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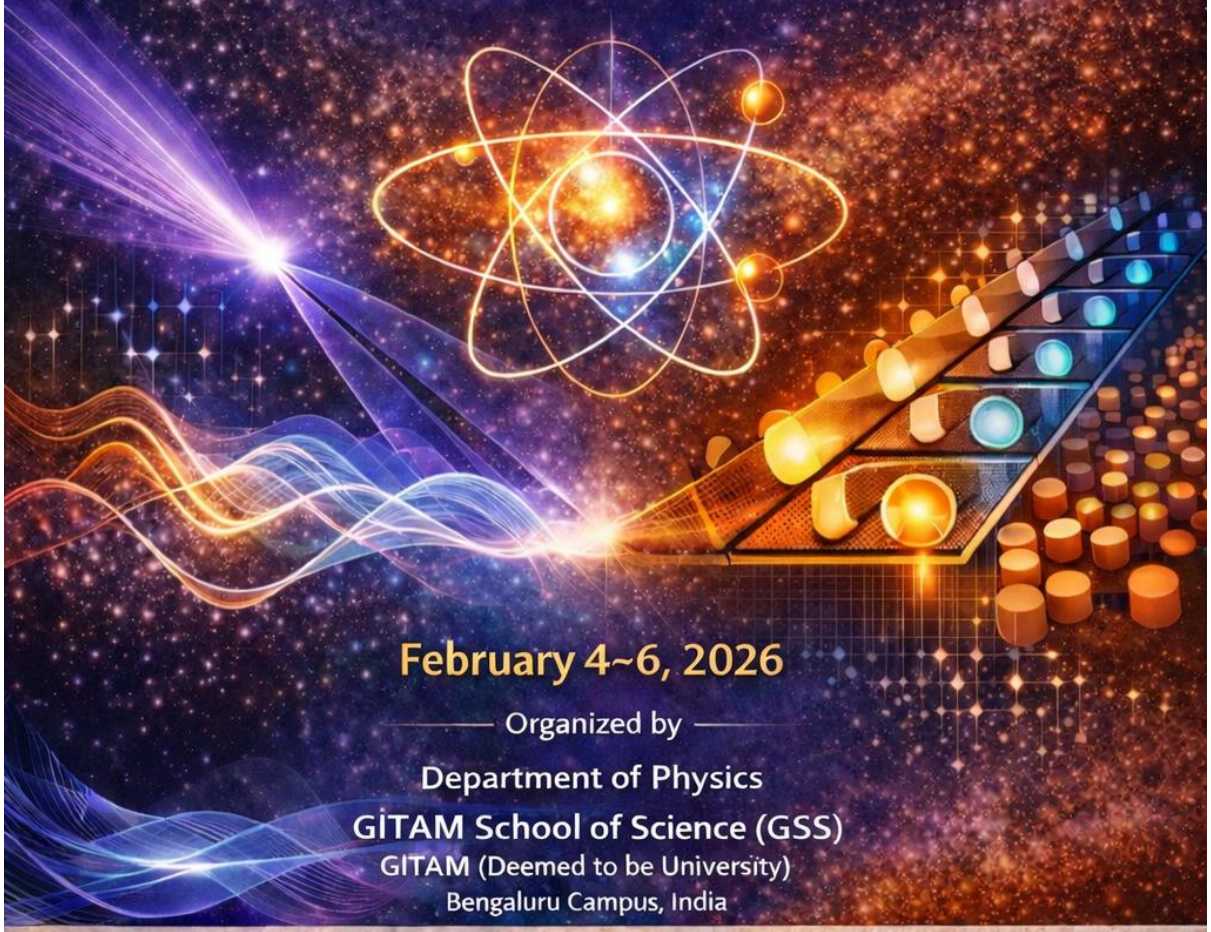
ABSTRACT BOOK

International Conference on

Advances in Light-Matter Interactions: Fundamentals to Frontiers



February 4~6, 2026

Organized by

Department of Physics

GITAM School of Science (GSS)

GITAM (Deemed to be University)

Bengaluru Campus, India

CERAMICS INTERNATIONAL | ELSEVIER | CRYSTAL Research & Technology | WILEY

About GITAM – Bengaluru Campus

GITAM (Deemed to be University), Bengaluru Campus is a modern and vibrant academic hub set amidst a serene and eco-friendly environment. The campus is designed to foster excellence in education, research, and innovation through interdisciplinary programs, state-of-the-art infrastructure, and advanced laboratories. With a strong focus on experiential learning, industry collaboration, and global standards, GITAM-Bengaluru nurtures competent professionals, ethical leaders, and innovative thinkers to address contemporary scientific, technological, and societal challenges.

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International Conference on Advances in Light-Matter Interactions: Fundamentals to Frontiers (ALMIC)

Dates: 4th to 6th February 2026

Organized by

Department of Physics,
GITAM School of Science (GSS),
GITAM-Bengaluru,
Karnataka-562163, India.

In association with

Indian Radio Science Society (InRaSS).

Partner Scientific Journals

Ceramics International
(Scopus & WoS Q1 and I. F: 5.6)

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Special Issue (S. I)

Advances in Light-Matter Interactions: Fundamentals to Frontiers.

Themes

Theme 1: Quantum Phenomena & Exotic States

- Quantum materials
- Strongly correlated systems
- Topological insulators
- Spin-orbit coupling
- 2D materials
- Spintronics
- Magnetic heterostructures

Theme 2: Energy Materials, Metamaterials & Nanostructures

- Metamaterials
- Photonic crystals
- Nano-photonics
- Optical sensing
- Fiber optics
- Photonic devices
- Energy materials
- Photocatalysis
- Ultrafast dynamics in functional materials

Theme 3: Biological Systems & Soft Matter

- Photoinduced dynamics
- Biological materials
- Soft materials
- Complex environments

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SRIBHARAT MATHUKUMILLI
PRESIDENT

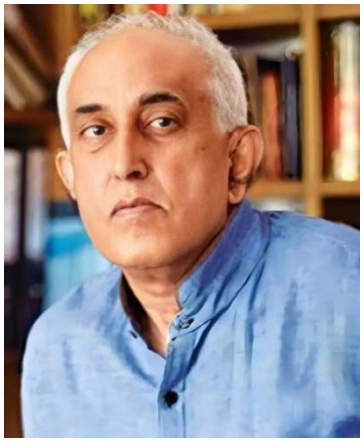
Message from President

It is my pleasure to extend warm greetings to all participants of the **International Conference on Advances in Light-Matter Interactions: Fundamentals to Frontiers (ALMIC) 2026**, being hosted at GITAM (Deemed to be University), Bengaluru Campus.

The conference represents a significant platform for global scholars, researchers, and industry experts to share cutting-edge advancements in light-matter interactions and allied disciplines. I believe that the diverse range of topics and discussions will stimulate interdisciplinary collaboration and inspire innovative research. Institutions like GITAM thrive when ideas transcend boundaries and bring together the best minds from around the world.

I thank the organizing committee, participants, and partners for their dedication and contribution to this important event. May ALMIC-2026 lead to new insights, meaningful partnerships, and lasting impact for science and society.

I extend my sincere best wishes to all participants. Welcome to ALMIC 2026, and welcome to GITAM (Deemed to be University).



PROF. VIRANDER SINGH CHAUHAN
CHANCELLOR

Message from Chancellor

It is a matter of great pleasure for me to convey my greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The focus on light–matter interactions reflect one of the most vibrant and rapidly evolving domains of modern science, underpinning significant advances in photonics, quantum technologies, nanomaterials, optoelectronics, and interdisciplinary research. By addressing both fundamental concepts and emerging frontiers, this conference provides an intellectually stimulating platform for advancing scientific understanding and innovation.

I am pleased to note that this international conference brings together eminent scientists, academicians, researchers, and young scholars from across the globe. Such academic forums play a vital role in promoting research excellence, encouraging cross-disciplinary dialogue, and fostering global collaborations—values that are central to GITAM's mission of creating knowledge-driven societal impact.

I congratulate the Department of Physics, GSS, and the organizing committee for their vision, commitment, and meticulous efforts in hosting this prestigious event. I also extend my appreciation to the keynote speaker, plenary speakers, invited experts, delegates, and all contributors for their active participation and support. I am confident that the deliberations and outcomes of this conference will lead to meaningful insights, innovative research directions, and long-lasting collaborations in the field of light–matter interactions.

I wish the conference every success and all participants a productive and enriching academic experience.

PROF. ERROL D'SOUZA
VICE CHANCELLOR

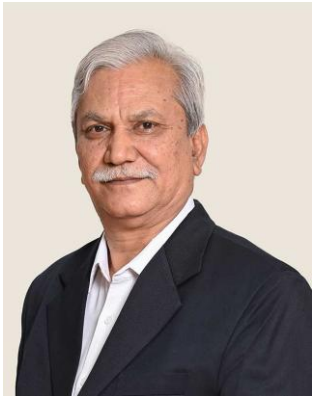
Message from Vice Chancellor

It gives me immense pleasure to extend my warm greetings on the occasion of the International Conference on **"Advances in Light–Matter Interactions: Fundamentals to Frontiers" (ALMIC 2026),** being organized by the **Department of Physics, GITAM School of Science (GSS), Bengaluru Campus,** during **February 4–6, 2026.**

This prestigious conference addresses one of the most dynamic and transformative areas of contemporary science, where fundamental understanding seamlessly converges with technological innovation. Light–matter interaction lies at the heart of numerous breakthroughs in physics, chemistry, materials science, photonics, nanotechnology, quantum technologies, and biomedical applications. By bringing together eminent scientists, academicians, researchers, and young scholars from across the globe, this conference provides an excellent platform to exchange ideas, share cutting-edge research, and foster meaningful collaborations that transcend disciplinary and geographical boundaries.

I am confident that the deliberations, keynote talks, plenary sessions, invited talks, oral presentations, and poster presentations will not only enrich scientific knowledge but also inspire innovative thinking among participants. Such academic gatherings play a vital role in nurturing research culture, promoting interdisciplinary approaches, and strengthening international cooperation-key pillars for addressing future scientific and societal challenges. I commend the organizers for their vision, dedication, and meticulous efforts in conceptualizing and executing this international event. I also extend my sincere appreciation to the speakers, delegates, sponsors, and all contributors whose support has made this conference possible.

I wish the conference every success and hope that it will lead to fruitful discussions, lasting collaborations, and significant advancements in the field of light–matter interactions. Welcome to ALMIC 2026 and to GITAM (Deemed to be University).



PROF. GUNASEKHARAN D
REGISTRAR

Message from Registrar

I am pleased to convey my warm greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The theme of the conference highlights a rapidly evolving and significant area of science that underpins many recent advancements in physics, materials science, photonics, and emerging technologies. By providing a platform that brings together fundamental concepts and advanced research frontiers, the conference offers valuable opportunities for academic interaction, knowledge sharing, and collaborative research.

I appreciate the efforts of the Department of Physics and the organizing committee for their dedication and efficient planning in hosting this international event. I am confident that the deliberations and discussions during the conference will lead to meaningful outcomes, inspire innovative research, and strengthen global academic collaborations.

I wish the conference great success and all the participants a productive and enriching academic experience.

PROF. BASAVARAJ G KATAGERI
PRO VICE CHANCELLOR
(BENGALURU CAMPUS)

Message from Pro Vice Chancellor

I am happy to extend my warm greetings on the occasion of the International Conference on "**Advances in Light–Matter Interactions: Fundamentals to Frontiers" (ALMIC 2026)**, being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The theme of this conference is both contemporary and impactful, as light–matter interactions constitute a cornerstone of modern scientific inquiry and technological progress. Advances in this domain continue to drive innovation in areas such as photonics, quantum science, nanotechnology, advanced materials, and interdisciplinary applications. By encompassing both fundamental concepts and emerging frontiers, the conference promises to stimulate meaningful dialogue and inspire novel research directions.

I am pleased to note that this event brings together distinguished scientists, academicians, researchers, and young scholars from across the world. Such platforms are invaluable for fostering interdisciplinary collaboration, strengthening global academic partnerships, and nurturing vibrant research ecosystem-key priorities of GITAM's academic vision. I commend the Department of Physics, GSS, and the organizing committee for their commitment, vision, and meticulous efforts in hosting this prestigious event. I also extend my appreciation to the keynote speaker, plenary speakers, invited experts, delegates, and sponsors for their enthusiastic participation and support. I am confident that the deliberations and outcomes of this conference will contribute significantly to the advancement of knowledge and will pave the way for enduring collaborations in the field of light–matter interactions.

I wish the conference every success and all participants a rewarding and enriching academic experience. Welcome to ALMIC 2026—a celebration of knowledge and collaboration at GITAM (Deemed to be University).

PROF. ANANTHA RAMAKRISHNA S
DEAN OF SCIENCES

Message from Dean

I am delighted to extend my warm greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The theme of the conference reflects a rapidly advancing and intellectually stimulating area of science that bridges fundamental understanding with emerging technological applications in photonics, quantum science, nanotechnology, and advanced materials. By bringing together researchers and academicians from diverse institutions and countries, the conference provides an excellent platform for scholarly exchange, interdisciplinary dialogue, and collaborative research.

I commend the Department of Physics and the organizing committee for their dedication and meticulous efforts in organizing this international event. I am confident that the technical sessions, keynote/plenary/invited lectures, and interactions during the conference will inspire innovative ideas and contribute meaningfully to the advancement of science.

I wish the conference every success and all the participants a productive and enriching academic experience.

PROF. B. V. R. TATA
DISTINGUISHED PROFESSOR-PHYSICS

Message from Distinguished Professor

I am happy to convey my warm greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

Light–matter interactions represent a cornerstone of modern physics, driving significant advances in photonics, quantum science, nanotechnology, and advanced functional materials. This conference, with its focus on both fundamental principles and emerging research frontiers, offers an excellent platform for meaningful scientific exchange and the dissemination of cutting-edge research.

I commend the Department of Physics and the organizing committee for their initiative and dedicated efforts in hosting this international forum. I am confident that the technical sessions and scholarly interactions will inspire new ideas, promote collaborative research, and contribute substantially to the advancement of this important field.

I wish the conference every success and all participants a stimulating and enriching academic experience.

PROF. RAVI KUMAR GURAZADA
DISTINGUISHED PROFESSOR-PHYSICS
Head, MURTI-Research Centre, GITAM

Message from Distinguished Professor

I am pleased to extend my warm greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The theme of this conference addresses one of the most dynamic and intellectually stimulating areas of contemporary physics. Advances in light–matter interactions continue to drive progress in photonics, quantum technologies, nanoscience, and advanced materials, with wide-ranging scientific and technological implications. By bringing together fundamental concepts and emerging research frontiers, the conference provides a valuable platform for the exchange of ideas and dissemination of high-quality research.

I commend the Department of Physics and the organizing committee for their initiative and dedicated efforts in hosting this international event. I am confident that the keynote/plenary/invited lectures, technical sessions, and scholarly interactions will inspire innovative thinking and foster meaningful collaborations among participants.

I wish the conference every success and all the participants a productive and enriching academic experience.

PROF. REJI PHILIP
PRINCIPAL
(GSS, BENGALURU CAMPUS)

Message from Principal

I am delighted to extend my warm greetings on the occasion of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The theme of the conference highlights one of the most vibrant and impactful areas of modern science, where fundamental understanding of light–matter interactions continues to drive major advancements in photonics, quantum science, nanotechnology, advanced materials, and interdisciplinary research. By covering topics from foundational principles to emerging frontiers, the conference offers an excellent platform for scholarly exchange and innovation.

I am pleased to note that this international forum brings together eminent scientists, academicians, researchers, and young scholars from across the globe. Such academic gatherings play a crucial role in strengthening research culture, fostering interdisciplinary collaboration, and enhancing global academic engagement—goals that resonate strongly with GITAM's vision of excellence in education and research.

I commend the Department of Physics and the organizing committee for their dedication, vision, and meticulous efforts in organizing this prestigious event. I also extend my sincere appreciation to the keynote speaker, plenary speakers, invited experts, delegates, sponsors, and all contributors for their valuable support. I am confident that the deliberations and outcomes of this conference will lead to meaningful insights, innovative research directions, and lasting collaborations in the field of light–matter interactions.

I wish the conference every success and all participants a fruitful and enriching academic experience.

PROF. N. V. KRISHNA PRASAD
HoD-PHYSICS
(GSS, BENGALURU CAMPUS)

Message from HoD & Chair, ALMIC-2026

It gives me immense pleasure to welcome you to the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

Light–matter interaction is a central theme in contemporary physics, underpinning remarkable developments in photonics, quantum technologies, nanoscience, advanced functional materials, and interdisciplinary applications. The objective of this conference is to provide a vibrant academic platform that bridges fundamental concepts with emerging research frontiers, encouraging the exchange of ideas among researchers from diverse backgrounds.

