demonstrate a substantial increase in conductivity and a corresponding decrease in resistivity as film thickness increases, with Mo films on Si (100) exhibiting superior electrical performance compared to those on quartz. The observed differences are attributed to the intrinsic properties of the substrates, including crystallinity, carrier concentration, surface energy, and nucleation behavior. This study highlights the crucial role of substrate selection in tailoring thin-film properties, indicating that Mo films on Si (100) are more suitable for electronic applications, while those on quartz are promising for optical and optoelectronic devices.

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Experimental and DFT Investigation of Vibrational and Nonlinear Optical Properties of 3NPP Chalcone for Optical Limiting Applications

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Abstract

This study examines the experimental nonlinear optical properties (NLO) of 3-(4-nitrophenyl)-1-(pyridin-3-yl)prop-2-en-1-one [3NPP] with density functional theory (DFT). All computational studies were executed in the gas phase at the B3LYP/DFT level with the 6–31+G(d,p) basis set. The simulated and experimental infrared spectra of the molecule were investigated, and vibrational assig nments were performed. Additionally, the third-order NLO properties of the 3NPP molecule were studied under a continuous wave (CW) regime. The two-photon absorption coefficient of 3NPP was found to be 2.44×10^{-4} cm/W at a 0.01 M concentration. The reverse saturation absorption (RSA) condition is justified by the ground-state and excited-state absorption cross sections. The threshold for optical limiting drops at 50% of the linear transmittance, yielding 1.46 kJ/cm^2 for the 3NPP molecule. A decreased limiting threshold of 3NPP molecule shows the potential optical limiting performance.

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NMSF-EPM-044

Enhanced Stability and Reliable Resistive Switching in Au/Zr-doped HfO_2/TiN RRAM for High-Density Non-Volatile Memory

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Abstract

Resistive random-access memory (RRAM) based on high-k oxide materials is considered a key technology for future non-volatile memory due to its scalability and low power operation. In this study, Au/Zr-doped HfO_2/TiN RRAM devices are fabricated and systematically investigated to achieve improved switching stability and reliability. The incorporation of zirconium into HfO_2 effectively tailors the defect landscape and promotes favorable phase formation, leading to consistent resistive switching behavior. The devices exhibit stable bipolar switching with a significant resistance window and reduced cycle-to-cycle variation. Electrical transport analysis indicates that conduction follows ohmic behavior in the low-resistance state, while the high-resistance state is dominated by trap-controlled mechanisms. In addition, the devices demonstrate strong endurance and long retention capability, confirming the robustness of conductive filament formation and rupture processes. The enhanced performance is primarily attributed to controlled oxygen vacancy distribution and improved interface characteristics within the device stack. These findings demonstrate that Zr-doped HfO_2-based RRAM devices are strong candidates for reliable and high-density non-volatile memory applications.

Keywords: *Resistive Random-Access Memory (RRAM), Zr-Doped HfO_2 (HZO), Resistive Switching, Non-Volatile Memory, Device Reliability*

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NMSF-EPM-045

Rigorous Analysis of X-Ray Diffraction Data of Ni-doped FeNbSb Alloy

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Abstract

Iron based Heusler alloys have shown the simultaneous behavior of thermoelectric and magnetic via controlled doping of magnetic element especially in FeNbSb thermoelectric material. Here, we report the X-Ray Diffraction (XRD) measurement results of Ni substituted FeNbSb alloys. Rigorous analysis of XRD data have been performed through Rietveld refinement and standard data for the refinement has been created by Vesta. In order to find the preferential site of the Ni in the parent alloy, we have tried to eliminate the different possibilities and corresponding simulated XRD data have been extracted for reducing the value of refined parameters especially χ^2 along with other relevant parameters. Although, magnetic characteristics with a particular structure have been reported previously but we were expected much better explanation through rigorous structural analysis. Hence, we have explored the XRD data and obtained the best possible structure with exact amount of swapping. We have also calculated the macrostrain, dislocations and crystallites size from the XRD data. Super reflection peaks (111 and 200) have been shown to be very sensitive for the small amount of swapping and disorder. Therefore, we have focused on the ratio of intensity of both the peaks. All the other peaks are also found to be affected with the swapping but not so significantly. This study will help to understand the XRD data more accurately.

Keywords: *Simulation, Rietveld Refinement, XRD Data, Super-Reflection Peaks, Swapping etc*

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Growth, Spectral, Linear, and Nonlinear Optical Characterization of S-Mandelic Acid Single Crystals: Next-Gen Materials for Sustainable Future

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Abstract

Single crystals of S-mandelic acid (SMA) were grown via low-temperature solution evaporation at 37 °C, positioning them as promising next-gen materials for sustainable future photonic applications. Single-crystal XRD confirmed a monoclinic system with lattice parameters $a = 8.666(19)$ Å, $b = 5.870(6)$ Å, $c = 15.206(20)$ Å, $\beta = 102.87°$, $V = 754(2)$ Å^3, corroborated by powder XRD indexing. FTIR (4000–400 cm^{-1}) and FT-Raman (4000–50 cm^{-1}) analyses identified key vibrations: O-H stretch at 3450 cm^{-1} (IR), C=O at 1722/1712 cm^{-1}, C-H stretches ~3000 cm^{-1}, and C-O bends ~640 cm^{-1}, affirming molecular integrity. SHG efficiency reached 0.71 times KDP (6.39 mJ output) under Nd : YAG laser (1064 nm), producing green emission for deep-UV potential. Z-scan with He-Ne laser (632.8 nm) revealed negative nonlinearity (n_2=-6.5 $\times$ 10^{-11} cm^2/W, self-defocusing via peak-valley), saturable absorption (α_2=-4.9 $\times$ 10^{-4} cm/W), and $\chi^{(3)} = 4.9 \times 10^{-6}$ esu, positioning SMA for optical sensors, Q-switches, and eco-friendly NLO devices.

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Detailed Analysis of X-Ray Diffraction Data of $Mn_2NiSb_{1-x}Sn_x$ (0.02 ≤x ≤ 0.10) Through Rietveld Refinement

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Abstract

Mn_2-based full-Heusler alloys have been proven to be a promising candidate due to its valuable magnetic features and high demanding for the spintronic applications. In view of this, Mn_2NiSb and Mn_2NiSn based alloys have been explored proprietarily in order to achieve best magnetic properties in their stable structure. In this report, we show the X-Ray diffraction (XRD) results for the Sn substituted at Sb site $Mn_2NiSb_{1-x}Sn_x$ ($0.02 \leq x \leq 0.10$) alloy. Although, we have already reported the magnetic properties of this series of alloys in a particular structure, but rigorous analysis of the structure has remained yet. Now, we report a detailed analysis of XRD results of $Mn_2NiSb_{1-x}Sn_x$ (0.02 ≤x ≤ 0.10) through Rietveld refinement in different possible swapping via Vesta. In spite of the fact that two types of stabilization have been found in the ground state of the Mn_2NiSb; Cu_2MnAl and Hg_2CuTi prototype. Most commonly, Mn_2NiSb and Mn_2NiSn have been found to be stabilized in Cu_2MnAl and Hg_2CuTi prototype structure respectively. Therefore, in order to make the combined structure of both prototype is very tough task. Hence, we have implemented the controlled substitution of Sn at Sb site in Mn_2NiSb and lattice parameters have decreased appropriately. Magnetic moments have also been found to be decreased as valance electron count of Sn was less than Sn. All the refined parameters have been given in the table. Crystallite size, micro-strain and dislocation density have also been calculated from the XRD data.