I am delighted to note that this event brings together eminent scientists, academicians, industry professionals, research scholars, and students from across the globe. Such interactions are invaluable for fostering collaborative research, promoting interdisciplinary approaches, and inspiring young minds to pursue excellence in scientific research.

On behalf of the Department of Physics, I sincerely thank the university leadership for their constant support and encouragement. I also extend my heartfelt appreciation to the organizing committee, keynote, plenary and invited speakers, delegates, sponsors, and all contributors whose efforts have made this conference possible. I am confident that the deliberations, discussions, and outcomes of this conference will lead to meaningful insights, innovative research directions, and long-lasting collaborations in the field of light–matter interactions.

I wish the conference grand success and all participants a productive, enriching, and memorable academic experience.

DR. PRASUN BANERJEE
ASSO. PROFESSOR-PHYSICS
(GSS, BENGALURU CAMPUS)

Message from Co-Chair, ALMIC-2026

It is a pleasure to welcome you to **ALMIC-2026 – Advances in Light-Matter Interactions: Fundamentals to Frontiers**, to be held at **GITAM (Deemed to be University), Bengaluru Campus,** during **4–6 February 2026**.

The conference focuses on contemporary theoretical, experimental, and computational advances in light–matter interactions, encompassing quantum phenomena and exotic states, energy and functional materials, metamaterials and nanostructured systems, as well as biological and soft matter. ALMIC-2026 aims to provide an interdisciplinary forum for the exchange of ideas, critical discussions on emerging directions, and the initiation of collaborative research.

I extend my sincere appreciation to all speakers, delegates, sponsors, and organizers, and wish the participants a stimulating and impactful conference experience.

DR. KADIYALA CHANDRA BABU NAIDU
ASSOC. PROFESSOR-PHYSICS
(GSS, BENGALURU CAMPUS)

Message from Convener

It is with great pleasure that I welcome you to the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The primary objective of this conference is to provide a dynamic and inclusive platform for scientists, academicians, and research scholars to share recent advances, exchange innovative ideas, and discuss emerging challenges in the broad field of light–matter interactions. By encompassing topics that span fundamental concepts to cutting-edge research frontiers, the conference aims to foster interdisciplinary dialogue and collaborative research.

We are honoured to host eminent keynote, plenary and invited speakers from leading institutions across the globe, whose expertise will greatly enrich the technical sessions and discussions. The enthusiastic participation of delegates from academia, research organizations, and industry reflects the growing importance and global relevance of this field.

I sincerely thank the leadership of GITAM for their constant encouragement and support. I also express my heartfelt gratitude to the organizing and advisory committees, session chairs, reviewers, sponsors, and student volunteers whose dedicated efforts have been instrumental in bringing this conference to fruition. I am confident that the interactions, deliberations, and outcomes of this conference will lead to meaningful scientific insights, innovative research directions, and enduring professional collaborations.

I wish all the participants a stimulating, productive, and memorable academic experience, and I look forward to the success of this conference.

DR. SUDESHNA SAMANTA
ASST. PROFESSOR-PHYSICS
(GSS, BENGALURU CAMPUS)

Message from Co-Convener

I am pleased to extend a warm welcome to all the participants of the International Conference entitled **"Advances in Light–Matter Interactions: Fundamentals to Frontiers,"** being organized by the **Department of Physics, GITAM School of Science (GSS), GITAM (Deemed to be University), Bengaluru Campus**, during **February 4–6, 2026**.

The conference aims to provide a vibrant platform for academicians, researchers, and research scholars to share recent advances, exchange innovative ideas, and discuss emerging challenges in the broad field of light–matter interactions. By bringing together fundamental concepts and cutting-edge research frontiers, the conference encourages interdisciplinary dialogue and collaborative research.

I sincerely appreciate the support and encouragement extended by the leadership of GITAM and acknowledge the dedicated efforts of the organizing committee, advisory members, speakers, reviewers, and student volunteers who have worked tirelessly to make this event possible. The enthusiastic response from participants across the globe reflects the relevance and importance of this theme.

I am confident that the technical sessions, keynote/plenary/invited lectures, oral & poster presentations and interactions during the conference will lead to meaningful scientific insights and foster lasting academic collaborations.

I wish all the participants a productive, engaging, and memorable conference experience.

CONTENTS

Invited Scientific Talks

Oral & Poster Presentations

ABSTRACTS

Prof. M.S. Ramachandra Rao
Department of Physics,
Quantum Centre for Diamond and Emergent Materials (QuCenDiEM),
India Centre for Lab-grown Diamond (InCent-LGD),
Nano Functional Materials Technology Centre,
and Materials Science Research Centre,
Indian Institute of Technology (IIT) Madras, Chennai-600036, India.
Email: msrrao@iitm.ac.in

Diamond and other wide bandgap materials for electronic and quantum applications

Our group focusses on the physics, doping and electronic correlations, defect-engineering and applications of thin films and nano-structures of Transition metal-oxides (TMOs) and diamond. During the past two decades, we have been focusing on utilizing diamond, the most versatile ultra-wide bandgap material for many technological applications. Diamond is a fascinating allotrope of carbon that offers half a dozen different applications, and its lattice is amenable to doping. Nano-crystalline diamond (NCD) coatings reduce carbon footprint in many mechanical applications. Diamond, despite being one of the most resistive materials, is driven to a semiconducting to superconducting state by boron doping and boron doped diamond (BDD) is considered as the most useful next generation granular superconductor useful for quantum-interface devices requiring high kinetic inductance. We have also demonstrated the use of boron doped diamond electrodes in the waste-water treatment. We are focusing on the quantum applications of diamond using nitrogen and other dopants. I will give a summary of our research and development journey of TMOs and diamond.

Prof. Urbasi Sinha
Raman Research Institute (RRI), Bangalore, India.
Email: usinha@rri.res.in

Quantum at the speed of light: Exotic photonic states, certified randomness, and quantum-secure technologies

Quantum mechanics is at its most striking when it produces states that have no classical counterpart, superpositions that refuse to behave like "either/or," correlations that outlive distance, and measurement outcomes that cannot be explained by any classical hidden-variable story. Photons are the ideal stage for this drama: they propagate at the speed of light, preserve coherence over long distances, and can be sculpted into high-dimensional and multi-photon quantum states that are both experimentally accessible and technologically actionable. In this plenary, I will trace a "discovery-to-deployment" arc for photonic quantum technologies, grounded in our experience across fundamental experiments and translational engineering. Starting from core quantum resources in light, such as superposition, interference, and entanglement, I will discuss how foundational tests of non-classicality and measurement can be repurposed into practical capabilities within **quantum communications**: trustworthy entropy generation, certified key material, and protocols whose security rests on experimentally verifiable quantum behaviour rather than assumptions about computational hardness.

I will highlight the role of **certified quantum randomness** as a central primitive for quantum communications. Nonclassical correlations enable certification of unpredictability, including device-independent approaches based on Bell nonlocality and single-system certification using temporal inequalities (Leggett–Garg). These tools illustrate a broader theme: "exotic" quantum behaviour can be engineered into an operational guarantee and then used directly in communication and cryptographic stacks. Building on this, I will discuss progress in **quantum-secure communication**, including quantum key distribution and its evolution from controlled laboratory demonstrations to field-relevant implementations. I will touch on atmospheric free-space links, pointing-acquisition-tracking for moving platforms, and the pathway toward satellite-based quantum communication. Finally, I will look ahead to scalable quantum networks, where multi-node entanglement distribution, quantum repeaters, and photon–matter interfaces (quantum memories) become essential. The talk will close with lessons from translating photonic quantum prototypes into products, including reliability engineering, validation standards, and the practical constraints that determine whether an exotic quantum state remains a beautiful experiment or becomes a working technology.

Prof. Giovanni Hearne
Department of Physics, University of Johannesburg, Auckland Park, Johannesburg, South Africa.
Email: grhearne@uj.ac.za

Advances in recoilless nuclear resonance spectroscopy for investigating light-matter interactions: Fundamentals to frontiers

Rudolph Mössbauer discovered nuclear resonance absorption of γ-photons in 1957. At the time he was a PhD student investigating nuclear resonance fluorescence, as the analogue to the well-known atomic-electronic resonance fluorescence. He developed an ingenious experimental setup involving the 129 keV nuclear transition in ^{191}Ir, which to his initial surprise showed an enhanced resonance absorption effect at cryogenic temperatures. Mössbauer recognised the stringent requirements for this nuclear resonance absorption and that that this would only be possible if nuclear transitions were recoilless. He further recognised that these conditions could best be fulfilled in a solid matter collection of quantum harmonic oscillators, i.e., crystal lattice. This earned him the Nobel Prize in 1961. Thus, his discovery of the recoilless emission of γ-photons by crystalline emitter nuclei (source) and recoilless resonance absorption of those photons by identical probe nuclei in an absorber (sample of interest), became known as the Mössbauer effect (ME). There was further recognition that such recoilless events occurring in the emitter lattice, rendered a radiation source of unprecedently narrow bandwidth, due to the linewidth of the nuclear excited state being only several neV. Such a highly monochromatized source of γ-photons enabled measurements of the 10−100 neV hyperfine shifts in nuclear levels of the Mössbauer probe atom in the absorber. Such shifts are due to interactions between the probe atom and its local atomic environment. Out of these fundamental discoveries emerged Mössbauer effect spectroscopy, constituting a local probe equally effective at providing atomic scale information of both amorphous/disordered and crystalline solids. The ME is now a very well-established investigative probe and analytical technique in a broad spectrum of disciplines, i.e., in the physical, earth and biological sciences as well as in engineering and materials science. I will exemplify how this neV-resolution spectroscopy has been evolved to investigate current and new-age problems. Examples will include a selection from ^{57}Fe ME studies of (i) magnetic-electronic phenomena in quantum matter under extreme pressure conditions [1], (ii) pressure tuning the spin-flop in hematite (Fe_2O_3) [2], (iii) H-bonding proton dynamics influenced by host lattice electron dynamics [3], and (iv) in situ spatio-temporal study of Fe-phase evolution in Fischer Tropsch synthesis [4].

References:

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4. E. de Smit and B.M. Weckhuysen, Chem. Soc. Rev. 37, (2008) 2758–2781.
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Prof. Venu Gopal Achanta
Director,
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Exotic coupling states in coupled exciton-plasmon systems

Light-matter interaction is one of the well-studied experimental areas after the invention of the laser. Theoretically, it is studied by modelling a two-level system, such as an atom or a quantum dot, inside a cavity. The cavity mode and the two-level system have different dynamics. However, depending on the coupling strength and its relationship with the decay rates of the two-level system and the cavity photon, different coupling regimes are possible. These are the weak, strong, ultra-strong, and deep strong coupling regimes. In a solid-state system, an exciton in a quantum dot or a defect in a 2D material or nanodiamond can be a two-level system, and the cavity can be an external cavity or a plasmon-mediated structure. In plasmonic structures with embedded nanoparticles, I will present enhanced emission in the weak coupling regime, anti-crossings in the strong coupling regime, and long-range coherent oscillations in the ultra-strong coupling regime, as observed in time-resolved measurements. Some of the applications of these in single-photon emission will be presented.

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Terahertz (THz) spectroscopy: Sources and detectors with applications

Terahertz (THz) spectroscopy offers large opportunities in the ultrafast study of materials of various kinds. We have developed several Terahertz (THz) spectroscopic techniques to study different materials from single crystals to metamaterials. There are no cheap and compact high-power sources or sensitive detectors of THz radiation. They are either expensive or difficult to fabricate. Using Laser driven THz sources and detectors, we can build THz time domain spectroscopy (TDS) setup. We developed different designs of the THz sources using different materials like SI-GaAs, GaAs: C and Germanium. We characterized Germanium based Sources and Detectors grown on many different substrates. **We first demonstrated detection of THz pulses using Germanium based detector [**1]. We have studied many pharmaceutical materials for their unique identification and were able to find molecular resonances in the THz region. We have studied Metamaterials of different types for various applications. We studied THz optical properties of Vanadium doped [100] β-Ga_2O_3 using THz-TDS [2]. The V-doped β-Ga2O3 crystal shows strong birefringence in the 0.2-2.4 THz range. We measured phase retardation over the whole THz range by developing THz Time-Domain Polarimetry (THz-TDP). We have also studied Metamaterials of different types for various applications. Polarization dependent transmission through an array of subwavelength apertures can have practical applications. We studied THz transmission through such surfaces. We developed a Near Field Scanning THz Microscope for this purpose. Whatever is seen by using Computer simulation, those near field patterns can be observed using this unique microscope. We studied numerically and experimentally excited bound state in the continuum (BIC) mode with a high Q-factor in the THz meta-molecule (composition of meta-atoms) system, leveraging a unique method of selective symmetry breaking in a ring-shaped metamolecule system. The experimental transmission spectrum and the near-field scanning images firmly validate [3], the existence of the high Q BIC mode under this strategic symmetry-breaking approach.

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Laser annealing: A light -matter interaction process to make crystalline oxides compatible with polymer substrates

Light -matter interactions are many and some of them are capable of modifying the structure of the material itself, especially if we use a pulsed laser with pulse durations less than a nano second. The laser parameters play a crucial role in these interactions and there are different models to understand their role in structure modification of materials. One such application, the laser annealing, is highlighted in this Talk.

There are phenomena which are exhibited only by crystalline state of the matter. Ferroelectricity is one such phenomena. But the crystallization of oxide ferroelectrics is a high temperature process while most of the ferroelectrics which give highly desirable properties are oxides. They crystallize at about 700°C, a temperature beyond the reach of polymers and nanoscale silicon processes. Hence ways suitable for their non thermal crystallization is to be explored. A comfortable temperature for both the above mentioned applications is 250-300°C. It has been found that laser annealing is a suitable process to get these oxide films crystallized at these temperatures. Because of penetration depth related issues, the crystallization archived is not complete but good enough for them to exhibit their characteristic piezoelectric properties. The process requires extensive optimization as the number of parameters involved are many. These studies were carried out primarily with the PLD grown films of $Ba_{0.5}Sr_{0.5}TiO_3$ (BST) and the studies were primarily in terms of their dielectric properties in the microwave range and their DC field dependence. The polymer substrate used is modified PTFE composite known by the trade name as RT Duroid. This process is significant considering the Semiconductor technology roadmap goal of integrating functional oxides with nanoelectronics in Si by 2028.

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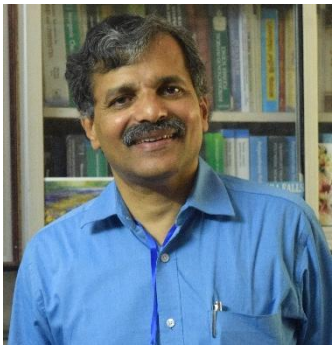

Interfacial modification in nanocomposites to tailor functionalities

The talk will concentrate on various approaches being used to engineer materials at the nanoscale for various applications in future technologies. In particular, the case of clay, carbon nanostructures (e.g. nanotubes, graphene), metal oxides, bionanomaterials (cellulose, starch and chitin) will be used to highlight the challenges and progress. Several polymer systems will be considered such as rubbers, thermoplastics, thermosets and their blends for the fabrication of functional polymer nanocomposites. The interfacial activity of nanomaterials in compatibilizing binary polymer blends will also be discussed. Various self-assembled architectures of hybrid nanostructures can be made using relatively simple processes. Some of these structures offer excellent opportunities to probe novel nanoscale behavior and can impart unusual macroscopic end properties. I will talk about various applications of these materials, considering their multifunctional properties. Some of the promising applications of clay, metal oxides, nano cellulose, chitin, carbon nanomaterials and their hybrids will be reviewed. Finally, the effect of dewetting up on solvent rinsing on nanoscale thin films will also be discussed.

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Raman spectroscopy investigations of isostructural phase transition in tin-based alloys under compression

Pressure of the order of few to few tens of GPa, is an excellent external tool to controllably tune the electronic wavefunction overlapping in the condensed matter systems, without any chemical doping. Thus, with the application of pressure one can fine tune the electronic structure. In several cases, such fine tuning can take the system to unconventional ground states hosting novel functionalities or interesting collective excitations. Systematic data on the high-pressure (HP) evolution of the structural and the local structural parameters is an important experimental input needed in comprehending such phenomena. From the crystallographic point of view, such transitions may not always necessarily involve a symmetry changing structural phase transition, though the Fermi surface can have a topological transition. In particular, transitions which does not require a lattice symmetry change – generally termed as isostructural phase transitions leave imprints in systematic datasets such as HP Raman spectroscopy. Such data coupled with other complementary computational and experimental investigations provides a wealth of knowledge. Recently we have applied HP Raman spectroscopy to a number of systems, particularly tin based intermetallics. Thanks to its relatively low melting temperature, tin is employed as a technologically strategic system. Low melting temperature also permits tin to form a variety of intermetallic compounds with vastly varying functional properties. We have been investigating several such compounds under HP: the intermetallic Ru_3Sn_7 [1], a few stannide based quasi-skutterudite superconductors [2,3], noncollinear antiferromagnetic Mn_3Sn [4], the topological nodal line semimetal $PtSn_4$ [5], *etc.* Several of these systems are found to have pressure-induced isostructural phase transitions. Details about such investigations will be presented.