Keywords: *Keywords- Rietveld Refinement, Swapping, Magnetics, Lattice Parameters, Crystallite Size, Micro-strain etc*

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Effect of Ru Substitution on Spiral Ordering in $CoCr_2O_4$

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Abstract

$CoCr_2O_4$ is a normal spinel compound (AB_2O_4) crystallizing in the cubic $Fd\bar{3}m$ space group, where the B-site ions form a pyrochlore sublattice, giving rise to strong geometric frustration. The interplay between A–B and B–B exchange interactionleads to competing magnetic correlations and complex magnetic ordering. The coexistence of geometric frustration and competing magnetic interaction is very interesting from physics point of view. In $CoCr_2O_4$, the AFM interactions between the Co-Co, Co-Cr and Cr-Cr ions lead to a rich sequence of magnetic transitions viz., ferromagnetic transition (T_c), spiral spin transition (T_S) and spin lock-in transition (T_L) [Winkler et. al, PRB 80, 104418 (2009)]. So it is of great significance to tune the sublattice magnetic interactions in $CoCr_2O_4$ by doping magnetic ions viz., Ru and modifying the exchange interaction and thereby study its effect on the magnetic behaviour.

In this work, single phase $CoCr_{2-x}Ru_xO_4$ (x = 0, 0.2) compounds were synthesized by solid state reaction method and their dc and ac magnetization properties were investigated. M(T) curves of $CoCr_2O_4$ and $CoCr_{1.8}Ru_{0.2}O_4$ showed ordering at $T_C \sim 98$ K and 101 K respectively followed by ZFC–FC bifurcation below $T_{irr} \sim 96$ K and 98 K resp. At further lower temperature, $CoCr_2O_4$ showed transitions at $T_S \sim 26$ K and $T_L \sim 15$ K as reported earlier [Tomiyasu et.al, PRB 70, 214434 (2004)], while $CoCr_{1.8}Ru_{0.2}O_4$ showed only one transition at $T_S \sim 23$ K but no transition at T_L. dM/dT curve show only a small kink at 23K indicating that spiral orderings get suppressed in $CoCr_{1.8}Ru_{0.2}O_4$. ZFC-FC bifurcation in M(T), presence of broad peak in the imaginary part of ac susceptibility ~ 75 K in $CoCr_{1.8}Ru_{0.2}O_4$ and the peak shifting to higher temperature with increasing frequency, confirms the presence of spin glass state similar to $CoCr_2O_4$ [Tomiyasu et.al], arising due to short range ordering of spiral component. The frustration factor f (θ_{CW} / T_c) in both the systems is ~ 6 indicating the presence of frustration in the compounds.

Spiral spin structure of $CoCr_2O_4$ has been predicted to be due to the comparable JAB and JBB exchange interaction [Das et. Al, J. Phys.: Condens. Matter **28**, 446001 (2016)]. Increase in Tc with Ru doping can be ascribed to increase in JAB exchange interaction. Furthermore, doping Ru, average B site moment decreases as a result JBB decreases. Doping Ru^{3+} changes JAB and JBB exchange interactions leading to suppression of the spiral spin structure.

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NMSF-OTH-017

Exploring the Potentialities of Reduced Graphene Oxide for Sulphur Detection in Wastewater

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Abstract

Reduced Graphene Oxide (RGO) have revealed the high efficiency of such materials in the detection and removal of sulphur from wastewater. Properties such as an ordered structure, good electrical conductivity, and high specific surface area, crystalline graphene allows a high number of adsorption sites for the binding of sulphur species like sulphides (S^{2-}), sulphates (SO_4^{2-}), and sulphur-containing organic compounds. Such functional materials allow fast detection and low detection limits as well as stability in aqueous solutions, which makes them good materials for the detection and elimination of sulphurs in water bodies. In the present study, RGO has been utilised for the early detection of the Sulphur ions in the waste water bodies. Physico-chemical characterisations of pristine RGO and its applications for Sulphur interactions and simultaneous detection with its presence has been characterised using Fourier Transform Infra-Red spectroscopy (FTIR), Field Emission Scanning Electron Microscopy (FE-SEM) and High Resolution-Transmission Electron Spectroscopy (HR-TEM) respectively. Sulphur (S) is ascertained to be detected at ~16.39% in the presence of RGO sheets. FTIR Bands observed in the region ~700 cm^{-1} are attributed to C–O, C–N, or C=C stretching vibrations. These peaks indicate the possible interaction taking place between RGO surface and the sulphur ions. HR-TEM reveals the complexation behaviour of graphene along with showing the lattice fringes, apart from demonstrates the dispersal of nanoparticles/sulphur clusters on the graphene surface at atomic level. The changes and alterations observed in these bands is due to the adsorption of sulphur, which further confirms the interaction between graphene and sulphur atoms, along with the process of redox-based charge transfer mechanism. Advanced developments in graphene structures have proven to be an efficient material for identifying and eliminating sulphur in the wastewater due to their unique physico-chemical properties, such as orderly structures, high electrical conductivity, and high surface area, respectively. Nanoparticle or heteroatom functionalization improves binding capability and charge transfer, making detection swift and easy at low limits in water stability. This advance 2D material could

prove a beneficial material in the area of heavy metal remediation in water treatment processes, providing thereby an efficient and reliable sulphur detection and removal paradigm in contaminated water bodies.

Keywords: *Graphene, Sulphur, Wastewater Treatment, Adsorption Mechanism*

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NMSF-OTH-020

Advanced Substrate Utilizing Metasurface-Assisted Antenna Technology for Communication Systems

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Abstract

The growing demand for miniature and high-performance wireless devices in modern communication systems has driven significant interest in advanced substrates for antenna technologies. This work investigates the design and performance enhancement of antenna devices for engineered dielectric substrates, artificial surfaces, and metasurface-inspired structures to achieve multifunctional characteristics such as wide impedance bandwidth, improved gain, polarization diversity, and radiation pattern. The proposed antenna configurations are used for operation at sub-6 G Hz and millimeter-wave frequency bands, addressing the requirements of 5G and beyond wireless standards. The electromagnetic simulations are carried out to analyze the performance parameters including reflection coefficient, radiation efficiency, gain, and cross-polarization levels. The influence of substrate properties and metasurface geometries on antenna size and performance enhancement is systematically evaluated. The applications in smart wireless devices, IoT systems and wireless body area networks are discussed to demonstrate the relevance of the proposed designs. The results confirm that the integration of advanced substrates and metasurface concepts offers an effective pathway for realizing compact, efficient, and multifunctional antenna devices for future communication systems.