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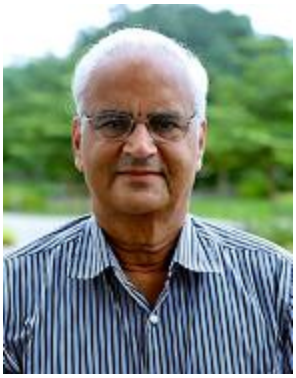

Microwave sintering studies on bulk and nano ceramics

Microwave sintering is one of the recent techniques to synthesize the nano materials. Most Recently, Dielectric and Magnetic ceramics, Carbon nano materials and Metals are synthesized using Microwave sintering process. Many of the physico chemical properties are observed with enhancement for device applications. A comparison between conventional sintering and microwave sintering has revealed the enhancement of density and uniformity of grain size and intrinsic properties like ionicity and reduction of damping coefficient of lattice vibrations with improved dielectric and magnetic properties. In this presentation, High energy ball milled nano ceramic composites with ferrite and ferroelectric composites were synthesized by Microwave sintering. The uniformity of grain size, single phase nature and increase in density of individual ceramic oxides were well observed. The composites showed retention of nano crystallinity. These composites showed enhancement of dielectric properties for Magneto Electric behavior. Increase of ionicity was also observed and its effect on dielectric properties are presented. A comparison with bulk materials of micron size and nano size ceramics synthesized by conventional and microwave sintering are also presented. The importance of ceramic oxides and development for ceramic tape for Low Temperature Co-Fired Ceramic devices are also discussed.

Role, concepts, design and development of some EMI materials for EM shielding

Recent advancements in material science and engineering have encouraged miniaturized and integrated electronic devices and gadgets that contributed to electronic interference (EMI) at low and high frequency of EM spectrum and in turn affecting additional signals to the supporting devices. Choice of materials with their design and development with suitable specifications play a vital role for electromagnetic shielding. This comprehensive tutorial lecture deals with role, concepts and design and development of some EMI materials apart to some ongoing industrially productionized materials for our country needs on EM shielding.

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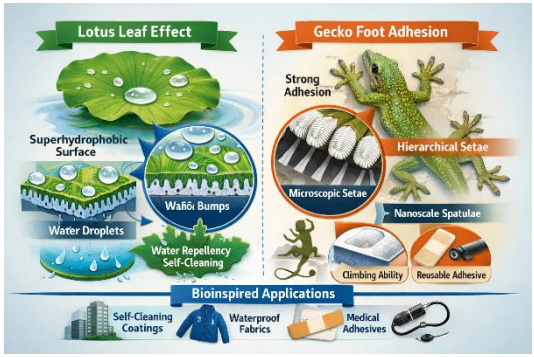
Bio-inspired hierarchical materials: Nature inspired technologies

Bioinspired hierarchical materials, such as those that resemble the lotus leaf and gecko foot, are being investigated for their self-cleaning and sticky capabilities. These functions are related to their hierarchical structures at the micro- and nanoscale levels. Several creatures, including insects, spiders, and geckos, have built intriguing nanoarchitectures to increase and control adhesion. The hydrophobicity of the lotus leaf surface and the extraordinary adhesive capabilities of gecko feet are only two examples that have been successfully reproduced and employed in various technological applications. Geckos' exceptional adhesion and climbing agility over uneven terrain are believed to stem from the multiscale hierarchical structures on their feet. Hundreds of thousands of elastic hairs termed "setae," each of which splits into multiple spatulas, form a high number of contact points, resulting in significant adhesion via van der Waals interactions. Gecko adhesives are glue-free, self-cleaning, reusable, and insensitive to a wide range of surface chemistry and roughness. Gecko-inspired adhesives have numerous industrial applications, including robotic endoscopy, biomedical cleaning, medical bandage tapes, rock climbing adhesives, and tissue adhesives. Gecko toes and spider filament could spur innovation in the glue and adhesives industry, as well as the building and textile industries. Nature's miracle inspired scientists to create a dry and self-cleaning glue. A Superman toy has also been made based on a similar sticky tape that adheres to glass surfaces. Gas endoscopy is a very promising discipline in which many patients could benefit from bioinspired adhesives. Super hydrophobicity, often known as the Lotus Effect, is an extraordinary phenomenon. The lotus effect is characterized by a surface's exceptional water repellence and self-cleaning due to its micro/nanostructures. It has been employed in numerous fields. For example, it is used in self-cleaning façade paints and waterproof, anti-rain fabrics. This presentation discusses these details.



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One dimensional nanostructured materials for applications in energy conversion and environmental pollution control

One-dimensional nanostructure holds special importance in nanoscience because of directional charge transport and higher specific surface area, that make them useful for reduced recombination of photogenerated charges. In particular, vertically aligned structures directly grown from an underlying substrate offer high flexibility and advantage in device design and implementation. In this talk, I shall discuss fabrication of three metal oxide systems such as TiO_2 nanotubes/nanorods, CuO-nanowires and $BiFeO_3$ nanorods in vertically oriented morphology and their heterostructures. Further, the charge transport mechanisms in single/individual nanostructure have been studied and their photo-electrochemical properties are explored. Also, our work on ion beam irradiated TiO_2 nanorods will be discussed. In the final part, I will present recent developments on photocatalytic CO_2 reduction using TiO_2-Graphene oxide nanocomposites and our innovations in both materials engineering and reactor design.

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Ultrashort pulse laser ablation for multi-functional nanomaterials

Pulsed laser light-matter interaction is a fascinating phenomenon with profound underlying physics, chemistry, and materials' properties. Further, it and has potential applications such as high-precision micromachining/processing/fabrication, surface functionalization, sensing, etc. The interaction of focused pulsed (picosecond and femtosecond duration) laser light with matter (in air and liquids) results in (a) novel phases of the matter, (b) novel colloidal nanoparticles and surface nanostructures in a single experiment using the technique of laser ablation in liquids, and (c) novel practical applications (anti-corrosion, hydrophobicity, hydrophilicity, complete absorption) [1-4]. In this presentation, we will discuss the effects of the interaction of pulsed laser light with diverse materials such as metals (Ag, Au, Ag-Au-Cu), semiconductors (Si, Ge, GaAs, SiC, InP), 2-D materials (WS_2, MoS_2, MXenes), and high-entropy alloys [5-19]. We discuss the formation of functional nanomaterials/nanostructures resulting from this interaction (ablation/irradiation), consequential in surface-enhanced Raman scattering (SERS)-based sensing applications, photonics, and defense.

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Ultrafast spectroscopy and dynamics of singlet exciton fission

Organic semiconductors have shown immense potential as replacements for traditional inorganic materials in optoelectronics applications, particularly in organic light emitting diodes (OLED) and organic photovoltaics (OPVs), to be mentioned specifically. At the core of the device physics governing the stability and efficiency of these devices are formation, lifetime, migration and annihilations of tightly bound electron-hole pairs, known as excitons, as well as the charge carriers, namely electrons and holes. Following optical or electrical excitation of organic semiconductors in these devices singlet and triplet excitons are generated. Singlet excitons usually decay radiatively and quickly (typically in nano-second) to the ground state. In contrast, triplet excitons, which are frequently non-radiative and longer lived (typically microseconds), can play important roles in organic optoelectronic devices. In recent decades, increasing attention has been paid to increase and utilize the triplet excitons in organic semiconductors. Additionally, the Shockley-Queisser (S-Q) limit is the theoretical maximum power conversion efficiency for a single-junction solar cell, capped at around 33.7. Among several strategies, using multi-junction cells and multi-exciton generation (MEG) methods have been successfully implied to overcome the S-Q limit.

MEG method involves generating more than one electron-hole pairs or excitons from a single high-energy photon. Towards this endeavor, search for molecules, which undergo efficient singlet exciton fission (SEF) to generate two triplet excitons following absorption of a single photon, has been very intense during the last two decades. Tetracene, pentacene and its derivatives have shown great potential to become efficient SEF materials and so, the dynamics of SEF reactions in nanoscale media have been extensively studied. In this consideration, the detailed photophysics and dynamics of the SEF process in Naphtho-[2,1,8-qra]-Tetracene (NpTc), which satisfies the energetic requirement of SEF, has recently been investigated by our group in polycrystalline media using ultrafast spectroscopic methods. This work has identified two sequential steps of the SEF process involving two spin correlated triplet pair states (CTP1 and CTP2), namely interacting and noninteracting CTPs, respectively, prior to generating two triplet excitons in sub-50 ps time-domain with the triplet exciton generation efficiency of about 85%.

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Nanostructured biowaste-based electrodes: A sustainable path to high-energy storage

The growing demand for sustainable energy has driven significant progress in developing environmentally friendly materials for energy storage systems. Biomass-derived electrode materials have attracted considerable attention due to their natural abundance, renewability, low cost, strong chemical and thermal stability, minimal environmental impact, and the ability to tailor structural properties for specific applications. Various biomass sources including agricultural waste, lignocellulosic materials, and biopolymers, are being explored for their potential to produce high-performance carbon-based electrodes. This research focuses on recent advancements in eco-friendly carbon electrodes synthesized from biomass for high-performance supercapacitors, highlighting agricultural and organic waste sources such as banana peels, tea residues, coconut shells, jackfruit peels, cauliflower, and other agricultural residues. Key fabrication techniques, including pyrolysis, chemical activation, and heteroatom doping, are discussed in relation to their influence on porosity, conductivity, and energy storage capacity. Activated carbons derived from biomass exhibit highly porous structures (surface area often exceeding **1500 - 2500 $m^2 \cdot g^{-1}$**) and large pore volumes, enabling excellent ion transport and charge storage. These materials achieve specific capacitances up to **300 - 450 $F \cdot g^{-1}$**, energy densities of **20 - 35 $Wh \cdot kg^{-1}$**, and power densities above **10 $kW \cdot kg^{-1}$**, making them ideal for supercapacitors and other applications such as hydrogen storage, catalysis, and adsorption. The paper also addresses current challenges, such as scalability, consistency, and integration into commercial devices, while outlining future research directions for the systematic development of biomass-derived electrode materials.

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Next-generation smart windows: Efforts towards the development of smart windows for sustainable energy applications

There is a great demand for smart partitions to serve as wide-area switchable gates for light transactions across defined spaces at offices, public locations, as well as homes. In addition, smart partitions can serve as canopy glasses for greenhouses, aiding in efficient crop harvesting. However, current partitions and windows only provide transparency and require permanent fixtures such as screens or curtains for adequate see-through visibility. Household ventilation and indoor lighting and temperature control are responsible for over 40% of global energy consumption, making energy-saving technologies critical. Smart windows have gained prominence as they optimize indoor light and heat transmission, reducing the usage of air conditioners, lights, and heaters. The challenge lies in developing cost-effective, power-efficient, and simple-to-fabricate smart windows. Our team has been working on designing affordable and functional smart windows that I will be discussing in this talk. By attending, you will gain insights into the latest technological advancements in smart windows and their potential for energy-saving applications.

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2D materials for quantum technologies and novel Physics

Two-dimensional (2D) materials are next-generation materials relevant for optoelectronics and electronics, as well as integrated photonics and quantum technologies. In this talk, I will first present a broad overview of why 2D semiconducting materials are interesting for both technologies, and fundamental physics [1]. I will discuss aspects on useful defects and twisted heterostructures.

I will present our group's work on the creation of low density of defects in monolayer MoS_2, using ultralow energy electron irradiation, for hosting single photon emitters (SPEs) [2,3]. I will then discuss our recent work on exciton dynamics in reconstructed 2D systems [4].

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Random laser based high-resolution biomedical imaging

Lasers, owing to their narrow bandwidth, high brightness, and spectral tunability, are one of the preferred excitation sources for fluorescence imaging. However, the presence of parasitic coherent artefacts in the laser illumination causes uneven excitation of fluorophores, and has a critical impact on the reliability, resolution, and efficiency of fluorescence imaging. The control of the laser's coherence is possible with modified cavity lasers. Of particular interest is the random laser, in which highly scattering particles dispersed in a gain medium act as a cavity for trapping the light and provide sufficient feedback for lasing through multiple scattering. In the first part of the talk, I will discuss the development random laser based artefact-free wide-field fluorescence bioimaging modality to obtain superior contrast fluorescence images, even of highly diffusive biological samples with sub-micron resolution. In an alternate perspective, the randomness inherent in biological tissues can trap light through multiple scattering events and provide optical feedback to generate random lasing emission. The emerging random lasing signals carry sensitive information about the scattering dynamics of the medium, which can help in identifying abnormalities in tissues, such as cancer. Utilizing the random lasing emission from tissues, a bimodal system capable of identifying and imaging tumour polyps as small as 1 mm2 in phantom tissue samples for the early diagnosis of tumour growth is developed. The integration of random lasing principles with sensing and imaging modalities has the potential to provide an efficient, minimally invasive, and cost effective means of early detection and treatment of diseases such as cancer.

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Spin-Orbit coupled Dirac fermions

Spin-Orbit coupling allows for newer implementation of microscopic symmetries. In this talk I shall discuss the rich set of phases that arises in proximity to a spin-Orbit coupled Dirac semimetal. The nature of both normal and superconducting phases bears distinct signatures of the underlying intertwining of spin and real spaces.

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Tunability in double perovskites by comparing structural, magnetic and dielectric properties on Tb_2CoMnO_6, Tb_2NiMnO_6

In quest of materials for futuristic industrial/device applications, double perovskite (DP) materials are intensively being explored by research group across the world. The interest is majorly driven due to exhibition of unique structural and physical properties viz. ferroelectricity, electrical conductivity, magnetodielectric, magnetoresistance etc in this class of compound [1-4]. Structurally these compounds are driven out by doubling simple perovskite (ABO_3) formula as $A_2B_2O_6$ and replacing B ion by another ion B' where large electropositive cation and small transition metal anion occupies A and B (B') sites. Several research articles in the literature suggests that due to availability of suitable elements at A and B (B') site, DP compounds exhibit wide physical properties and thus provide opportunity to optimize the properties as per the requirement. This aspect is driving research in these compounds in condensed matter research [5]. Research on these materials also enriches our understanding of fundamental physical principles and leads to development of advanced materials. Here, we discuss the case for tunability in double perovskite by studying structural, magnetic, dielectric and other physical properties on Tb_2CoMnO_6 and Tb_2NiMnO_6. These were synthesized in polycrystalline form by employing solid state route. Phase formation was confirmed by X-ray diffraction (XRD) and neutron diffraction (ND) recorded at PD-III diffractometer at Dhruva, India [6]. Rietveld refined XRD and ND patterns were fitted with monoclinic $P2_1/n$ space group by employing Fullprof suite [7]. Magnetization study carried out by employing PPMS in VSM mode (M/s. Quantum Design) on $Tb_2Ni/CoMnO_6$ ascertain, paramagnetic to antiferromagnetic transition. Isothermal magnetization study further elucidate ordering. Physical and structural properties are also comprehended by temperature dependent neutron diffraction, dielectric, specific heat, AC Susceptibility study and will be discussed in the talk. We have found evidence which elucidates the role of Ni and Co ion in tailoring properties and magnetic structure in respective double perovskite compounds.

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Emergent sub-Ohmic zero gap state at Mott quantum criticality

Quantum phase transitions driven by electron correlations lie at the heart of some of the most intriguing phenomena in condensed matter physics. In this talk, I will introduce the concept of Mott quantum criticality (MQC) and highlight how it manifests in experiments on correlated materials. I will then outline the conventional theoretical framework based on the Hubbard Hamiltonian in the infinite-dimensional limit, which has shaped our current understanding of the Mott transition. Going beyond this standard picture, I will present our recent work based on a modified periodic Anderson model, where we uncover a striking and unexpected result: exactly at the Mott quantum critical point, the system hosts an emergent zero-gap state with a sub-Ohmic (soft-gap) low-energy spectrum. This critical state is neither a Fermi liquid nor a conventional insulator, but represents a distinct, correlation-driven quantum phase. I will conclude by discussing clear, experimentally testable signatures of Mott quantum criticality in dc and optical transport, providing direct routes for connecting theory to ongoing and future experiments.