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Keywords: *Advanced Substrates, Metasurface, Multifunctional Antenna Devices, Modern Wireless Communication Systems*

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NMSF-OTH-021

Green Synthesis of Ag-ZnO Associated Nanocomposite using Polyherbal Extract and their Efficacy against Dental Caries

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Abstract

The goal of the current study is to create environmentally acceptable zinc oxide (ZnO) nanoparticles (NPs) doped with silver (Ag). Soxhlet extraction is applied to Mentha arvensis and Piper betel using ethyl acetate. Standard techniques were used to quantify phenols, flavonoids, and alkaloids. Silver-zinc oxide nanocomposites (Ag-ZnO NCs) were created using polyherbal extract and the sol-gel technique. Scanning electron microscopy and UV–visible spectroscopy was used to validate the reduction of metal ions. Compared to native plants, polyherbal plants have greater quantities of phenols, flavonoids, and alkaloids. Fourier Transform Infrared Spectroscopy (FTIR) spectroscopy and a zeta size analyzer were used to identify the functional group of Ag-ZnO NCs. The spherical shape of the Ag-ZnO NCs was verified by scanning electron microscopy. For every examined pathogen, the compounded Ag-ZnO NCs' antimicrobial efficacy outperformed that of the extract. Ag-ZnO NCs exhibit the strongest antibacterial activity at 50 µg and extract at 200 µg. At a low concentration of 500 µg/mL, biosynthesized nanoparticles show a strong anti-inflammatory impact of 68%, which is more effective than diclofenac sodium. Furthermore, the produced Ag-ZnO nanoparticle exhibited excellent antibacterial qualities against lactobacillus isolated from dental cavities and showed stability for 90 days. Dental caries can be reduced by phytocompounds. The antibacterial effectiveness of herbs is assessed by measuring the diameter of each herb's zone of inhibition against isolated bacterium species using AST. It was discovered that Mentha arvensis has the largest zone of inhibition, measuring 18 mm, and that it can be utilized to reduce dental cavities.

Keywords: *Nanocomposite, Dental Caries, Lactobacillus, Piper betel, Phytochemical Screening, Mentha Arvensis*

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NMSF-OTH-026

GO, rGO and Ag-rGO Nanocomposite as Promising Bacterial Removal with Antibacterial Activity

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Abstract

This research work focuses on the synthesis and detailed characterization of graphene oxide (GO), reduced graphene oxide (rGO), and silver-reduced graphene oxide (Ag-rGO) nanocomposites for their effective applications in removing bacteria and antimicrobial activity. Characterization of the prepared nanocomposites was performed using UV-Vis Spectroscopy, FTIR, XRD, and FESEM. The finding substantiates the effective reduction of graphene oxide (GO) to reduce graphene oxide(rGO) and efficient functionalization with silver nanoparticles. Antibacterial assessment against Escherichia coli revealed significant inhibition, with silver (AgNP)-reduced graphene oxide (rGO) showing the highest activity due to a synergistic interaction between silver nanoparticles (AgNPs) and reduced graphene oxide (rGO). Ag-rGO indicates the largest inhibition zone of 18mm, while graphene oxide shows the smallest inhibition zone, and reduced graphene oxide shows a moderate amount of inhibition zone. Physical disruption of the cell membrane impairs bacterial inhibition and induces oxidative stress by generating reactive oxygen species (ROS), thereby affecting various cellular components. These results demonstrate the potential of Ag-rGO as a capable nanomaterial for environmental and biomedical applications, including bacterial removal and water purification.

Keywords: *GO, rGO, Silver Nanoparticles, Nanocomposite, Antibacterial Activity, Bacterial Removal, Water Purification, Reactive Oxygen Species*

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NMSF-OTH-029

Effect of External Magnetic Field on the Phase Diagram of Antiferromagnetism and Superconductivity in Hole-Doped Cuprate Superconductors

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Abstract

We present a theoretical study of the effect of an external magnetic field on antiferromagnetism (AFM) and superconductivity (SC) in hole-doped cuprate superconductors, along with the construction of magnetic-field-dependent phase diagrams. The model Hamiltonian is formulated within a generalized BCS-type mean-field framework, incorporating electron dispersion, staggered magnetization for AFM, superconducting pairing interactions, and coupling to an external magnetic field. The system is analysed using the equations-of-motion approach with Zubarev single-particle Green's functions, enabling the derivation of correlation functions in terms of quasiparticle energies. The AFM and SC order parameters, along with the chemical potential, are obtained self-consistently as functions of temperature and doping.

Our results show that, in the absence of a magnetic field, AFM and SC orders compete, with AFM progressively suppressed upon hole doping and superconductivity emerging beyond a critical doping level. Superconductivity strengthens over an intermediate doping range and weakens in the overdoped regime. The application of an external magnetic field leads to a suppression of the superconducting order parameter and modifies the AFM order, indicating strong sensitivity to field-induced perturbations. These results highlight the intricate interplay between AFM and SC orders in cuprates and show qualitative agreement with experimental observations, offering insight into the phase evolution of high-temperature superconductors under external magnetic fields.

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NMSF-OTH-030

Study of Change in Thermodynamic Parameters Specific Heat and Gibbs Free Energy for Ge_ySe_{94}-yIn_6 Chalcogenide Glasses During Glass/Crystal Phase Transformation

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Abstract

Present paper discuss the change in specific heat and Gibb's free energy during glass/crystal phase transformation for $Ge_ySe_{94-y}In_6$(y=10, 15&20) chalcogenide glasses. $Ge_ySe_{94-y}In_6$(y=10,15 &20) chalcogenide glasses have been prepared by rapid quenching of melt techniques. For structure characterization XRD and EDAX techniques have been used. For measurement of specific heat Differential Scanning Calorimetery have been used.DSC scans have been recorder from room temperature to 823K at different heating rates i.e 5, 10, 15 &20K/min. DSC scans for measurements of specific heat have been carried out at heating rate 20K/min from room temperature to 823K under non isothermal conditions. Gibb's free energy difference during glass/crystal phase transformation provides information about stability of glassy alloys. $Ge_{10}Se_{84}In_6$ glass having minimum value of Ggc is most stable composition in $Ge_ySe_{94-y}In_6$ glassy series.