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Strange metals with spatially random interactions, and their universal transport properties

The recently developed paradigm of spatial randomness in electron interactions in strongly correlated metals has shown great promise in explaining certain aspects of the experimental phenomenology of strange metals within the framework of large-N theories. I will describe numerically exact hybrid Monte Carlo simulations of two-dimensional metals with spatially random antiferromagnetic interactions, which are free from artificial constructions such as large-N limits. Our simulations reproduce strange metals' key experimental signature of linear-in-temperature resistivity with a universal 'planckian' transport scattering rate $\Gamma_{tr} \sim 2\pi k_B T/\hbar$ that is independent of coupling constants. We further find that strange metallicity in these systems is not associated with a quantum critical point and instead arises from a phase of matter with gapless antiferromagnetic fluctuations that lacks long-range correlations and spans an extended region of parameter space: a feature that is also observed in several experiments. These gapless antiferromagnetic fluctuations take the form of spatially localized overdamped modes, whose presence could possibly be detected using recently developed nanoscale magnetometry methods. I will also describe signatures in the magnetic structure factor $S(q, \omega)$ of the low energy regime of spin fluctuations controlled by these localized modes, which can be measured in neutron scattering experiments. Finally, using dynamical mean field theory methods, I will show that the tendency of electrons to localize due to Hubbard-U Coulomb repulsion leads to a non-perturbative enhancement of strange metal behavior arising from spatially random antiferromagnetic interactions.

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Spin–valley Physics and interlayer excitons in two-dimensional TMDCs

Two-dimensional transition metal dichalcogenides (TMDCs) have emerged as a key platform for valleytronics and exciton-based optoelectronics due to their coupled spin–valley degrees of freedom. While pristine monolayers and heterostructures have been widely explored, TMDC alloys offer an additional and largely untapped degree of freedom through band-gap and symmetry engineering. In this talk, I will present a comprehensive experimental and theoretical investigation of spin–valley physics and excitonic phenomena in TMDC alloy systems.

I will first demonstrate valley polarization and helicity-dependent photocurrent generation in monolayer and bilayer $MoS_{2x}Se_{2(1-x)}$ via the circular photogalvanic effect. Piezoelectric force microscopy reveals an intrinsic out-of-plane electric field in the alloy, breaking mirror symmetry and enabling electrical control of the photocurrent. First-principles density functional theory calculations support the experimental observations and elucidate the role of alloy-induced symmetry breaking. Building on this concept, we introduce alloying as a novel route to realizing interlayer excitons in bilayer $WS_{2x}Se_{2(1-x)}$ without the need for conventional type-II heterostructures. The internal electric field drives an effective band alignment that promotes spatial separation of charge carriers across layers. Circularly polarized photoluminescence measurements reveal interlayer excitons with a negative degree of circular polarization that increases with temperature. A simple theoretical model shows that this behavior is dominated by spin polarization rather than valley polarization, reflecting the spin–valley–layer coupling intrinsic to TMDC bilayers.

Our results establish TMDC alloying as a versatile strategy for controlling valley-dependent transport and excitonic states, opening new pathways toward room-temperature valleytronic and quantum optoelectronic devices.

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The influence of samarium on structural and magnetic properties of $CoFe_2O_4$

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The structural and magnetic properties of $CoFe_{2-x}Sm_xO_4$ (x = 0, 0.05, 0.1, 0.15, and 0.2) compounds are discussed and the results are reported. The materials were synthesized using a tactical process such as a solid-state conventional reaction technique. The formation of the compounds in the cubic inverse spinel phase with space group $Fd\bar{3}m$ was confirmed from their Rietveld refined x-ray diffraction (XRD) patterns and Raman spectra. Upon the partial substitution of Fe^{3+} by Sm^{3+}, the lattice constant is found to increase then decrease. The lattice constant values, bond angles, bond lengths, coordination numbers, interatomic distances, and other factors were estimated with the help of Rietveld refinement. The substitution of higher the ionic radius of Sm^{3+} (0.964 Å) by Fe^{3+} (0.69 Å), resulted in the formation of small amount of secondary phase from x = 0.15 onwards. The Raman spectra gave the peaks corresponding to the tetrahedral and octahedral groups. The right shift of the peaks indicates the presence of massive Sm^{3+} ions at the octahedral sites. The surface morphology is depicted through scanning electron micrographs. The investigated samples are found to be transparent, homogenous, and uniformly distributed. The obtained samples' elemental content and atomic ratios were confirmed using energy-dispersive spectroscopy. As the Sm^{3+} concentration x increase, the saturation magnetization (M_s) values were found to drop from 82.4 emu/g for x = 0 to 52.63 emu/g for x = 0.2. The magnetization (M) was also measured as a function of temperature T in the range of 300 – 900 K, at a field of 100 Oe. The Curie temperature (T_C) is extracted from the inflection point (in M vs T) which gives a minimum in dM/dT vs T at $T = T_C$. The effect of the doping of the higher ionic radius and high magnetic moment Sm^{3+} ions causing the reduction of Ms values, altered H_c values, T_C are discussed and explained in detail. In addition, the cubic anisotropy constant (K_1) values of all the compounds were calculated employing LAS method and the role of Sm^{3+} on K_1 is also discussed.

Keywords: Ferrites; Magnetization; LAS; Curie temperature.

Computational methods and statistical analysis for advanced ceramics

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Recent advances in statistical modelling and data-driven techniques have transformed the study and design of ceramic materials. This review highlights the application of regression analysis, Bayesian inference, multivariate statistical methods, and machine learning approaches in understanding and predicting ceramic properties. Key applications include mechanical strength and fracture toughness prediction, microstructural characterization, optimization of processing parameters in sintering and additive manufacturing, and phase

stability and thermal behavior modelling. Despite significant progress, challenges remain in the availability of high-quality datasets, integration of multiscale models, interpretability and reproducibility of machine learning predictions, and incorporation of uncertainty quantification. We discuss strategies to address these challenges, including the development of standardized databases, multiscale modelling frameworks, interpretable algorithms, and closed-loop materials discovery pipelines. The integration of statistical and computational methods with experimental data promises to accelerate the design of high-performance ceramics, enabling more efficient materials development for diverse applications.
Keywords: Ceramics; Statistical Modeling; Data-Driven Approaches; Machine Learning.

Efficiency of solar PV panel charging an electric vehicle battery via a DC to DC boost converter

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This paper investigates whether a simple MATLAB/Simulink model can be developed to charge an electric vehicle battery via a DC-DC boost converter from a Solar PV panel. The idea is to create a constant duty cycle for all input solar irradiance and temperatures. In the developed model, the continuous duty cycle is maintained at 38 %, and the efficiency of the solar PV panel's output to the battery charging power is above 98 %. The system is subjected to variable irradiance from 200 to 1000 watts per square and temperature from 25 to 45 ^{o}C for testing purposes. The simulation results show that the efficiency was above 99 %. It is noted that no PID controller is used in the present paper, making the implementation of hardware friendly. The output responses through Simulink diagrams show high efficiency power transfer from the PV panel output to the electric vehicle battery charging with a constant duty cycle.
Keywords: Solar photovoltaic, MPPT, boost converter, electric vehicle battery, charging efficiency, MATLAB/Simulink.

Tunable elastic wave band gaps and transmission in aluminum and silicon phononic metamaterials

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Phononic metamaterials offer tunable control over elastic waves in solids, with band gaps strongly dependent on material properties and geometry. In this study, a single unit cell with a circular hole was modelled using 3D Finite Element Analysis (FEA) in COMSOL's structural mechanics module, with aluminum and silicon assigned for their contrasting stiffness and density in separate simulations. Geometric parameters, including hole radius and thickness, were systematically varied to identify the configuration yielding the largest elastic band gap of ~28%. The optimized unit cell was then assembled into a finite multi-unit array, and elastic

waves were sent through the array to analyze transmission. The results showed that the array effectively suppressed elastic waves, with aluminum structures attenuating lower frequency waves and silicon structures shifting suppression to higher frequencies due to their higher stiffness. They showed combined influence of material choice and geometry with quantitative guidance for designing nanoscale devices for frequency selective elastic wave control.
Keywords: Metamaterials; FEA; Wave attenuation; Elastic band gap; COMSOL.

Smart algorithm for finding the MPPT parameters of solar PV panel

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The work aims to predict voltage, current, and power with corresponding MPPT input parameters, solar irradiance, and the solar PV panel temperature. The literature shows that there are different MPPT algorithms. Most algorithms refer to real-time Voltage and current sensing at least a couple of times before the algorithm converges. In phase-1 of this paper, Matlab m-file coding is done based on a 6^{th} degree polynomial prediction of v, I at maximum power based on data of the different irradiance levels. The 6^{th} order predicted v, I with 100% accuracy. The limitation of the 6^{th}-degree polynomial is that it does not take care of the difference in temperature variations at the solar panel. In phase 2 of the paper, a second-order linear regression model is developed in MATLAB M-file for predicting v, I corresponding to maximum power with respect to variations in irradiance and temperature. The fitted linear regression model achieved an efficiency of more than 98%. The advantage of a data prediction algorithm is that it takes only one time to collect the sample of irradiance and temperature. In contrast, MPPT algorithms require multiple sensing of v and I before convergence.
Keywords: Photovoltaic system; Maximum Power Point Tracking (MPPT); Renewable energy.

Hyperbolic dispersion of silver nanowire array metamaterial and purcell enhancement of the coupled CdSe-ZnS quantum dots

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Collective dielectric response of silver nanowires grown in a porous Aluminium oxide host, shows broadband hyperbolic dispersion in optical regime. The nanowire array material is called as hyperbolic metamaterial (HMM), due to the nature of dispersion. The nanowires were grown by electrodeposition of Silver in Alumina matrix, to have a nanowire filling fraction of 15%. The collective dielectric response is modelled by Maxwell-Garnet effective medium theory (EMT) predicts that the set-in of the hyperbolic dispersion is at 589 nm in reflection spectrum and the sharpness of transition depends upon the losses of the HMM. A sharp transition in the differential reflection spectrum is observed at 590 nm, which is in good

agreement with EMT modelling of HMM. The hyperbolic dispersion results in diverging photonic density of states, for HMM. As a consequence, light emitters placed in the near field region of HMM are predicted to show significant radiative decay rate enhancement. To validate this, CdSe-ZnS alloyed quantum dots (QDs) were synthesized with Photoluminescence (PL) peak emission at 591 nm. The QDs were deposited onto HMM samples with polymer spacer by spin coating. The observed spectral shape and linewidth of QDs on HMM was unchanged, whereas the radiative lifetime of QDs showed significant modification. The Purcell factor of QDs at 10 nm separation from the HMM surface, was observed to be 4.8 ± 0.2. This confirms that the interaction of QDs with HMM modes is in the weakly coupled, Purcell regime. It was also observed that the Purcell factor of QDs has reduced, when they were deposited at a further distance from the HMM surface. This behaviour is explained by the variation of photonic density of states with distance from the surface of HMM. The HMM system shows potential to serve as a platform to probe emission dynamics of faint light emitters, due to its broadband hyperbolic dispersion and scalability of the metamaterial fabrication.

Keywords: Silver nanowires; Hyperbolic metamaterial; Quantum dots; Lifetime; Purcell effect.

Metal-free heteroatom-doped graphene quantum dots for hydrogen evolution in proton exchange membrane water electrolysis

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Electrolytic hydrogen production by proton exchange membrane (PEM) water electrolysis still relies heavily on precious-metal catalysts, motivating the search for durable, metal-free alternatives, especially at the anode where oxygen evolution reaction (OER) is demanding. Here, we developed and test multi-doped GQDs as high-performance, metal-free anode catalysts for proton eexchange membrane water electrolysis (PEMWE). The GQDs were prepared by rapid, infrared-assisted carbonization of citric acid, urea, boric acid, and Nafion®, yielding uniformly nanoscale particles co-incorporating nitrogen, fluorine, and boron. These heteroatoms generate abundant surface-active sites and tune the electronic structure to accelerate the OER phenomenon. In single-cell PEMWE evaluations coupled with either conventional Pt or barbituric-acid (BTA)–modified Pt cathodes, the N/F-co-doped GQD with BTA-modified Pt delivers the enhanced hydrogen evolution performance, reaching 350 L kWh^{-1} at 2.5 V and 50 °C, and sustaining 10 h of operation with only a 2.3% loss in current density. Mechanistic analysis indicates that the dopants redistribute charge, enhance hydrophilicity, and lower activation barriers for both OER and HER, while the pairing of N/F-co-doped GQDs with H-rich Pt improves proton transport, water adsorption, and catalytic turnover. Collectively, these results position multi-doped GQDs as a practical, sustainable class of metal-free electrocatalysts for next-generation PEM water electrolyzers.

Keywords: Graphene Quantum Dots (GQDs); Metal-Free Electrocatalysts; Hydrogen; Oxygen.

Fabrication of novel PANI/STO/AC heterojunction for enhanced photocatalytic reduction of 4-nitrophenol

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The present study involves the synthesis and fabrication of a novel dual Z-scheme heterojunction photocatalyst composed of Polyaniline, $Sr_3Ti_2O_7$, and Activated carbon (PANI/STO/AC). The heterojunction was synthesized by an in-situ polymerization method and characterized by various techniques like X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscopy (SEM), BET surface area, photoluminescence emission spectra (PL), and UV-Vis diffuse reflectance spectroscopy (UV-DRS). The band gap of the PANI/STO/AC was found between 1.1 to 1.5 eV. The photocatalytic activity of the heterostructures was evaluated for the reduction of 4-nitrophenol to aminophenol for various concentrations ranging from 10^{-4} M to 10^{-3} M under sunlight and visible light. Results indicate that heterojunction has a superior reduction of 4-nitrophenol, with 90-100% removal efficiency under sunlight than visible light, compared to individual materials. This study presents a novel approach for constructing dual Z-scheme PANI/STO/AC-based materials with promising applications in photocatalytic reduction of organic pollutants.
Keywords: PANI, Activated carbon, Z-scheme heterostructure, photocatalyst, sunlight.

Control of re-entrant localization transitions in non-Hermitian quasiperiodic chains via Rashba spin-orbit coupling

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We explore the unconventional localization properties of non-Hermitian one-dimensional systems with a quasiperiodic potential of the form $V_n = V_0 + \lambda(-1)^n$ along with Rashba spin-orbit coupling (RSOC), where n is the site index and λ modulates a staggered on-site component. This system without RSCO exhibits a striking re-entrant behavior wherein increasing the potential strength V_0 drives the system through successive phases: from localized to delocalized and back to localized states. This re-entrant localization transition challenges conventional single-transition paradigms and arises from the competition between the quasiperiodic disorder and the bipartite lattice structure. Our central finding is that RSOC provides a powerful mechanism to suppress this re-entrant phenomenon. Through numerical analysis of the inverse participation ratio and energy spectrum, we demonstrate that increasing RSOC strength progressively diminishes the intermediate extended phase, eventually restoring a direct localization transition. This tunable control over phase transitions via an external coupling parameter offers significant potential for engineering quantum states in synthetic matter and developing switching devices based on non-Hermitian systems.
Keywords: Quantum phase transitions; Quasiperiodic systems; Spin-orbit coupling.

Ballistic performance of epoxy-based hybrid laminates reinforced with banana and areca fibers

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The development of sustainable, lightweight, and cost-effective materials for ballistic protection is a growing area of interest in both defense and civilian sectors. Conventional ballistic materials such as aramid fibers and ultra-high molecular weight polyethylene (UHMWPE) offer excellent performance but are expensive, non-biodegradable, and energy-intensive to manufacture. As an eco-friendly alternative, this study investigates the ballistic performance of epoxy-based hybrid laminates reinforced with banana and areca fibers, two abundant natural fibers known for their favorable mechanical properties and biodegradability. Banana and areca fibers were selected due to their complementary characteristics: banana fibers exhibit high tensile strength and stiffness, while areca fibers contribute good energy absorption and impact resistance. Both fiber types were alkali-treated to remove lignin, hemicellulose, and other impurities, enhancing fiber–matrix adhesion. The treated fibers were arranged in various stacking sequences and orientations to form hybrid laminates using an epoxy resin matrix via the compression molding technique. The fabricated composite laminates were categorized into different configurations: pure banana fiber composite, pure areca fiber composite, and several banana-areca hybrid combinations (e.g., alternate, sandwich, and gradient layering). The areal density and thickness of the laminates were maintained within standard limits for personal body armor to allow for practical application and comparison with commercial armor materials. Ballistic performance was evaluated through low- and high-velocity impact testing, with a focus on resistance to projectile penetration, energy absorption, backface signature (BFS), and damage morphology. Testing followed NIJ (National Institute of Justice) Level IIA and II standards using 9 mm FMJ (Full Metal Jacket) projectiles fired at controlled velocities. Post-impact analysis included digital image correlation (DIC) for deformation mapping, Scanning Electron Microscopy (SEM) to assess failure modes, and mechanical testing (tensile, flexural, and interlaminar shear strength) to correlate structural integrity with ballistic behavior. Results demonstrated that the hybrid composites significantly outperformed the single-fiber laminates in terms of energy absorption and damage resistance. Laminates with alternating layers of banana and areca fibers exhibited improved ballistic limit (V_{50}), lower backface deformation, and enhanced delamination resistance. The hybrid structure enabled a more efficient distribution of impact energy, with the stiffer banana fibers resisting penetration and the tougher areca fibers dissipating energy through fiber pull-out and matrix cracking. Failure analysis revealed a combination of fiber breakage, matrix cracking, delamination, and fiber pull-out, indicating complex energy absorption mechanisms active during ballistic events. Among all configurations, the banana–areca–banana (sandwich-type) hybrid laminate provided the best balance between stiffness and toughness, meeting critical performance benchmarks for body armor applications. This study confirms the potential of banana and areca fiber hybrid

composites as sustainable materials for ballistic protection. The synergy between these natural fibers, when properly processed and layered, provides a viable route toward lightweight, biodegradable, and cost-effective armor solutions. Future research will explore nano-fillers for matrix toughening, dynamic strain rate testing, and long-term durability under environmental exposure to advance these materials toward real-world applications.

Keywords: Banana Fibers, Ballistic, NAOH.

Enhanced ammonia sensing performance of UV-activated WO_3 thin films deposited by RF magnetron sputtering

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A WO_3 thin film with an approximate thickness of 300 nm was deposited on the sapphire substrate by means of RF magnetron sputtering technique. The effect of exposure to UV light on the NH_3 sensing behavior of WO_3 thin film has been systematically investigated. The results showed that UV-activated WO_3 thin films has the remarkable ability to detect ammonia, with a high sensitivity, excellent selectivity, a rapid response and recovery time, and a very low detection limit of 0.1 ppm. The enhanced sensing efficiency under UV illumination is attributed to the photocatalytic oxidation of ammonia on the WO_3 surface, the planar structure of the thin film, which facilitates effective absorption of UV light, and the increased surface-to-volume ratio arising from the film's roughness and porous morphology.

Keywords: WO_3 thin films; UV light; Ammonia Sensing; Sensitivity; and Selectivity.

Hybrid composite fabrication using areca fibers and metal mesh for enhanced impact resistance

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The growing demand for lightweight, cost-effective, and sustainable materials has accelerated research into natural fiber-reinforced composites for structural and impact-resistant applications. However, despite their biodegradability and reasonable mechanical properties, natural fiber composites often suffer from limited impact strength and poor durability under dynamic loading. To overcome these limitations, this study presents the development of a hybrid composite material combining areca fibers with metal mesh reinforcement, aiming to enhance impact resistance while retaining eco-friendly characteristics. Areca fibers, extracted

from the husk of the Areca catechu (betel nut) palm, offer advantages such as low density, renewability, and good specific strength. However, their use in impact-critical components is constrained by relatively low toughness. To address this, a hybrid reinforcement strategy was employed by embedding stainless steel wire mesh within an areca fiber-epoxy matrix composite. The synergy between the ductile nature of metal mesh and the energy-absorbing capacity of natural fibers was investigated to develop a robust hybrid structure suitable for low-velocity impact applications such as automotive interior panels, protective gear, and structural cladding. The fabrication process involved alkali treatment of areca fibers to improve fiber-matrix interfacial bonding, followed by drying and orientation into various configurations (unidirectional and bidirectional). The metal mesh was integrated into single and multiple layers within the laminate using hand layup and compression molding techniques with epoxy resin as the matrix. The composite laminates were cured under pressure and post-cured to ensure proper consolidation and adhesion between layers. A comprehensive experimental study was conducted to evaluate the mechanical and impact performance of the fabricated composites. Low-velocity impact tests were carried out as per ASTM D7136 to measure parameters such as peak force, energy absorption, damage area, and residual strength. Results indicated a significant improvement in impact resistance for the hybrid composites compared to those reinforced with areca fibers alone. In particular, samples with bidirectional fiber orientation and double-layer metal mesh exhibited the highest energy absorption capacity and minimal delamination or surface cracking. Fractographic analysis using Scanning Electron Microscopy (SEM) revealed effective load transfer between the fibers and matrix, as well as a strong mechanical interlock between the metal mesh and the surrounding matrix. The dominant failure modes observed included fiber pull-out, matrix cracking, and localized deformation of the mesh, all contributing to enhanced energy dissipation. This study concludes that the hybridization of areca fibers with metal mesh reinforcement offers a promising approach to overcoming the limitations of natural fiber composites, enabling their application in areas demanding higher impact resistance.

Keywords: Areca Fibers; SEM; NAOH.

Investigation of structural and magnetic properties of polycrystalline $Y_3Fe_5O_{12}$

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Polycrystalline $Y_3Fe_5O_{12}$ (YIG) garnet was synthesized via the sol–gel auto-combustion technique and investigated for its structural and magnetic characteristics. Rietveld refinement of the x-ray diffraction data, supported by Raman spectroscopy, confirms the formation of single-phase YIG with a cubic (space group *Ia3d*) crystal structure. Field emission scanning electron microscopy (FESEM) reveals a homogeneous distribution of nearly spherical particles

with an average size of approximately 80 nm. The temperature-dependent magnetization measurements indicate a ferrimagnetic Curie temperature (T_C) of around 566 K. Furthermore, the variation of saturation magnetization with temperature follows the Bloch $T^{3/2}$ law, signifying dominant spin-wave excitation behavior.

Keywords: Garnets; Sol-Gel; Structure; Magnetization; Electron Microscopy.

A facilely synthesized MoS_2-ZnS-rGO composite: A bifunctional platform for enhanced electrocatalysis (OER) and photocatalysis

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The design of efficient, low-cost, and durable bifunctional catalysts for both sustainable energy conversion and environmental remediation remain a considerable challenge. Here, we present a straightforward, one-step hydrothermal synthesis of a MoS_2-ZnS-rGO nanocomposite. The material's structural, morphological, and chemical properties were thoroughly examined. The XRD and Raman spectroscopy verified the successful formation of MoS_2 and ZnS phases anchored on the reduced graphene oxide (rGO) sheets. FESEM and HRTEM analyses displayed a close heterojunction interface between MoS_2 and ZnS nanoparticles, which were well-distributed on the rGO support. The composite also exhibited a high specific surface area, as validated by BET analysis. This novel composite demonstrated impressive bifunctional catalytic activity. As an electrocatalyst, the MoS_2-ZnS-rGO composite performed excellently in the oxygen evolution reaction (OER) within alkaline media, reaching a low overpotential of 310 mV at 10 mA cm^{-2} and a modest Tafel slope of 75 mV dec^{-1}, indicating favourable kinetics. Simultaneously, the material acted as a high-performance photocatalyst for degrading Congo red dye under visible light irradiation, achieving 92% degradation within 120 minutes. The improved bifunctional activity is ascribed to the synergistic effects within the composite: (i) the MoS_2-ZnS heterojunction enhances effective separation of photogenerated charge carriers, (ii) the rGO substrate offers excellent electrical conductivity and a substantial surface area, and (iii) the multicomponent system provides plentiful active sites for both oxygen evolution reaction (OER) and photocatalysis. These results establish the MoS_2-ZnS-rGO composite as a promising, cost-effective material for dual applications in energy and environmental sectors.

Keywords: Bifunctional Catalyst; MoS_2-ZnS; rGO; Photocatalysis.

Enhanced structural, optical and magnetic properties of Gd and Bi-doped yttrium iron garnet (YIG) nanoparticles synthesized via a modified sol-gel auto-combustion method

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$Y_{2-x}Gd_xBiFe_5O_{12}$ (x = 0, 0.25, 0.50, 0.75, 1.0) garnet ferrites were synthesized via a sol–gel route to examine the influence of Gd substitution on structural, optical, and magneto-functional properties. X-ray diffraction confirmed phase-pure garnet formation with systematic lattice expansion upon Gd incorporation. SEM analysis showed grain coarsening up to x = 0.50, followed by refinement at higher Gd levels, consistent with controlled densification. FTIR spectra displayed characteristic Fe–O stretching modes that red-shifted with increasing Gd content, indicating lattice distortion. UV–Vis., absorption spectra revealed a direct optical band gap in the range of 2.15–2.30 eV, with only minor variations across compositions, reflecting the structural robustness of the garnet framework despite substitution. (Bi, Gd) co-doped YIG garnets exhibit enhanced permittivity (ε′ ≈ 30–45 versus 12–15 for YIG) with an optimum at x=0.5, while maintaining low dielectric loss (tan δ < 0.02 at >1 MHz), suggesting suitability for high-frequency devices. Magnetization studies demonstrated a maximum saturation magnetization (M_s = 38.75 emu/g) at x=0.50, with coercivity (H_c) increasing steadily with Gd content due to enhanced anisotropy. The magnetoelectric coefficient (α_{ME}) peaked at ~29.3 mV/cm·Oe for x=0.75, illustrating a strong correlation between optimized magnetic ordering and ME coupling. Collectively, these results highlight that judicious Gd substitution simultaneously tunes lattice dynamics, electronic transitions, grain morphology, and magnetoelectric functionality, rendering Gd-doped Bi–YIG garnets promising for multifunctional spintronic and sensor applications.

Keywords: Yttrium Iron Garnet; Sol-gel; Magnetic Properties; Magnetoelectric Coefficient.

Non-destructive detection of water adulteration in rum

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An optical device is designed and implemented to investigate the adulteration of rum with water. Water serves as a prevalent adulterant in alcoholic beverages, particularly rum, due to its cost-effectiveness and its widespread accessibility. The rum used is composed of approximately 42.8% alcohol by volume (ABV), with the remaining significant constituents being water, along with trace amounts of sugars and phenolic compounds. Given that water constitutes the predominant component of rum, discerning its presence when blended in lesser quantities proves to be challenging. For this investigation, eleven distinct samples of

water in rum were systematically prepared, and samples were named as RW1 to RW11, corresponding to 0%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, and 100% water in rum. These samples underwent rigorous analysis to ascertain the efficacy of the developed low-cost optical fiber device (refer to Fig. 1(a)) in quantifying water concentrations. The findings illustrated in Fig. 1(b) reveal that the device possesses the capability to accurately detect water levels, thereby contributing to improved safety in the consumption of alcoholic beverages. The sensitivity of the device was determined to be 0.017 µW per 1% (v/v) of water concentration present in rum. The total average power variation recorded approximates 1.68 µW across the spectrum of 0% to 100% water concentration in the rum. The average error associated with the reflected power measurements has been documented as 0.05 µW. Even at the minimal percentage of adulteration, this device successfully identifies the presence of water in rum. To evaluate the detection thresholds of water concentration in rum, measurements were meticulously conducted over 800 instances on various days and at different temporal intervals for each sample. The straightforward configuration of this economical device demonstrates commendable repeatability and reversibility. The operational efficacy of the device underscores its potential for extensive application in quality assurance within the alcoholic beverage sector. This validated optical fiber device represents a dependable instrument that fulfils the objective of contactless monitoring of water adulteration in rum in a non-destructive and rapid manner.

Keywords: Non-destructive, Adulteration, Alcoholic beverages, Reflected Power.

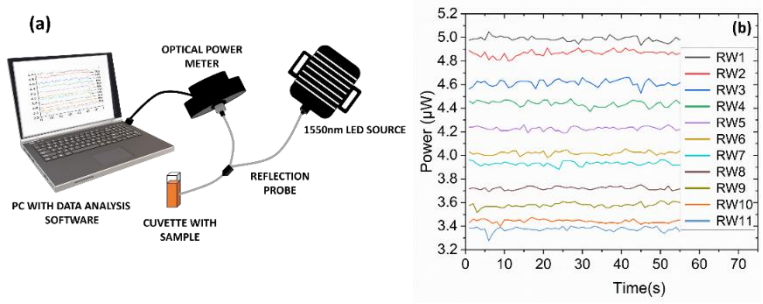

Fig. 1. (a) Schematic diagram of the optical device arrangement. (b) Reflected power corresponding to the different water concentration percentages in rum.

Quantum-accelerated defect modelling: Variational quantum eigen solver study of correlated oxygen vacancies in zirconia

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Accurate prediction of point defect formation energies (ΔE_f) in functional ceramics remains a major challenge for electronic structure theory. In zirconia (ZrO_2), a benchmark oxygen-ion conductor used in solid oxide fuel cells (SOFCs) and related energy devices, the presence of localized and strongly correlated oxygen vacancies (V_O) pushes the accuracy limits of conventional density functional theory (DFT). Determining ΔE_f precisely is essential for

describing ionic transport and device performance, yet empirical corrections such as DFT+U often reduce predictive reliability. This limitation constrains the design of next-generation oxide materials. To address this, we present a quantum–classical hybrid framework that attains chemically accurate defect energetics on near-term quantum hardware (NISQ). The method integrates Quantum Embedding Theory (QET) with a Variational Quantum Eigensolver (VQE) to solve a reduced active-space Hamiltonian ($N \leq 8$ qubits) representing the correlated region surrounding V_O. QET isolates localized defect states from the extended lattice, while VQE captures static and dynamic correlation effects beyond mean-field DFT. The workflow implemented using PySCF and Qiskit Nature, with Qiskit Aer noise benchmarking, employs a hardware-efficient ansatz optimized through gradient-based updates and shot-frugal measurement strategies. The approach mitigates decoherence and achieves convergence within ~1 kcal mol^{-1} of high-level DFT+U energies. A resource analysis further quantifies qubit requirements, circuit depth, and measurement overhead for achieving chemical accuracy on current NISQ processors. This study demonstrates a scalable quantum-accelerated pathway for predictive modelling of strongly correlated point defects, opening avenues for data-driven and quantum-enhanced materials discovery in complex oxides.
Keywords: Variational Quantum Eigen solver; Quantum–Classical Hybrid Simulation.

Modelling error-resilient quantum key distribution in hybrid Si_3N_4–InP waveguides: Towards long-haul secure communication

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The work shows modelling and performance analysis of hybrid Si_3N_4–InP waveguide platforms for long-distance, error-resilient QKD. The architecture synergistically combines the ultra-low propagation loss (<0.1 dB/cm) and CMOS-compatible fabrication of silicon nitride (Si_3N_4) with the high-speed electro-optic modulation and active photonic functionalities of indium phosphide (InP). Through detailed numerical and system-level simulations, we demonstrate gigahertz-clock-rate QKD operation with quantum bit error rates (QBER) below 1% under >20 dB channel attenuation. The hybrid design enables secure key exchange over distances up to 250 km in standard single-mode fiber and achieves bidirectional secret key rates exceeding 1.8 Mbps at 10 dB loss. We quantify critical performance metrics that including optical loss budget, error tolerance, polarization stability, and finite-key effect, which confirming that Si_3N_4–InP integration significantly enhances both transmission reach and robustness compared to homogeneous photonic platforms. Furthermore, the co-integration of passive and active components on a single chip reduces coupling losses and environmental sensitivity, improving practical deplorability. Our results establish hybrid Si_3N_4–InP photonics as a scalable, high-performance pathway toward field-deployable QKD systems capable of meeting the stringent requirements of real-world quantum-secured communication networks.
Keywords: QKD-Quantum Key Distribution, Photonic qubit; Quantum networks.

Localized thermal gradient-assisted hydrothermal reactor for controlled ZnO nanowire growth and room-temperature ethanol sensing

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In this work, high aspect ratio Zinc oxide (ZnO) nanowires have been successfully synthesized using a customized hydrothermal set-up on n-type (100) silicon substrate. The customized set-up has been developed in such a manner to improve the efficiency of the traditional hydrothermal method for synthesizing high aspect ratio zinc oxide (ZnO) nanowires (NWs). The morphological study by Field Emission Scanning Electron Microscopy (FESEM) and Transmission Electron Microscopy (TEM) reveals high aspect ratio thread-like ZnO nanowires of around 130, and a superior growth rate of ~2.2 µm/hour. Furthermore, prominent peaks correspond to (002), (100) and (101) plane have been observed from the structural investigation by X-ray diffraction which indicates good crystallinity of the samples. Besides, the elemental mapping images also validates the presence of Zn and O atoms only with uniform distribution. A considerable sensitivity has been observed, with the sample exposed to 500 ppm has shown the highest sensitivity at room temperature. Additionally, the ethanol sensing response and the recovery time of nanowires were significantly found to be around 17.5 second and 15 seconds, respectively at room temperature at a detection limit of 500 ppm. The sensor performance results potential application as an ethanol nano-gas sensor.
Keywords: Thermal gradient; Localized; high aspect ratio; Nanowires.