Keywords: *Chalcogenide Glass, Specific Heat, Gibb's Free Energy*

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NMSF-OTH-031

Acid-Modified Fly Ash as a Low-Cost Adsorbent for Efficient Phosphate Removal from Aqueous Systems

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Abstract

Phosphate contamination, primarily arising from agricultural runoff, domestic wastewater, and industrial effluents, is a major environmental concern due to its role in eutrophication, which leads to harmful algal blooms, oxygen depletion, and degradation of water quality. Addressing this issue through sustainable and economical treatment methods is therefore essential. The research focuses on enhancing the adsorption capacity of fly ash, an abundant industrial by-product, through acid modification using mineral acids such as hydrochloric acid, sulfuric acid, and nitric acid. This modification is expected to improve the physicochemical properties of fly ash, including surface area, porosity, and the availability of active adsorption sites. Both raw and modified fly ash samples will be characterized using techniques such as XRF, XRD, FTIR, and BET surface area analysis to evaluate structural and surface changes. The batch adsorption experiments were conducted under varying conditions of pH, adsorbent dosage, contact time, and initial phosphate concentration to determine optimal removal efficiency. Adsorption behavior was analyzed using isotherm models (Langmuir, Freundlich, and Dubinin–Radushkevich) and kinetic models (pseudo first order and pseudo-second-order) to understand the mechanism and rate of adsorption. The findings demonstrate that acid-modified fly ash exhibits significantly higher phosphate removal efficiency compared to raw fly ash, with optimal performance under mildly acidic to neutral pH conditions. Overall, this research highlights the potential of utilizing industrial waste materials for sustainable wastewater treatment, contributing to environmental protection and resource recovery.

Keywords: *Fly Ash, Acid-Modification, Adsorption, Phosphate removal, Wastewater Treatment*

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NMSF-OTH-033

Synthesis, Characterization, and Gas Sensing Performance of Chemically Synthesised Cu-doped SnO_2 Film Sensor

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Abstract

SnO_2 and Cu-doped SnO_2 materials were prepared by using the co-precipitation method. The sensor element required for gas sensing investigation was prepared by using the screen-printing method. The effect of copper inclusion on the structure, the electrical conductivity, and the gas sensing properties of SnO_2 was examined. The interaction of SnO_2 and Cu-doped SnO_2 thick films with H_2S, LPG, CO_2, and NH_3 gases was studied at temperatures ranging from 50 °C to 300 °C. Powder XRD analysis revealed that the prepared materials crystalline in the cassiterite phase of SnO_2 and that the crystallite size of SnO_2 decreases as the copper percentage increases. Morphological and elemental analysis were done by using SEM and EDX spectroscopy. The addition of 5 wt.% Cu significantly increased the sensitivity of SnO_2 at 150 OC. The average crystallite size of 5 wt.%Cu was around 4 nm and was confirmed by transmission electron microscopy (TEM). The band gap of the synthesised samples was found using UV-visible spectroscopy.

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NMSF-OTH-035

Assessment of Heavy Metal Contamination in the Tunia River Around the Petroleum Refinery Area of Daligaon, Assam

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Abstract

Rapid industrialization and refinery operations in this region have raised significant environmental concerns, particularly regarding the discharge of untreated or partially treated effluents into nearby water bodies. Heavy metals such as lead (Pb), cadmium (Cd), chromium (Cr), mercury (Hg), arsenic (As), manganese (Mn), zinc (Zn), nickel (Ni), vanadium (V), and iron (Fe) are persistent, non-biodegradable pollutants that can accumulate in aquatic systems, posing serious ecological and human health risks for sustainable future. This study presents a comprehensive assessment of heavy metal contamination in the Tunia River surrounding the petroleum refinery area of Daligaon, Assam. The primary objective of this study is to evaluate the concentration and spatial distribution of heavy metals in the Tunia River and to assess their relationship with key physicochemical parameters, including pH, temperature, dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), and total dissolved solids (TDS). Standard analytical techniques such as Atomic Absorption Spectroscopy (AAS) are employed for accurate quantification of metal concentrations, while statistical tools are used to analyze trends and correlations. The study also incorporates pollution indices such as the Heavy Metal Pollution Index (HPI) and Contamination Factor (CF) to evaluate the overall water quality and degree of contamination. Measured values are compared with national and international standards, including BIS and WHO guidelines, to determine the suitability of water for domestic and drinking purposes. The findings revealed slightly higher levels of heavy metals, particularly in areas proximal to refinery activities, indicating some anthropogenic influence. This study provides essential baseline data for environmental monitoring and contributes to a better understanding of pollution dynamics in industrial regions. It also highlights the urgent need for effective wastewater treatment, stricter regulatory enforcement, and sustainable remediation strategies such as biosorption and phytoremediation.

Keywords: *Heavy metal, Contamination Factor, Heavy Metal Pollution Index, Water pollution, Water quality*

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NMSF-OTH-037

Photo-luminescence in Synthetically Derived Hydroxyapatite: Biomedical Applications

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Abstract

Synthetically derived Hydroxyapatite (HAp) has emerged as a promising multifunctional biomaterial exhibiting intrinsic photoluminescence (PL) without the need for extrinsic dopants. This study explores the origin and tunability of defect-induced PL in HAp synthesized via sol–gel routes. Structural and morphological analyses confirm phase-pure apatite formation with nanoscale crystallinity, while spectroscopic investigations reveal emission spanning the blue to green spectral regions under ultraviolet excitation. The observed luminescence is attributed primarily to lattice imperfections, including oxygen vacancies, hydroxyl deficiencies, and calcium vacancies, which introduce localized energy states within the band gap. These defect states act as radiative recombination centers, enabling electron–hole pair relaxation via photon emission. The concentration and nature of defects are found to be strongly dependent on synthesis parameters such as pH, and calcination temperature. Increased thermal treatment enhances crystallinity but reduces defect density, leading to diminished PL intensity, whereas low-temperature synthesis favors higher defect concentrations and stronger emission.

Additionally, surface states and nanocrystal size effects contribute to emission variability through quantum confinement and surface recombination pathways. Time-resolved PL studies indicate multi-exponential decay behavior, reflecting the coexistence of shallow and deep trap states. The ability to engineer defect chemistry in HAp offers a pathway for tailoring its optical response for applications in bioimaging, sensing, and theranostics. Importantly, the inherent biocompatibility and bioactivity of HAp make it an attractive candidate for developing luminescent biomaterials for non-invasive diagnostics and real-time monitoring in biological environments. This work highlights defect engineering as a key strategy in advancing the functional versatility of hydroxyapatite.

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NMSF-OTH-038

Development of Biomimetic Nanocomposites as Bone Extracellular Matrix for Human Osteoblastic Cells

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Abstract

Bone tissue engineering has emerged as a promising alternative to traditional methods such as autografts and allografts, which often suffer from limitations like infection risk, donor site morbidity, and limited availability. To mimic natural bone, composed of organic collagen and inorganic nano-hydroxyapatite (HAP), researchers have developed organic–inorganic hybrid nanocomposites. Chitosan (CTS), a natural polysaccharide, is widely used due to its biocompatibility, biodegradability, and non-toxic nature. However, its osteoconductivity is relatively low. Incorporation of HAP enhances osteoconductivity by promoting calcification and improving osteoblast adhesion and proliferation. However, increasing HAP content leads to brittleness and reduced mechanical strength. To overcome this limitation, CTS is combined with poly(vinyl alcohol) (PVA), a biodegradable polymer known for its good mechanical strength and stability. An ideal scaffold should be biodegradable, biocompatible, porous, mechanically strong, and capable of supporting cell growth, nutrient diffusion, and vascularization. Additionally, antimicrobial properties are essential to prevent infection, which can be achieved by incorporating metal ions such as zinc. In this study, a biomimetic nanocomposite of CTS, PVA, and nano HAP–ZnO was developed. The composite exhibited improved tensile strength, high porosity similar to cancellous bone, good water uptake, biodegradability, and antimicrobial properties. It also showed excellent compatibility with human cells and supported osteoblast growth without toxicity, making it a promising material for bone tissue engineering applications.