Latest advancements in rice wastes derived heterogeneous catalytic conversion of biomass to fuels (biodiesel): A review

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Fossil fuels are the main source of energy, but its extensive usage causing severe environmental pollution. So, to get rid of this, there is an urgent need of generating fuels as a sustainable energy source from the biomasses like waste cooking oil, soyabean oil, palm oil, seed oil etc. which are biodegradable, environment friendly and easily available everywhere. And catalytic conversion of these biomasses into biofuels like biodiesel by using heterogeneous catalysts derived from the agriculture wastes such as rice straw and rice husk offers a sustainable alternative to traditional fuel production processes. Since, rice straw and husk are the major lignocellulosic agriculture waste materials produced every year all over the world especially in India and the catalysts prepared from these wastes has advantages like low cost, ecofriendly, more availability, heterogeneous nature and highly stable than the catalysts prepared from the chemicals. So, this study highlights the utilization of these rice straw and husk to synthesize environmentally friendly green catalysts to produce biodiesel from the different available biomass oils through transesterification/esterification process and also

suggests clear idea about the recent developments, advancement in the technology used by different researchers around the world to synthesize green catalyst for conversion of biomass to fuels like biodiesel. This review also focuses on the research gaps, advantages and disadvantages of the process and the future way to utilization of the biomass and to increase the yield of the biofuels.

Keywords: Fossil fuels, Biomass, Rice straw & husk, Green catalyst, Biodiesel.

Numerical modelling and simulation of fiber Bragg grating for cryogenic temperature sensing using COMSOL multi-physics

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Precise and reliable thermometry in the cryogenic regime underpins technological innovation in diverse fields, including aerospace engineering, high-energy physics, and superconducting technologies [1]. Fiber optics sensors offer a superior alternative to conventional electronic sensors, providing immunity to electromagnetic interference, multiplexing capabilities, a lightweight design, and resistance to harsh environmental conditions [2]. Fiber Bragg Grating (FBG) is a type of optical fiber sensor in which a small element of the core has a periodic variation of refractive index, because of which a particular wavelength of light is reflected, called the Bragg wavelength. Any variation in the external parameter, such as strain and temperature, will lead to a shift in the reflected Bragg wavelength [3]. This study presents a comprehensive modelling and simulation of FBG using the Finite Element Method (FEM) within the COMSOL Multiphysics Software. The research focuses on the temperature-dependent shift in Bragg Wavelength, especially in the cryogenic temperature range. In the modelling software, we utilized the Wave Optics, Heat Transfer, and Solid Mechanics modules to investigate the spectral response of the FBG. In the model, we have created the standard single-mode fiber geometry-based FBG. To reduce computational complexity, the uniform periodic geometry features a square-wave refractive index profile for the grating. To characterize the sensor's response, the parametric sweep was performed from room temperature to 77 K. At each temperature point, the spectrum was computed over a wavelength range of 1450 to 1600 nm. The electric field distribution along the core of the fiber is also investigated (Fig. 1(a)). Over this temperature range, the blue shift was observed with a total shift of 2 nm (Fig. 1(b)). The average sensitivity calculated in the studied temperature range is 0.01 nm/K. The validity of the computational model is established by comparing the simulated wavelength shifts with theoretically predicted values, demonstrating strong agreement. The developed FBG model provides an accurate and reliable tool for predicting the performance of FBG sensors in cryogenic environments. This computational approach facilitates the design & optimization of FBG-based cryogenic sensing systems by enabling the analysis of grating parameters without extensive and costly experimental prototyping.

Keywords: Fiber Bragg Grating, Cryogenic, Finite Element Method.

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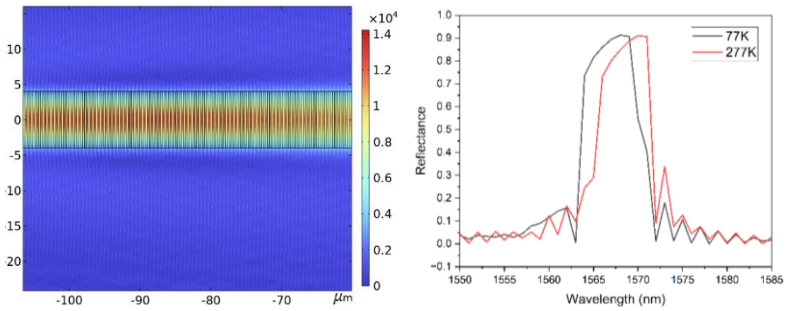

Fig 1(a). Out-of-plane electric field distribution along the core of the fiber, (b)Bragg Wavelength for temperatures of 277K and 77K.

Low-cost fabrication of flexible Sn-doped CuS photodetector by chemical bath deposition method

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The covellite phase of copper sulphide (CuS) thin film, being a constituent of the copper-based chalcogenide family, has emerged as a low-cost semiconductor with various applications, particularly photovoltaics, due to its economical availability. In this research work, the CuS thin film has been deposited on the flexible PET (polyethylene terephthalate) substrate at 70 °C by the low-cost chemical bath deposition (CBD) method. The structural, morphological, wettability, mechanical, and optoelectronic properties of CuS thin film have been further investigated along with the effect of Sn dopant by varying the molar concentration of Sn-dopant from 1 % to 5 %. The X-ray diffraction studies of Sn-doped CuS thin film reveal an increase in crystallinity with an increase in Sn-dopant concentration up to 3 %. The substitutional doping of 3 % Sn in CuS thin film reveals a maximum crystallite size of 23.6 nm with the lowest structural defects. The higher Sn-dopant concentration leads to a decrease in crystallinity with a rise in vacancy and defects. The FESEM micrograph reveals the largest grain size of 79 nm for 3 % Sn doping in CuS. The post-annealing treatment of 3 % Sn-doped CuS reveals a further enhancement in crystallinity with an increase in annealing temperature from 50 °C to 110 °C. The mobility of 3 % Sn-doped CuS thin film is increased with an increase in annealing temperature. The 3 % Sn-doped CuS thin film, annealed at 110 °C, being more crystalline in nature, possesses the higher mobility of 87.03 $cm^2/V.s$ due to the larger grain size, and shows a lower resistivity of 1.12×10^{-1} Ω.cm. The positive Hall coefficient reveals the p-type nature of Sn-doped CuS thin film. The contact angle study reveals a maximum contact angle of 102.2° (hydrophobic), with a minimum surface energy 11.19 mN/m. The photo-response and bending study of 3 % Sn-doped CuS thin film annealed at 110 °C (Al/Sn-doped CuS/PET – 110), exhibiting optimised responsivity of 0.52 mA/W, and detectivity of 3.75×10^8 Jones, could be a suitable for modern flexible and wearable optoelectronic devices.
Keywords: covellite phase (CuS); chemical bath deposition (CBD); photo-response; resistivity.

Facile hydrothermal synthesis of $NiCo_2O_4$@MWCNT for high-performance supercapacitors and electrocatalytic oxygen evolution

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The development of cost-effective, high-performance bifunctional materials for energy storage and conversion systems is a critical research challenge. In this work, we report the facile synthesis of a nickel cobaltite-multi-walled carbon nanotube composite via a simple one-step hydrothermal method. The structural, morphological, and compositional properties of the as-prepared composite were systematically investigated. The XRD and Raman Spectroscopy confirmed the successful formation of the cubic spinel phase $NiCo_2O_4$. The FESEM and HRTEM revealed ultrafine nanoparticles of $NiCo_2O_4$ uniformly anchored onto the conductive MWCNT framework. The BET analysis confirmed a high specific surface area of 53.6 m^2/g, which is crucial for electrochemical applications. When evaluated as a supercapacitor electrode, the $NiCo_2O_4$@MWCNT composite exhibited outstanding electrochemical performance. It delivered a high specific capacitance of 1210 F/g at a current density of 1 A/g. It demonstrated remarkable cycling stability, retaining 95% of its initial capacitance after 5000 charge-discharge cycles. Furthermore, the material's electrocatalytic activity for the OER was assessed in 1.0 M KOH. The $NiCo_2O_4$@MWCNT catalyst showcased excellent OER performance, requiring a low overpotential of only 375 mV to achieve a current density of 10 mA/cm^2 and a slight Tafel slope of 125 in mV/dec. This superior bifunctional performance is attributed to the strong synergistic coupling between the highly active $NiCo_2O_4$ and the conductive MWCNT scaffold, which facilitates rapid ion/electron transport and provides a large number of accessible active sites. These findings highlight the $NiCo_2O_4$@MWCNT composite as an auspicious electrode material for next-generation supercapacitors and electrocatalysts.

Keywords: $NiCo_2O_4$; MWCNT; Supercapacitor; Oxygen Evolution Reaction (OER).

Analysis of vibration behavior in CNC machining of advanced engineering materials

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Advanced engineering materials are being used rapidly in the vast area, so the manufacturing of the products related to them is essential. The intent of this study is to demonstrate the real time vibration monitoring to enhance the predictive maintenance strategies, reduce downtime and improve machine performance in the machining of advanced engineering

materials. The present study explores the relationship between the tool geometry, specifically the insert nose radius and machine tool vibration during milling operation of the titanium alloy Grade 5 (Ti-6Al-4V). Experiments were conducted using carbide inserts under the set of machining parameters. A tri-axial accelerometer, mounted on the spindle head of CNC vertical milling machine was used to capture the induced machine tool vibrations. The vibration data were correlated with machining parameters and insert geometry to identify the optimum values for permissible machine tool vibration, highlighting the potential of vibration analysis as a diagnostic tool for early detection of tool deterioration and machine health assessment.
Keywords: Tool geometry, Advanced material, Machine tool Vibration, Machining parameters

Photoresponse study of $MoTe_2$ films with various configuration

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Two-dimensional (2D) materials have emerged as transformative candidates for next-generation electronic and optoelectronic devices. Among those, molybdenum ditelluride ($MoTe_2$) stands out for its ideal bandgap, making it highly suitable for infrared (IR) detection applications. In particular, $MoTe_2$/Si heterojunctions hold significant promise for photodetector technologies. In study the synthesis of $MoTe_2$ thin films is done by rapid thermal processing (RTP) technique, with molybdenum (Mo) deposition using a sputtering system prior to the thermal evaporation of tellurium (Te). Thereafter, the Mo/Te-coated substrates are treated in an RTP furnace with a growth temperature of 600 °C and a growth time of 10 minutes, with working pressure and argon gas flow of 2 torr and 160 sccm respectively. This study presents a comprehensive investigation of the photoresponse characteristics of $MoTe_2$-based infrared detectors fabricated in various device configurations. Current–time measurements were employed to evaluate near-infrared performance through responsivity, specific detectivity, and temporal response under illumination at 850 nm, 940 nm, 1060 nm, 1300 nm and 1550 nm. These current-time results indicate effective carrier generation and transport in the $MoTe_2$ layer, demonstrating its strong potential for use in IR photodetection technologies. Among the metal–semiconductor structures, the Al/ $MoTe_2$ Schottky junction exhibited a responsivity of 1255.41 mA/W and a detectivity of 1.46×10^{11} $cm.H_Z^{1/2}.W^{-1}$, attributed to the enhanced built-in potential at the interface. For heterostructure devices, the rGO/ $MoTe_2$ stack achieved improved performance, with responsivity and detectivity reaching 1385.71 mA/W and 4.12×10^{11} $cm.H_Z^{1/2}.W^{-1}$, respectively, under 1060 nm illumination, along with rise and fall times of 0.6 s and 0.7 s. The highest photoresponse was observed for the $MoTe_2/MoS_2$ stack layer, yielding a responsivity of 1728 mA/W and a detectivity of 66.52×10^{11} $cm.H_Z^{1/2}.W^{-1}$, accompanied by symmetric rise/fall times of 0.6 s. Meanwhile, $MoTe_2$ photoconductors demonstrated the fastest temporal dynamics (0.6 s rise and fall), owing to the absence of interfacial barriers. Overall, these results highlight the critical role of device architecture in tuning and enhancing the infrared detection capabilities of $MoTe_2$-based photodetectors.
Keywords: $MoTe_2$ thin film, IR detector, Stack layer, Schottky junction, Heterojunction, IT.

Phase-engineered $Ni_{0.8}Mn_{0.2}Fe_2O_4$–$BaFeO_3$ nanocomposites with tunable functional properties

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Nanocomposites of (1–x) $Ni_{0.8}Mn_{0.2}Fe_2O_4$ + x ($BaFeO_3$) (x = 0.2-0.8) were synthesized via a hydrothermal route and studied structural, microstructural, dielectric and magnetic characteristics. XRD (Xray diffraction) data confirmed the formation of both spinel and perovskite phases in all the composites. Morphological studies including FESEM (Field Emission Scanning Electron Microscopy) and TEM (Transmission Electron Microscopy) showed well grown grains with high densities and spherical nanoparticles, respectively. The obtained particle sizes were consistent with size distributions estimated from XRD studies using W-H (Williamson-Hall) plots. Along with these, thermal stability and phase formation was tested using TGA (Thermogravimetric Analysis) and DSC (Differential Scanning Calorimetry) studies. Dielectric spectroscopy revealed significant low-frequency dispersion due to Maxwell–Wagner interfacial polarization and hopping conduction, as described by Josher's power law. Magnetic investigations with VSM validated the soft ferrimagnetic characteristics of these samples. The interaction of microstructure, interfaces, and composition facilitates the adjustment of dielectric and magnetic characteristics for prospective high-frequency and multifunctional applications.

Keywords: Ni–Mn ferrite; Hydrothermal synthesis; TEM; Dielectric spectroscopy; VSM.

Structural and optical properties of Pr^{3+} doped Li_2O-CdO-Al_2O_3-B_2O_3 glasses: suitable for optical fibers and photonics

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Praseodymium doped lithium cadmium alumino borate glasses are synthesized by the melt-quenching technique. XRD analysis confirms amorphous nature of glass. FTIR and Raman studies reveal the presence of intermediate range order (IRO) structural groups such as boroxol $B_3\emptyset_6$, pentaborate $B_5\emptyset_{10}^-$, dipentaborate $B_3\emptyset_{11}^{2-}$, diborate $B_4\emptyset_9^{2-}$ and metaborate $B_3\emptyset_9^{3-}$ groups. Addition of cadmium converts diborate and dipentaborate into metaborate units. These structural variations affect the radiative properties of praseodymium. UV-Visible studies show absorption peaks which are signatures of Pr^{3+} 4f - 4f transitions. Nephelauxetic ration and bonding parameters confirm the covalent bonding nature of glasses.

Photoluminescence studies reveal red luminescence at 600 and 640 nm which are due to $^1D_2$ – $^3H_4$ and $^3P_0$ – $^3F_2$ transitions. Lifetime studies reveal the stability of $^1D_2$ state suitable for radiative emission. Structural, UV-visible and PL studies reveal praseodymium doped lithium cadmium alumino borate glasses are suitable for fiber amplifiers and photonic devices.
Keywords: Diborate, Praseodymium, Photoluminescence, Raman spectroscopy, UV-vis.

Influence of Tb^{3+} substitution on the structural, optical, and dielectric properties of cobalt ferrites with thermoelectric assessment

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Terbium (Tb)-substituted cobalt ferrites ($CoTb_yFe_{2-y}O_4$, where y = 0.0 to 0.025 with a step of 0.005) were synthesized using the sol-gel auto-combustion method. The structural properties were analyzed using X-ray diffraction (XRD) with Rietveld refinement, confirming a single-phase cubic spinel structure with minor secondary phases. The cation distribution was evaluated by comparing theoretical lattice constants for various site occupancies with experimental values obtained from XRD. Optical properties were investigated through UV-visible spectroscopy, revealing a decrease in band gap with increasing Tb^{3+} content, consistent with the semiconducting behavior observed in these materials. Fourier Transform Infrared (FTIR) spectroscopy was used to explore the elastic properties and functional groups, while dielectric properties and DC-conductivity were studied across a wide frequency and temperature range (35 to 400 °C). The positive Seebeck coefficient across all doped samples indicated p-type semiconductor behavior, making these materials potential candidates for thermoelectric applications. The analysis of these properties provides valuable insights into the development of rare earth-doped cobalt ferrites for advanced technological applications.
Keywords: Cobalt Ferrite; Optical properties, Dielectric properties, Thermoelectric effect.

Fabrication, structure, bandgap, and dielectric study of $Al_{0.8}Zn_{1-x}Ni_xTiO_{3+\delta}$ (x = 0.04, 0.08, 0.12 & 0.16)

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A series of $Al_{0.8}Zn_{1-x}Ni_xTiO_{3+\delta}$ (x=0.04,0.08,0.12,0.16) (AZNT) nanoparticles were synthesized via low temperature hydrothermal method. The X-ray diffraction patterns were used to confirm the structure while the FESEM, and TEM used for evaluating the microstructure. The optical bandgap was determined using the Tauc's plots. The frequency dependent dielectric behavior was studied as a function of frequency, and composition.
Keywords: Nanoparticles; Perovskites; Bandgap; Dielectric.

Optimized magnetic and optical performance in Sm^{3+}-doped Ni–Co ferrites for functional device applications

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A series of Sm^{3+}-doped $Ni_{0.5}Co_{0.5}Fe_{2-x}Sm_xO_4$ (x = 0.000–0.025) ceramics were synthesized via a conventional sol–gel auto-combustion method, followed by sintering. The phase purity and structural modifications were examined using X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, and electron microscopy. XRD results confirmed the formation of a single-phase spinel structure with a decreasing lattice parameter (8.35–8.33 Å) and crystallite size (35–22 nm) upon Sm^{3+} substitution, attributed to lattice distortion and dopant-induced strain. Photoluminescence spectra revealed visible emissions (400–500 nm) corresponding to the $^4G_{5/2} \rightarrow {}^6H_{7/2}$ and $^4G_{5/2} \rightarrow {}^6H_{9/2}$ transitions of Sm^{3+} ions. Magnetic measurements indicated an enhanced saturation magnetization of 40.11 emu/g at x = 0.010, followed by a decline at higher concentrations due to spin disorder. The optical band gap increased from 1.66 to 1.90 eV, and dielectric studies confirmed normal dispersion behavior with improved dielectric constant and loss tangent. These findings demonstrate that controlled Sm^{3+} substitution effectively tailors the structural and electronic characteristics of Ni–Co ferrites, enhancing their suitability for spintronic and optoelectronics.
Keywords: Ferrites; Magnetic; Optical; Functional properties.

Mesoporous silica nanoparticles in modern cancer therapies: An engineering review

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Cancer is the second most common cause of death globally, after cardiovascular disease. Conventional cancer therapies, including chemotherapy, radiotherapy and surgery, still have several limitations such as the low water solubility of many anticancer drugs, damage to healthy tissues during radiotherapy, and the risk of infection associated with surgical procedures. This review focuses on the biomedicine applications of mesoporous silica nanoparticles (MSNs) especially in cancer treatment strategies and their ability to overcome the drawbacks of current treatment strategies. Mesoporous Silica Nanoparticles possess several advantageous features that make them suitable for their use in biomedicine, such as adjustable pore size and volume, controlled drug release capability, high loading capacity, the ability to convert crystalline drugs into amorphous form, and good biocompatibility and

biodegradability, making them highly suitable carriers for improving the solubility and delivery of hydrophobic chemotherapeutic agents. This review highlights the recent progress in the use of mesoporous silica nanoparticles for cancer diagnosis and therapy, including advancements in the stimuli responsive gatekeepers for on demand drug release, surface modification strategies for active targeting, and the development of multifunctional MSN based drug delivery systems. Moreover, this review also discusses the major challenges associated with the use of mesoporous silica nanoparticles in a cancer treatment particularly regarding their biosafety, long-term stability and cytotoxicity. Overall, mesoporous silica nanoparticles show significant potential that enhances the effectiveness and precision of currently used modern cancer therapies.

Keywords: Nanoparticles; Silica; Cancer Therapies.

Design, synthesis and physical studies of cerium based MOFs with isonicotinate linker for advanced functional applications

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Metal–Organic Frameworks (MOFs) are an emerging class of highly porous crystalline materials constructed from metal ions and organic linkers. Owing to their exceptionally high surface area, tunable pore structure, and adjustable chemical functionality. Cerium-based MOFs are particularly promising because cerium exhibits unique redox properties, enabling reversible transition between Ce^{3+} and Ce^{4+} states, along with strong Lewis's acidity, which enhances catalytic and electrochemical activity. In the present study, Cerium based MOFs with isonicotinate linkers were synthesized via facile hydrothermal method, yielding nanoscale crystalline materials. These prepared Ce-isonicotinate nano MOFs were structural characterised using X-ray diffraction (XRD) for confirmation of their crystalline phase formation and purity of the synthesized MOFs. The FTIR verified the coordination between Ce ions and the organic linker and detected the absence of major impurities. Surface morphology and textural properties were examined using SEM, BET surface area analysis and TGA for thermal stability studies. The catalytic performance of these Ce-MOFs was evaluated through the degradation of methylene blue dye under visible light irradiation. The degradation process was monitored by UV-Visible spectrophotometer, revealing rapid dye removal and high catalytic efficiency. Kinetic analysis indicated that the degradation follows a pseudo-first order kinetics, with a rate constant significantly higher than that of bulk CeO_2 and other control materials. The DFT calculations provided additional insight into the electronic structure, metal-ligand bonding interactions, and charge transfer properties. The results revealed strong orbital overlap and favourable energy stability, which support the improved redox behaviour and structural robustness of the synthesized Ce-MOFs. Overall, the combined experimental and theoretical findings highlight that Ce-MOFs derived from isonicotinate linkers possess excellent potential for applications in energy storage, catalytic oxidation, and gas adsorption. This shows a useful correlation between experimental and computational modelling for the rational design of materials as efficient, recyclable catalysts for environmental applications.

Keywords: Cerium MOFs, Hydrothermal synthesis, Energy storage, DFT modelling.

Optical, and electronic behavior of Ni-doped $BiFeO_3$ nanoparticles

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The $Bi_{1-x}Ni_xFeO_3$ (x=0.2-0.8) nanoparticles are synthesized by hydrothermal technique. The rhombohedral structure including few secondary phases are confirmed from the obtained X-ray diffraction patterns. The microstructure confirms the formation of nanospheres like structures including small nanorods. The agglomeration is noticed among the nanoparticles owing to the magnetic interactions. The Tauc's plots are drawn to evaluate the optical bandgap (E_g) as a function of Ni-content. The x=0.2-0.8 samples show the dielectric, magnetic, and ferroelectric behavior evidencing the multiferroic perovskite nature. The thermal analysis reveals the weight loss and few transition temperatures of the samples.
Keywords: Multiferroic; Perovskite; Microstructure; Nanoparticles; Dielectric.

Optical properties of $BaCoTiO_3$ quantum dots

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The $Ba_{1-x}Co_xTiO_3$ (x=0.2-0.8) perovskite nanoparticles are prepared via hydrothermal method. The X-ray diffraction confirmed the cubic perovskite structure while specifically, the x=0.4 sample shows the mixed structure. The microstructure, and selected area electron diffraction patterns clearly show the formation of quantum dots for x=0.4 having the average size of 4.01 nm which can be suggested for quantum technology applications. The Tauc's plots obtained from UV-Visible spectral analysis confirmed the decrease of optical bandgap (E_g) from 2.262-1.701 eV with increase in Co-content in the barium titanate system. The metal oxide bonds are confirmed using IR-spectra. The Raman spectra of BCT evidences the formation of perovskite structure disclosing the lattice vibrations, and Raman modes of BCT. Further, the PL spectra of x=0.2-0.8 show the perovskite formation pertaining to the emission of colours.
Keywords: Hydrothermal; Perovskite; Quantum Dot; Microstructure; Optical.

Electronic structure of CdS, Cu_2SnS_3, Cu_2SnSe_3, and $Cu_2Sn(S_{0.5}Se_{0.5})_3$: A systematic assessment of DFT exchange–correlation functionals

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We investigate the electronic structure and band gaps of CdS, Cu_2SnS_3 (CTS), Cu_2SnSe_3 (CTSe), and the mixed compound $Cu_2Sn(S_{0.5}Se_{0.5})_3$ (CTSSe) using first-principles DFT calculations to assess their suitability for thin-film photovoltaic applications. Semi-local PBE and SCAN functionals reproduce structural properties but fail to open the band gap due to missing nonlocal exchange. The DFT+U corrections applied to Cu-3d states show negligible effect, confirming the absence of strong electronic correlations. In contrast, the HSE hybrid functional accurately reproduces experimental band gaps, with tunable exact exchange providing quasiparticle-level agreement. The low-energy electronic states are dominated by p–s and p–p hybridizations from S, Se, and Sn, making nonlocal exchange essential for realistic modeling. We also compute effective masses, work functions, and optical responses, demonstrating the functional dependence of key photovoltaic parameters. These results offer validated electronic and optical benchmarks for optimizing composition and device design in chalcopyrite-based solar absorbers.

Keywords: DFT; Electronic Structure; Bandgap.

Ce doping-induced structural and electrochemical performance enhancement in octahedral $ZnMn_2O_4$ microcrystallites for hybrid supercapacitor applications

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Doping is an effective strategy to enhance the electrochemical performance of battery-type electrode materials by improving electrical conductivity and promoting rapid electron transport for efficient redox reactions. In this work, cerium (Ce)-doped octahedral $ZnMn_2O_4$microcrystallites were successfully synthesized via a solution combustion synthesis method and systematically evaluated as a battery-type electrode for hybrid supercapacitor applications. Three samples with varying Ce content—undoped, 0.5 %Ce-$ZnMn_2O_4$, and 1%Ce-$ZnMn_2O_4$—were prepared to evaluate the effect of doping concentration. The structural, morphological, and surface properties of the materials were comprehensively characterized using X-ray diffraction (XRD), Raman spectroscopy, field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), and BET surface area analysis. The 1 % Ce-doped $ZnMn_2O_4$ sample showed notable enhancements in structural and surface characteristics, with reduced crystallite size, well-defined octahedral morphology, and a high specific surface area of 42.71 $m^2\ g^{-1}$ compared to other samples, facilitating improved ion and electron transport and a greater number of electroactive sites. Electrochemical evaluation confirmed the battery-type nature of all samples, with 1%Ce–$ZnMn_2O_4$ delivering a superior specific capacity of 426.1 C g^{-1} at 1 A g^{-1}, far exceeding the undoped (145.5 C g^{-1}) and 0.5%Ce–$ZnMn_2O_4$ (401 C g^{-1}) electrodes. Even at 20 A g^{-1}, the 1%Ce–$ZnMn_2O_4$ electrode retained 60% of its initial capacity and maintained 85% stability after 5000 cycles. These results demonstrate that rare-earth doping is an effective approach to optimizing $ZnMn_2O_4$-based battery-type electrodes for next-generation hybrid supercapacitors.

Keywords: $ZnMn_2O_4$, Combustion synthesis, Specific capacity, Electrochemical performance.

Electron correlations, itinerant magnetism and *DMI* strength in $Fe_{1-x}Co_xSi$ (x = 0.4 and 0.6): A comparative investigation

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We study the magnetic, thermodynamic, and transport properties of $Fe_{1-x}Co_xSi$ alloys with nominal compositions of x = 0.4 and x = 0.6. A comparative analysis of magnetization, specific heat, and electrical resistivity has been carried out to understand the influence of Co concentration on the itinerant magnetic character of these alloys. Magnetization measurements reveal distinct magnetic transition temperatures: 53.71 K for x = 0.4 and 30 K for x = 0.6. The saturation and spontaneous magnetic moments, as well as the technical saturation field, are reduced in the x = 0.6, although the dimensionless ratio θ_W/T_C remains nearly equal for both compositions. Interestingly, despite weaker magnetic interactions inferred from these observations, the Rhodes–Wohlfarth ratio is found to be 2.3 times larger for x = 0.6, highlighting its enhanced itinerant nature. Furthermore, the effective magnetic moment of x = 0.6 composition is 1.3 times greater than that of x = 0.4, accompanied by a relatively strong paramagnetic, temperature-independent background. In addition, the Dzyaloshinskii-Moriya interaction (DMI) strength is found to decrease largely in x = 0.6 in comparison with that of an itinerant system MnSi. Specific heat measurements provide additional insight into the electronic and magnetic correlations. The C/T versus T^2 plots exhibit linearity for x = 0.4, while a low-temperature rise is observed for x = 0.6, suggesting subtle differences in the density of states and low-energy excitations. Electrical resistivity further distinguishes the two compositions: the x = 0.4 alloy shows an unusual upturn below the ordering temperature, indicative of enhanced scattering mechanisms, whereas the resistivity of x = 0.6 remains nearly temperature independent in the ordered state, consistent with itinerant electron behaviour. Taken together, these results demonstrate that increasing Co concentration from 0.4 to 0.6 drives $Fe_{1-x}Co_xSi$ towards a more itinerant magnetic regime, as evidenced by the larger Rhodes–Wohlfarth ratio, stronger paramagnetic background, and resistivity characteristics. In contrast, the x = 0.4 alloy retains features of localized magnetism, manifested in its resistivity upturn and lower effective moment. The comparative study thus highlights the delicate balance between localized and itinerant magnetism in Fe-Co-Si alloys and underscores the role of chemical composition in tuning their fundamental properties. These findings provide valuable insights into the interplay of magnetic and electronic correlations in transition-metal monosilicides and guide for functional applications.

Keywords: Strongly correlated systems; Quantum interference; Magnetic interactions.

Magnetic disorder-manifested deviation from Fermi liquid mechanism in the correlated electron metal $Mn_{0.5}Fe_{0.5}Si$

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We investigate the transport and thermodynamic properties of the half magnetically doped itinerant magnet $Mn_{1-x}Fe_xSi$ with nominal composition x = 0.5, focusing on resistivity and specific heat measurements. The alloy crystallizes in the B20 cubic structure, and the chosen composition lies above the quantum critical point of $Mn_{1-x}Fe_xSi$, making it an ideal candidate to probe non-Fermi liquid behaviour and strong electron correlations. Resistivity decreases steadily with temperature from 300 K but fails to exhibit the quadratic dependence expected for a conventional Fermi liquid at low temperatures, nearly signalling non-Fermi liquid features. Moreover, the resistivity magnitude at 2 K is nearly 70 times larger than that of pure MnSi, underscoring the pronounced influence of magnetic disorder. Zero-field resistivity analysis is employed to disentangle the contributing scattering mechanisms. Specific heat measurements provide complementary evidence of enhanced correlations. On a C/T versus T^2 scale, the data reveal a pronounced upturn, with C/T reaching approximately 66 $mJ.mol^{-1}\cdot K^{-2}$. This represents a significant enhancement of quasiparticle effective mass in B20 itinerant systems. To further probe electron correlations, magnetic fields up to 140 kOe are applied, and both resistivity and specific heat are measured under these conditions. The combined results show no evidence of magnetic ordering down to 2 K, while the low-temperature features consistently support strong electron correlation effects. The findings highlight the critical role of spin fluctuations and magnetic disorder in shaping the electronic ground state of $Mn_{0.5}Fe_{0.5}Si$. The absence of ordering, together with the large resistivity and enhanced specific heat, point to a correlated itinerant regime dominated by disorder-induced scattering. These observations emphasize the delicate interplay between itinerancy, magnetic disorder, and electron correlations in B20 silicides. A detailed investigation of spin fluctuations in $Mn_{0.5}Fe_{0.5}Si$ is therefore essential to fully understand the unconventional transport and thermodynamic behaviour observed above the quantum critical point. The present study provides new insights into the physics of doped itinerant magnets and contributes to the broader understanding of correlated electron systems in transition-metal monosilicides.

Keywords: Quantum phase transition; Strong electron correlations; Quasiparticles.

Tailoring the morphology and dielectric properties of RF sputtered Ta_2O_5 thin film by variation of RTA temperature and duration

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This study investigates the impact of post-deposition rapid thermal annealing (RTA) on the structural, morphological, and electrical properties of Ta_2O_5 thin films deposited by radio frequency (RF) sputtering. The Ta_2O_5 thin films were subjected to RTA at varying temperatures and durations to evaluate changes in their crystallinity, morphology, dielectric properties, and leakage current characteristics. X-ray diffraction (XRD), atomic force microscopy (AFM), and FESEM studies revealed the enhanced crystallinity and improved surface morphology with increasing annealing temperature up to 750 °C, and with further increase in RTA temperature, the roughness increases and diffraction peak intensity decreases. Electrical characteristics investigated using capacitance-voltage (C-V) and current-voltage (I-V) measurements. The results revealed that RTA significantly influences the dielectric constant, oxide charge density (Q_{ox}), interface charge density (D_{it}), and leakage current of the Ta_2O_5 thin film. The film, rapidly treated at 750 °C for 10 min, was found to have a high dielectric constant of 23, low Q_{ox} value of 0.98 × 10^{12} cm^{-2}, low D_{it} value of 1.06 × 10^{12} $eV^{-1}cm^{-2}$, and low leakage current of 1.01 × 10^{-8} A, which is the optimal RTA condition in optimizing Ta_2O_5 thin films for applications in advanced electronic and optoelectronic devices.
Keywords: Rapid thermal annealing, Sputtering, High-k dielectric, Ta_2O_5 thin film.