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NMSF-OTH-039

Low-Cost Particulate Matter Sensor Using Activated Carbon and LED- Photodiode Detection

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Abstract

This paper presents a low-cost particulate matter (PM) sensor for the detection of $PM_{2.5}$ and PM_{10} using readily available components. The proposed system operates on the light scattering principle, using a light emitting diode (LED) as the illumination source and a photodiode as a detector. Airborne PM scatters the incident light, and the resulting scattered intensity is converted into an electrical signal proportional to particle concentration. An activated carbon filter is integrated into the sensor setup to minimize interference from gaseous pollutants and enhance measurement reliability. The sensor provides the real time monitoring of PM with low power consumption and simple circuitry. Owing to its compact design and cost-effectiveness, the developed sensor is suitable for indoor and outdoor air quality monitoring applications, particularly in low resource environments. This work highlights the feasibility of affordable optical sensing techniques as an alternative to conventional particulate monitoring instruments.

Keywords: *Particulate Matter, Low-Cost Sensor, Air Quality Monitoring, Light Emitting Diode, Activated Carbon*

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NMSF-OTH-044

Hybrid Strategies for Flow Assurance in Heavy Oil: Synergistic Effects of Chemical, Thermal, and Nanomaterial-Based Approaches

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Abstract

Persistent asphaltene and paraffin deposition in heavy crude oil systems significantly impairs flow assurance by increasing viscosity, causing pipeline blockages, and elevating operational costs. Conventional chemical surfactants, while effective, raise environmental and sustainability concerns, necessitating greener alternatives. This review critically examines the role of sustainable biosurfactants in mitigating deposition and improving the flow behavior of heavy crude oils, focusing on their physicochemical mechanisms, efficiency, and industrial feasibility. Biosurfactants primarily glycolipids, lipopeptides, and polymeric bio emulsifiers produced by microorganisms exhibit excellent interfacial activity, biodegradability, and stability under extreme reservoir conditions. They reduce oil-water interfacial tension (IFT), modify wettability, and stabilize emulsions, thereby enhancing crude mobility and preventing aggregation of heavy fractions. Experimental studies report viscosity reductions exceeding 70% and oil removal efficiencies up to 98% under optimal conditions. Mechanistically, biosurfactants disrupt wax and asphaltene crystallization, alter crystal morphology, and weaken the structural network of heavy components. Additionally, microbial systems can facilitate in situ biodegradation of long-chain hydrocarbons, further reducing deposition tendencies. Bio-based flow improvers derived from renewable resources demonstrate comparable or superior performance to conventional additives in reducing viscosity, gel strength, and pour point, with improved environmental compatibility. Despite these advantages, challenges remain in large-scale production, cost-effectiveness, and field implementation. This review highlights recent advancements, identifies knowledge gaps, and suggests future research directions, emphasizing the integration of biosurfactants into sustainable flow assurance strategies. Overall, biosurfactants show strong potential as eco-friendly alternatives for controlling deposition and enhancing heavy crude oil transport.

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NMSF-OTH-048

Innovative Approach for Surface Analysis of Fe-doped ZnO Nanoparticles (NPs) for Biological Applications

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Abstract

ZnO-based nanoparticles possess various nanostructures, which in turn play significant roles in different applications, especially in the field of electronics and biology. When doped with metals, the materials are found to exhibit enhanced inhibition of Gram-positive and Gram-negative microorganisms due to their small sizes and large surface areas. The facets of the granules are rough and highly complex, thereby providing an enormous contact area with microbial cells for inhibition. The multifractal analysis (MFA) of the surface texture and fractals of nanoparticles describes their morphology and predicts the optimum quantification of inhibition of different pathogens. The parameters of nonlinear dynamics (NLD) namely the Lyapunov exponent and Correlation dimension, provide indices that relate to the size and roughness of the nanoparticles, which are noticeable factors in restraining the growth of microorganisms. With this view, an attempt has been made to synthesize four Fe-doped ZnO nanoparticles for nonlinear dynamical study with the help of nonlinear dynamical parameters and multifractal spectra. The study is extended to calibrations of various NLD, MFA, and biological parameters for various applications in material science, bioscience, medicine, and sensors. The comparisons of different information on hidden nonlinearity of the samples provided by the NLD tools and MFA spectra are done for better efficiency in analyzing samples of the same kind for various applications in our next paper.

Keywords: *NLD, MFA, Nanoparticles, Pathogens, Lyapunov Exponent, Correlation Dimension*

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NMSF-OTH-049

Synthesis of Nano-Metal Oxide and Nano-Sulfur and its Application in Synthesis of Symmetrical Disulfides from Aryl/Alkyl Halides

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Abstract

The one-pot formation of S-S linkage from halides instead of thiol can save both time and cost. Attention has been drawn to utilize halides with various sulfur sources such as alkali metal disulfides, thiourea, thiouronium salts, thiocarboamide, elemental sulfur, and others. But the reactions mentioned with halides are often slower and moderate yielding due to many steps involved and usually affected at high temperature. Metal-nanoparticle can be an efficient catalyst in enhancing reactivity of this halide transformed reactions. The nanostructured catalysts are used in organic reactions especially in coupling reactions, considering unidirectional or by-product bound synthesis. They furnish higher surface area and lower coordination sites responsible for its higher catalytic activity. In addition, straightforward recovery and reuse of catalyst from the reaction mixture by simple filtration or centrifugation are considerable advantages. Here, we have reported a novel approach towards dual-nano assisted synthesis of disulfides from coupling of alkyl/aryl halides and sulfur nanoparticles. The indium oxide nanoparticles as catalyst expedite the conversion and sulfur nanoparticle notably enhances the miscibility, providing a faster, high yielding and cost-effective process in ethanol water system. The method has synthetic advantages in terms of mild reaction framework, catalyst regeneration up to 5 times, and absence of any sulfide or polysulfide linkage as by-product. By this dual nano assisted method, a variety of alkyl, aryl and heteroaryl symmetrical disulfides are obtained in good to excellent yields up to exceeding 98%.

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NMSF-OTH-050

Optimization of ETL and Passivation Layers in Lead-Free Perovskite Solar Cells for Improved Photovoltaic Performance

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Abstract

Perovskite solar cells have emerged as promising candidates to replace conventional fossil fuel–based energy technologies due to their excellent optoelectronic properties and rapid advancements in power conversion efficiency. Over the past two decades, perovskite solar cells have achieved efficiencies exceeding 25%. Despite of high efficiency, perovskite solar sell face challenges due to low stability and toxicity of lead based materials. Consequently, current research is increasingly focused on the development of lead-free perovskite materials and the enhancement of their photovoltaic performance. In this context, tin (Sn)-based perovskite solar cells have attracted considerable attention as environmentally non toxic alternatives. Tin (Sn) based materials exhibit suitable properties such as a low band gap, high absorption coefficient, and excellent optoelectronic characteristics for photovoltaic applications. This work focuses on the systematic investigation and optimization of electron transport layers (ETLs) and ETL/passivation layer combinations in tin-based inverted (p–i–n) perovskite solar cells using numerical simulation. The device performance is analysed using SCAPS − 1D numerical simulation by evaluating key photovoltaic parameters such as open-circuit voltage, short-circuit current density, fill factor, and overall power conversion efficiency. The basic p-i-n device configuration opted for this study is FTO/Spiro-OMeTAD/ $CH_3NH_3SnI_3$/ZnO/Ag. Various ETL materials and interfacial passivation layers such as ZnO, PCBM, BCP, Al_2O_3 are incorporated to improve charge carrier extraction and minimize recombination at the perovskite/ETL and ETL/ metal contact interface. The simulation results demonstrate that the incorporation of suitable passivation layers significantly reduces interfacial recombination losses and enhances charge transport efficiency. An optimized PCBM/ZnO ETL/Passivation layer combination yields a power conversion efficiency of approximately 24%, accompanied by a high current density 33 mA/cm2, Voc of 0.99V and improved fill factor around 75%. The study highlights the critical role of interface engineering in improving the performance of lead-free perovskite solar cells and provides valuable insights for the design of efficient and stable tin-based photovoltaic devices.

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NMSF-OTH-051

Structural Study of Zinc Ferrite Nanoparticles Synthesized using Different Methods

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Abstract

Crystallite size and lattice strain are crucial structural parameters that strongly influence the physical properties of nanomaterials. This study presents a comparative analysis of these structural parameters in zinc ferrite (ZF) synthesized using different methods, such as citric acid-based, polyethylene glycol (PEG) and ammonium hydroxide (NH_4OH) reagent-based sol-gel method, and nanostructures obtained from different bulk precursors. X-ray diffraction (XRD) patterns of these synthesized materials exhibit the presence of a cubic spinal phase. These materials are further investigated using Fourier transform infrared spectroscopy to study the characteristic bands associated with spinel phase. XRD patterns were further employed to evaluate crystallite size and macrostrain using pseudo-Voigt, Williamson-Hall (W-H), and Halder-Wagner (H-W) approaches. The Voigt function is represented as the combination of Lorentzian (size broadening) and Gaussian (strain broadening) components, whereas the W-H and H-W methods provide more understanding by differentiating between size-induced and strain-induced broadening. These results reveal that the synthesis technique affects peak broadening, indicating variation in crystallite size and strain. Strain values of these nanoparticles using different approaches generally differ; however, these values exhibit similar trends with size or synthesis parameters. Values estimated from Halder-Wagner approaches may be considered more reliable as the correlation coefficient is close to 1.

Keywords: *Crystallite size, microstrain, Pseudo-Voigt, Williamson-Hall (W-H) and Halder-Wagner (H-W) approach*

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NMSF-OTH-052

Colorimetric Sensing of Anions with Bis(indolyl)methane Derivatives: A Study Based on Experimental and Computational Evidences

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Abstract

Amongst various strategies for anion sensing, colorimetric ion sensing is one of the most widely used techniques, as it enables the detection of ions in a sample via a visible colour change. In this work, ten bis(indolyl)methanes (BIMs) bearing different donor/acceptor substituents on the aryl and indolyl moieties have been designed, synthesized, and used as efficient colorimetric and selective sensors for fluoride and acetate ions. The mechanistic study based on spectroscopic and theoretical evidence confirms 1:2 interactions between BIMs and fluoride ions, leading to deprotonation of the BIMs to their corresponding di-anions. The lower HOMO-LUMO energy gap associated with the di-anion, as compared to its neutral state, is responsible for the corresponding spectral and visible color change. The H-bonded association-dissociation equilibrium between BIMs and its corresponding di-anion was studied in four different solvents, and it was found to depend on the polarity and basicity of the solvent, as in the given order DMF > DMSO > THF > acetone. Whereas, the ion selectivity of the optical chemosensors towards fluoride is reliant on the pKa of indole N–H of BIMs and found to be most selective in the case of the most acidic N–H over the least or moderately acidic N–H. Hence, better sensitivity and ion selectivity of BIMs towards a particular anion may be achieved by appropriate tuning of their substituent at aryl and indole moieties.

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NMSF-OTH-053

Analysis of Experimental X-Ray Diffraction Data for $Mn_{2-x}Ni_{1-x}Sb$ (x=0.25, 0.5) through Rietveld Refinement

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Abstract

Heusler alloys have been exhibited a tuneable magnetic property with minor change in their crystal structure. Hence, rigorous analysis of X-Ray diffraction (XRD) is very crucial. Among the others, Mn-based Heusler alloys have been found to be a significant due to the high magnetic moment associated with the parallel alig nment of magnetic moment between the Mn-Mn atoms and high Curie temperature which enables them to easily sustain at room temperature. However, two stable structures have been found for full-Heusler alloys: direct Heusler and inverse Heusler alloys. Hence, Exact evaluation of the structure is very tedious task. Here, we have performed the Rietveld refinement software of XRD data obtained for $Mn_{2-x}Ni_{1-x}Sb$(x= 0.25, 0.5) considering both the structures. All the refined data have given and least Chi^2 value has been considered to be a reliable in order to decide whether alloys have stabilized in either direct or inverse structure.

Keywords: *X-Ray Diffraction, Direct and Inverse Heusler, Cuire Temperature, Rietveld Refinement, Chi*^{2}

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NMSF-OTH-055

Fitting of XRD data of Mn_2NiSb in Cu_2MnAl and Hg_2CuTi Prototype Structure Including Disorder

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Abstract

Full-Heusler alloys have been generally preferred to stabilized in Cu_2MnAl and Hg_2CuTi prototype structure. In order to find the preferred structure, best fitting is required to achieve for the experimental X-Ray diffraction data. Here, we have successfully prepared the Mn_2NiSb alloy and performed the XRD measurement with slow scan rate. We have obtained very smooth data which revealed the highest ordering of the alloy in four interpenetrating face centred cubic lattices. However, swapping has always been associated with the structure having elements similar in their atomic size and electronegativity. In order to find the exact prototype structure, we have simulated the XRD data through Vesta of Mn_2NiSb alloy in both Cu_2MnAl and Hg_2CuTi prototype. With these simulated data, we have fitted the XRD data and tried to reduce the Chi2 value for both structures. We have also calculated the lattice parameter and other refined parameter from the fitting. Electronic density map has also been shown from the Fourier data obtained from the refinement. Crystalline size, dislocation density and macrostrain have also been calculated from the experimental XRD data.

Keywords: *Prototype, Vesta, Electronic Density, Crystalline Size, XRD data, Dislocation etc.*

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NMSF-OTH-056

Biosynthesis of Zinc Oxide Nanoparticles Using Madagascar Periwinkle Extract and its Application in Degradation of Toxic Methylene Blue Dye

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Abstract

Abstract: We have prepared zinc oxide nanoparticles (namely L5 and L10) using 5 mL and 10 mL Madagascar periwinkle leaf extract. These synthesized zinc oxide nanoparticles have been characterized using various techniques. The size and morphology of synthesized nanoparticles were determined using Scanning Electron Microscopy (SEM), Field Emission Scanning Electron Microscopy (FESEM), and Transmission Electron Microscopy (TEM). The Powder X-ray diffraction (PXRD) revealed that synthesized ZnO nanoparticles consist of a typical hexagonal wurtzite phase. The BET analysis shows that the measured surface areas of L5 and L10 nanoparticles are 10.202 m^2/g and 38.762 m^2/g respectively. The photocatalytic activity of both the synthesized nanoparticles was determined against methylene blue (MB) organic dye. It was evident from the results that L10 is a better catalyst than L5. Herein, MB dye was degraded (94.09%) in 600 min by ZnO (L5) photocatalyst and (97.92%) in 360 min by ZnO (L10) photocatalyst. Therefore, synthesized ZnO (L5) and ZnO (L10) nanoparticles could be employed as an efficient photocatalyst for the degradation of toxic organic dyes.

Keywords: *Biosynthesis, ZnO Nanoparticles, Photocatalytic Degradation, Organic Dye*

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NMSF-OTH-057

Study of Vibrational Modes of Coumarin 152 in Gas Phase and Solvents Using Density Functional Theory

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Abstract

The theoretical simulations on Coumarin 152 have been performed using Density Functional Theory (DFT). Positions of some of the calculated vibrational bands show noticeable change in the solvents. Assignments of various vibrational modes have been done using vibrational energy distribution analysis. The bands, which showed prominent shift, have contributions from the vibrational motion of the nitrogen, oxygen and fluorine atoms present in the molecule. These shifts arise due to simultaneous interaction of a number of solvent molecules at nitrogen, oxygen and fluorine atoms present in the dye molecule. Study of Molecular Electrostatic Potential (MEP) of the dye molecule shows highly electronegative and electropositive regions, which are responsible for interaction between the dye molecule and solvent molecules. The molecular parameters, atomic charge densities of coumarin 152 have been obtained using B3LYP functionals. Optimized structure of Coumarin 152 -methanol molecule complex has also been obtained using DFT calculations, which support these interactions. It has been observed that the interaction between dye molecule and methanol molecule are stronger as compared to interaction between dye molecule and carbon tetrachloride, which means that dipole-dipole interactions are responsible for change in frequency of vibrational bands in solvents. These interactions have been confirmed by studying possible donor-acceptor charge transfer interactions in coumarin6 for different solvents using NBO analysis and by studying the shapes of frontier molecular orbitals. In addition to dipole moment, the interactions between solvent and dye molecule also depend on the size of solvent molecule. This steric hindrance is also indicated in the solvent accessible surface of coumarin 152 in different solvents. This study may be helpful in understanding the behavior of coumarin 152 in different solvents and to identify the specific atoms of dye, which take part in various interactions with solvent molecules

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NMSF-OTH-058

Photocatalytic Degradation of Triclosan from Simulated Wastewater

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Abstract

Triclosan is a well-known antibacterial and antifungal agent that is widely used in consumer goods including paints, plastic materials, and toys as well as in a number of healthcare products like toothpaste, soaps, detergents, perfumes, deodorants, hand-wash and cosmetics. The extensive use of triclosan is a matter of great concern. It is poisonous and causes endocrine disruption in amphibians and mammals. It can limit algal photosynthesis, affecting aquatic plant growth. The chemical has an enormous effect on human health, causing immune suppression, abnormal embryonic development, and endocrine dysfunction. Triclosan is continuously discharged into the environment through sewage systems. Therefore, there is an urgent need to develop water treatment techniques for the effective removal of this contaminant.

Photocatalysis has gained significant attention as a powerful water treatment method in recent years. In the present work, we report photocatalytic degradation of triclosan using TiO_2. The experiments were carried out using one factor at a time analysis. The effect of various parameters such as initial concentration of triclosan, amount of photocatalyst, lamp intensity and pH on the degradation was studied. At optimum conditions, the reaction kinetics and mechanism was studied.

Keywords: *Triclosan; Water treatment, Photocatalysis,* TiO_2*, Kinetics, Mechanism*

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NMSF-OTH-059

Photo-Catalytic, Morphological, Structural and Optical Properties Of Green Synthesized Silver-Doped Zinc Oxide Nanoparticles

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Abstract

This study explores the green synthesis of Ag-doped ZnO nanoparticles using orange peel extract as a natural reducing and stabilizing agent. Structural and morphological characterization confirmed hexagonal wurtzite structure and uniform Ag distribution. The optical band gap decreased from 3.40 eV to 2.99 eV with Ag doping. Photocatalytic activity reached 90.99% dye degradation, and antioxidant activity also improved significantly. These results highlight the enhanced multifunctional properties of Ag-doped ZnO NPs for environmental and biomedical use.

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NMSF-OTH-060

pH-Dependent Adsorption and Ligand Exchange Dynamics of Amino Acids on Citrate-Stabilized Gold Nanoparticles: A UV–Vis Spectroscopic Study

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Abstract

The present work systematically examines the pH-dependent adsorption behavior and ligand exchange mechanisms of amino acids on citrate-stabilized gold nanoparticles (AuNPs). Colloidal AuNPs were synthesized via the classical citrate reduction method and subsequently functionalized with L-cysteine, L-glutamic acid, and L-arginine over a pH range of 5–11. The interaction dynamics and surface modification were probed using UV–Visible spectroscopy, with detailed analysis of surface plasmon resonance (SPR) band shifts (λmax), intensity variations, and spectral broadening.

The adsorption process is strongly governed by the protonation state of functional groups and their corresponding electrostatic and chemisorptive interactions with the AuNP surface. L-cysteine demonstrates a pronounced affinity toward AuNPs, attributed to the formation of strong Au–S bonds, resulting in efficient displacement of citrate ions and significant SPR modulation. In contrast, L-arginine exhibits minimal adsorption, likely due to electrostatic repulsion and weaker surface binding interactions, while L-glutamic acid displays intermediate behavior governed by carboxylate-mediated interactions.

Furthermore, L-cysteine-functionalized AuNPs exhibit enhanced pH-responsive optical properties, indicating significant alterations in surface charge distribution and interparticle interactions under varying pH conditions. These findings elucidate the critical role of amino acid structure and solution pH in dictating nanoparticle surface chemistry and colloidal stability. The study provides fundamental insights relevant to the rational design of biofunctionalized nanomaterials for applications in sensing, targeted delivery, and nanobioconjugation.

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NMSF-OTH-061

Improved Dye Degradation Performance of Green-Synthesized Ni^{2+} and Mg^{2+} Doped CeO_2 Photocatalysts

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Abstract

This study examines the improved degradation of Methylene Blue (MB) dye using photocatalysts of green-synthesized cerium oxide (CeO_2) nanoparticles and Ni^{2+} doped, Mg^{2+} doped CeO_2 nanoparticles. The nanoparticles of CeO_2 were synthesized through the plant-mediated method, which is eco-friendly in nature. Characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-vis spectroscopy confirmed that a cubic fluorite structure has been formed with crystallite sizes of CeO_2 6.15 nm, Ni^{2+} 5.59 nm-doped, and Mg^{2+} 5.19 nm-doped CeO_2. UV-Visible analysis shows band gap reduction to 3.36 and 3.24 eV, indicating improved visible-light absorption through doping. The tests of photocatalytic activity show that the CeO_2 has 79% degradation efficiency, and Ni^{2+} -doped and Mg^{2+} -doped CeO_2 have 93% and 94%, respectively. The findings show that the photocatalytic property of Ni^{2+} and Mg^{2+} doped CeO_2 nanoparticles is improved and this enhancement makes these nanoparticles suitable for environmental remediation applications.

Keywords: CeO_2 *Nanoparticles, Green Synthesis, XRD, SEM, Photocatalysis*

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NMSF-OTH-063

Integrating Sustainable Materials Science into STEM Education: A Review of Pedagogical Approaches, Challenges and Future Directions

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Abstract

Sustainable materials science is an emerging interdisciplinary field that addresses global challenges related to clean energy, environmental protection, climate change, and sustainable technological development. Next-generation materials such as nanomaterials, biodegradable materials, smart materials, photovoltaic materials, battery materials, supercapacitor materials, and green composites have wide applications in renewable energy, electronics, healthcare, and environmental remediation. Therefore, introducing these concepts in Science, Technology, Engineering and Mathematics (STEM) education is essential to connect classroom learning with real-world sustainability challenges. This review paper discusses the need to integrate sustainable materials science into school, undergraduate, and teacher education curricula. It highlights pedagogical approaches such as project-based learning, experiential learning, interdisciplinary teaching, virtual laboratories, simulation-based learning, and digital/AI-enabled tools for improving conceptual understanding and scientific thinking. The paper also examines the relevance of NEP-2020 in promoting multidisciplinary education, skill development, innovation, and sustainability-focused learning. Major challenges, including limited laboratory infrastructure, curriculum gaps, lack of trained faculty, and insufficient exposure to emerging research areas, are also discussed. The review concludes that integrating sustainable materials science into STEM education can strengthen scientific literacy, environmental responsibility, and readiness for future careers in green technologies and sustainable development.

Keywords: Sustainable materials science, STEM education, nanomaterials, renewable energy materials, green technology, NEP-2020, interdisciplinary learning.

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NMSF-OTH-064

Transition Metal Selenide as High-Performance Supercapacitor Electrodes: A Crystallinity Engineering and DFT Guided Approach

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Abstract

Bimetallic selenides have recently attracted significant attention as advanced electrode materials for high-performance supercapacitors due to their high electrical conductivity and multiple redox-active sites. In this study, $CuMnSe_2$ was synthesized via a hydrothermal method at different reaction temperatures (160, 180 and 2000 C) to investigate the influence of temperature on structural and electrochemical properties. X-ray diffraction (XRD) confirmed the successful formation of crystalline selenide phases, with crystallinity strongly dependent on synthesis temperature. The electrochemical behavior, evaluated through cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS), demonstrated remarkable capacitive characteristics. The optimized $CuMnSe_2$ electrode delivered a high specific capacitance of 276 F g^{-1} at 1 A g^{-1}, excellent rate capability, and an energy density of 58.13 Wh kg^{-1} at a power density of 799.97 W kg^{-1}. The superior performance is attributed to the synergistic effect of bimetallic ions and improved crystallinity, which collectively enhance charge-transfer kinetics and ion-diffusion pathways. This study highlights temperature-controlled synthesis as an effective strategy to tailor the structural and electrochemical properties of $CuMnSe_2$, confirming its great potential as a promising electrode material for next-generation energy storage applications.

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NMSF-OTH-065

Bimetallic $CuCo_2Se_4$ Spinel for High-Performance Supercapacitors: Experimental and Theoretical Insights into Structure–Performance

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Abstract

Achieving high energy density without compromising power density remains a central challenge in supercapacitor research. Herein, we report the hydrothermal synthesis and comprehensive investigation of bimetallic $CuCo_2Se_4$ spinel as a high-performance electrode material, integrating experimental studies with density functional theory (DFT) insights. $CuCo_2Se_4$ synthesized at 160, 180, and 200 C exhibited flower-like porous morphologies, providing abundant electroactive sites and efficient ion transport pathways. Structural and spectroscopic analyses (XRD, FTIR, Raman, FE-SEM) confirmed the successful formation and crystallinity of the spinel phase. Electrochemical measurements revealed a high specific capacitance of 527 F g^{-1} at 0.5 A g^{-1}, excellent rate capability, and ∼76 % capacitance retention over 2000 cycles. The optimized electrode delivered a higher energy density of 92 Wh kg^{-1} with a power density of 3970 W kg^{-1}. Complementary DFT calculations confirmed a high density of states near the Fermi level, strong Cu/Co–Se hybridization, and enhanced quantum capacitance (1620 $\mu F/cm^2$), underpinning the observed conductivity and pseudocapacitive behavior. Device-level demonstrations further validated its practical applicability in powering LEDs and small motors. This work highlights the synergistic redox activity of bimetallic $CuCo_2Se_4$, outperforming its monometallic counterparts, and establishes design principles for next-generation selenide-based energy storage devices.

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NMSF-OTH-066

Study of Structural, Electronic and Optical Properties of XN-MoS_2 (X= Al, B) Heterostructure

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Abstract

In this work, we investigate the structural, electronic, vibrational and optical properties of XN–MoS_2 (X = Al, B) van der Waals heterostructures using Density Functional Theory (DFT). The calculations were carried out within the framework of the GGA-PBE approximation. The optimized geometries confirm stable stacking configurations with favorable interlayer interactions. The calculated cohesive energies and phonon dispersion spectra, showing the absence of imaginary frequencies, verify the structural and dynamical stability of the heterostructures. Electronic band structure analysis reveals that both AlN–MoS_2 and BN–MoS_2 systems exhibit semiconducting behavior with band gaps around 1.27 eV. The projected density of states indicates significant contributions from Mo-*d* orbitals near the Fermi level, suggesting their important role in charge transport properties. Furthermore, optical investigations based on the dielectric function demonstrate strong absorption and optical response in the visible and ultraviolet regions. These findings suggest that XN–MoS_2 heterostructures are promising candidates for future nanoelectronic, optoelectronic and photovoltaic applications.

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