Photocatalytic dye degradation using CuO thin films prepared by the doctor blade technique

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In this study, CuO thin film was successfully synthesised on a glass substrate using the doctor blade method. The film was thoroughly analysed using XRD, FTIR, Raman spectroscopy and UV–visible spectroscopy to investigate its structural and optical characteristics. XRD analysis confirmed the formation of a single-phase CuO with a monoclinic structure and the crystallite size was determined to be about 34 nm using the Scherrer formula. FTIR analysis confirms the formation of CuO thin film by detecting the characteristic Cu-O bond vibrations. Raman spectrum shows the characteristics A_g and B_g modes of CuO, confirming the formation of monoclinic CuO thin films. Optical characterization using UV–visible spectroscopy and the Tauc relation indicated that the thin film exhibited an energy band gap of approximately 2.5

eV. The copper oxide thin film exhibited effective photocatalytic activity for dye degradation under UV-light illumination.

Keywords: Doctor blade method; Structural properties; Optical properties; Photocatalytic.

Structural, morphological and antibacterial evaluation of spinel cobalt ferrite nanoparticles

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Cobalt ferrite ($CoFe_2O_4$) nanoparticles with a spinel structure were successfully synthesized via the sol–gel auto-combustion method using glycine as a fuel. The X-ray diffraction (XRD) analysis confirmed the formation of a single-phase spinel structure, exhibiting a lattice parameter of 8.3758 Å and an average crystallite size of 13 nm. FTIR spectroscopy further supported the structural formation by characteristic metal–oxygen vibrational bands at 526.56 cm^{-1} (ν_1) and 410.83 cm^{-1} (ν_2), corresponding to tetrahedral and octahedral sites in the spinel lattice. Transmission electron microscopy (TEM) revealed well-defined, uniformly distributed nanoparticles with clear morphological features, indicating successful synthesis and controlled particle formation. The antibacterial activity of the synthesized $CoFe_2O_4$ nanoparticles was evaluated against *Bacillus subtilis* (Gram-positive) and *Escherichia coli* (Gram-negative), demonstrating effective inhibition of both bacterial strains. These results highlight the potential of cobalt ferrite nanoparticles for antibacterial applications and other functional nanomaterial-based systems.

Keywords: Cobalt ferrite; Sol–gel auto-combustion; Spinel structure; Antibacterial activity.

Influence of aluminum doping on the photocatalytic activity of nickel ferrite nanoparticles

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The present research work deals with the synthesis of Al-doped nickel ferrite nanoparticles with the generic formula $NiFe_{2-x}Al_xO_4$ (x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5) using a green synthesis approach. Ginger extract was used as a green fuel. The prepared nanoparticles were characterized structurally for phase purity and structural properties using the X-ray diffraction method reported earlier. The nanocrystalline nature of the materials was further validated by transmission electron microscopy (TEM), which revealed uniformly distributed nanoparticles with size values consistent with the nanoscale regime. Raman spectroscopy recorded in the 200-1000 cm^{-1} range exhibited five prominent vibrational modes, E_g, T_{2g} (1), T_{2g} (2), T_{2g} (3), and A_{1g} (1) characteristic of spinel ferrites, confirming the structural stability and local lattice symmetry. X-ray photoelectron spectroscopy (XPS) analyses identified core-level signals corresponding to Ni $2p_{3/2}$, Fe 2p, O 1s, C 1s, and Al 2p, confirming the successful incorporation of Al into the ferrite lattice and providing insight into the oxidation states of the constituent elements. Magnetic measurements conducted using field-cooled (FC) and zero-field-cooled (ZFC) protocols yielded blocking temperatures in the narrow range of 299-301 K, indicating superparamagnetic behavior near room temperature. The luminescence spectra show a decrease in peak intensity as the aluminium dopant is increased. The photocatalytic performance of the synthesized nanoparticles was evaluated using methylene blue dye under natural sunlight irradiation. Significant degradation activity was observed, demonstrating the potential of Al-doped nickel ferrite nanoparticles as efficient sunlight-driven photocatalysts.
Keywords: Al-doped nickel ferrite, TEM, Raman Spectroscopy, XPS, FC-ZFC, PL, Photocatalytic.

Enhanced structural and magnetic properties of cobalt ferrite nanoparticles prepared via glycine assisted sol-gel auto-combustion method

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In this work, we report the synthesis of pristine cobalt ferrite in nanocrystalline form using sol-gel auto-combustion method. Glycine in the ratio of 3:1 with metal nitrate was used as a chelating agent. Single phase formation and cubic spinel structure was established through X-ray diffraction technique. The nano-crystalline nature was confirmed through crystallite size (14 nm) obtained. The lattice constant, X-ray density, unit cell volume, lattice strain and other structural parameters obtained from XRD data are in good agreement with the literature report. The XRD pattern show the single phase diffraction peaks. The presence of two absorption bands near 400 cm^{-1} and 600 cm^{-1} observed in the FTIR spectra revealed the spinel ferrite formation. The absorption band were used to obtain force constants. FE-SEM images show uniform grain growth with less agglomeration of the nanoparticles. The EDS spectra reveals that all the constituent ions Co, Fe and O are in stoichiometric proportion. The saturation magnetization of the order of 76 emu/g was recorded through M-H hysteresis curve. The overall magnetic behaviour is explained through Neel's model.
Keywords: Cobalt ferrite, Nanocrystalline, XRD, FE-SEM, VSM.

Effect of copper oxide nanoparticles on the impedance and A.C. conductivity properties of borosilicate glass ceramics

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The present work investigates impedance spectroscopic properties of copper oxide (Cu_2O) nanoparticles modified Borosilicate glass ceramics. The Cu_2O was maintained with the weight ratio 0%, 10%, 30% in the Borosilicate matrix. The X-ray diffraction performed on the samples confirmed the crystalline phase along with glassy nature. The morphology of the synthesized samples established the smooth glassy surface with tiny chip-like ceramic structures. The impedance, AC conductivity and electrical modulus measurements were carried out on the cylindrical samples in the capacitor geometry. The Bode plots of the resulting samples indicated the decreased impedance with increase in Cu_2O. The Nyquist plot was carried out for all the samples and analyzed using the equivalent circuit. The circuit suggested the two major contributions to the electrical behavior of the samples. The AC conductivity revealed constant behavior followed by a frequency dependence and the overall conductivity was increased with Cu_2O. Hence, the present modifier Cu_2O nanoparticles can be used as an optimizer for the glasses to tune their electrical properties.

Keywords: Cu_2O Nanoparticles; Borosilicate Glass Ceramics; Impedance Spectroscopy.

Investigations of structural and optical properties of Fe doped $BaTiO_3$ nanopowder

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In this work, we report the synthesis and characterizations of bare barium titanate ($BaTiO_3$) and Fe doped $BaTiO_3$ ($BaTi_{1-x}Fe_xO_3$, x= 0.05) nanopowder using an advanced low temperature aqueous sol-gel auto combustion method. The synthesis method utilizes citric acid as a chelating agent (fuel). The metal nitrate to fuel ratio was maintained to as 1:3. The synthesized

nanopowder was well characterized by non-destructive X-ray diffraction tool to understand the phase purity and to investigate the structural parameters. The X-ray analysis confirmed the formation of homogeneous pure phase compound with crystalline size of the order of 124 nm to 128 nm. The crystal structure was found to be tetragonal with lattice constant a = b = 3.910 Å and c = 4.002 Å. Williamson-Hall (W-H) equation was used to obtain the lattice strain as well as crystallite size. The tolerance factor was estimated to confirm the perovskite structure. The optical properties were investigated by means of UV-Visible spectroscopy technique. The band gap energy determined using Tauc's plot is of the order of 3.06 eV.
Keywords: $BaTiO_3$, Fe doping, X-ray diffraction, UV-Vis.

Influence of V_2O_5 on the optical properties of $BaO–Li_2O–Bi_2O_3–WO_3–B_2O_3$ glasses

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In the present study, vanadium doped $BaO–Li_2O–Bi_2O_3–WO_3–B_2O_3$ glasses were synthesized using the conventional melt-quenching technique. The amorphous nature of the prepared samples was confirmed through X-ray Diffraction (XRD), ensuring the formation of a homogeneous glass network suitable for optical investigations. To understand the role of vanadium ions in modifying the optical behavior of the host matrix, detailed UV–Visible absorption studies were carried out. The spectra indicate systematic changes in the optical absorption edge, suggesting that the optical band gap energy (E_{opt}) and metallization criterion (M) increase with the incorporation of V_2O_5. Such behavior is characteristic of enhanced electronic localization, implying that these glasses exhibit semiconducting features in their amorphous state. In addition, a comprehensive set of optical parameters such as refractive index (n), absorption coefficient (α), extinction coefficient (K), optical conductivity (σ_{op}), optical polarizability (α_o), and theoretical optical basicity (Λ_{th}) were calculated across the studied wavelength range. These parameters explore the details on electronic transitions and polarizability effect imparted by the vanadium ions. This study ensures the prospect of using transition-metal-doped boro-bismuthate glasses in photonic components, nonlinear optical devices, and other emerging optoelectronic applications.
Keywords: Oxide glasses, UV-Vis, optical bandgap, absorption coefficient, Optical basicity.

Electrical conduction behaviour of NaI doped system: Applicability of Meyer–Neldel rule

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The thermally activated conduction behaviour of NaI-Ag_2S-Se-Te-Zn-S chalcogenide glassy system has been examined with emphasis on the Meyer–Neldel rule (MNR). Temperature-dependent AC conductivity has been compared with that of AgI doped oxide system, AgI – CdO – V_2O_5 – P_2O_5 –ZnO. The DC conductivities (σ_0) are analyzed from the linearly fitted curves of the AC conductivities using Arrhenius relation, $\sigma = \sigma_0 \exp(-\Delta E / K_BT)$, which exhibits thermally activated nature. The conductivity exhibited Arrhenius-type behaviour, allowing the extraction of the activation energy (ΔE) and pre-exponential factor (σ_o). Analysis performed by varying either frequencies at fixed composition or composition at fixed frequency revealed that the system follows the Meyer–Neldel rule. A clear correlation between σ_o and ΔE has been observed, and further examination using the relation $\sigma_o = \sigma_{oo} \exp(\Delta E/\Delta E_{mn})$ confirmed the presence of "Further MNR." The Meyer–Neldel energy (ΔE_{mn}), obtained from the slopes of σ_o versus ΔE plots, supports a multi-phonon excitation mechanism. This interpretation suggests that thermally stimulated electron or polaron hopping between localized states may be assisted by phonon-induced entropy contributions. The correlation between σ_o and ΔE_{mn} demonstrates that MNR provides a meaningful framework for understanding microscopic charge transport processes in NaI-Ag_2S-Se-Te-Zn-S chalcogenide glassy system. With all factors considered, the present study shows that employing mixed glass formers is crucial for enhancing electrical conductivity, optimising activation energy, and modifying conduction paths. These are therefore beneficial choices for advanced solid electrolyte applications.

Keywords: Chalcogenides, MN Rule Complex impedance, Polaron hopping.

$NiFe_2O_4$/ZnO heterostructure nanocomposites fir efficient photocatalytic dye degradation and hydrogen generation

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This investigation explores the successful fabrication of [$(NiFe_2O_4)_x$/ZnO] (x=25%,50%75%) nanocomposites via. sol-gel self-ignition method to optimize photocatalytic dye degradation and hydrogen (H_2) evolution. Crystalline analysis via X-ray diffraction (XRD) verified the presence of single-phase $NiFe_2O_4$ and ZnO, with mixed phases observed in the composite material. FTIR analysis validated the existence of characteristic functional groups, while FE-SEM and EDX verified the quasi-spherical structure and elemental composition of the nanocomposites. BET analysis revealed a higher surface area for $NiFe_2O_4$ (38.89 m^2/g) than for ZnO (28.21 m^2/g), contributing to improved photocatalytic performance. UV–Vis's spectroscopy revealed a tunable band gap to enhance visible light absorption, and photoluminescence (PL) characterizations verified mitigated electron-hole recombination, enhancing the overall photocatalytic activity. An increase in magnetic saturation was observed with the gradual addition of $NiFe_2O_4$, as confirmed by magnetic measurements. Remarkable

photocatalytic activity was observed for the $NiFe_2O_4$/ZnO (x = 75%) nanocomposite, with 99.56% breakdown of MB dye achieved in just 100 min of visible light exposure. Moreover, the nanocomposite exhibited excellent hydrogen generation activity, with a maximum H_2 yield of 814 µmol/h/g after 8 h. The nanocomposite exhibited outstanding long-term stability and maintained its effectiveness through repeated use. These outcomes emphasize the potential of $NiFe_2O_4$/ZnO nanocomposites as effective and robust photocatalysts for eco-friendly remediation and green hydrogen generation.

Keywords: Photocatalysis, Sol-gel auto-combustion, Photocatalyst, Hydrogen evolution.

Room temperature magnetoelectric properties of $CoFe_2O_4$ nanoflakes

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Magnetoelectric effects at room temperature are of great interest for advanced sensors, memory, and spintronic devices. In this work, cobalt ferrite ($CoFe_2O_4$) nanoflakes were synthesized using a chemical route and their structural, morphological, and magnetoelectrical properties were investigated. X-ray diffraction confirmed the formation of an inverse-spinel structure, while Raman spectroscopy identified the characteristic vibrational modes of cobalt ferrites. Field-emission scanning electron microscopy revealed well-defined flake-like morphologies. Room-temperature magnetoimpedance (MI) measurements showed strong frequency dependence, with a maximum negative MI of 1.6% under a 1.4 T field at 100 Hz, which decreased to nearly –0.1% at 1 MHz. Additionally, a significant change in electrical polarisation was observed under a small magnetic field of 0.3 T, demonstrating magnetoelectric coupling. These findings indicate that $CoFe_2O_4$ nanoflakes exhibit promising frequency-tuneable responses, making them suitable candidates for multifunctional applications in sensing and spintronic technologies.

Keywords: Nanoflakes; Cobalt ferrite; Magnetoimpedance; Magnetoelectric.

Fabrication of plasmonic nanoparticle-embedded PDMS substrates for surface enhanced Raman spectroscopy

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Surface-enhanced Raman spectroscopy (SERS) is a prominent technique in detecting molecular structures. With the presence of plasmonic metal nanoparticles on its detection surface, the Raman signal is amplified by several orders of magnitude. The plasmonic metal nano particle array will significantly contribute to local surface plasmon resonance and boost Raman scattering process. In the present report, we mentioned the work to amplify the

Raman attributes of rhodamine 6G (R6G) through the utilization of a polydimethylsiloxane (PDMS) substrate that is coated with surface gold nanoparticles (AuNPs) Array. The fabrication procedure, the AuNPs were integrated into the surface of the PDMS substrate. This integration ensured that the AuNPs were consistently distributed and demonstrated significant plasmonic coupling. The evaluation of the results pertaining to signal enhancement was conducted by scrutinizing the Raman spectra of R6G, illustrating a significant increase in signal intensity as opposed to the conventional PDMS substrate. The PDMS-based technology is characterized by its versatility and biocompatibility, offering low-cost and reproducible Raman enhancement, thereby rendering it a suitable candidate for biosensor and screening applications. In addition, the inclusion of gold nanoparticles amplifies the efficiency of the substrate by contributing to its stability and reusability at several intervals. Raman spectroscopy investigations were conducted on R6G to assess the effectiveness of various Raman modes related to R6G. This research broadens the methodological framework for the advancement of adaptable, versatile, and efficient SERS substrates suitable for applications in biological and chemical analysis and detection.

Keywords: SERS; Plasmonic Nanoparticles; PDMS substrate.

Pareto optimal approach for sparing normal brain using normal tissue objective function based static-field intensity modulated stereotactic radiosurgery of solitary brain metastasis

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The purpose of the study was to establish a pareto optimal approach for normal brain sparing using a distance driven normal tissue dose gradient function for static field intensity modulated stereotactic radiosurgery planning of solitary brain metastasis (SBM). A sample of twenty seven (n=27) SBM cases were planned to a 20 Gy dose using 6 MV static fields to determine the pareto optimal plans among the six NTO variations formed from slope = 0.2, 0.6, and 1.0 mm^{-1}, priority + end-dose = 100 + 10% and 200 + 30%. The greater the slope or smaller the end-dose values the stricter the NTO function in terms of dose gradient formation. For analysis, NTO function having a slope = 1.0 mm^{-1}, priority + end-dose = 100 + 10% was chosen as control group. All NTO variations were analysed for changes in field size (FS), normal brain dose volumes (V12 and V8), conformity index (CI), gradient index (GI), prescription isodose level (PIDL), and MU per Gy. Lower values of normal brain dose volumes, GI and CI value near unity implies optimal plan quality. Correlational analysis was conducted to find relevant associations between FS, V12 and GI for all the NTO function variations. Groups with priority = 200 plus slope ≥ 0.6 mm^{-1}, showed substantial reductions for FS, V12, V8, GI and PIDL ($P < 0.0001$). Significant decrease in normal brain dose volumes was observed due to increase in fluence conformity and consequent FS regression. No changes appeared in CI (±0.01), while significant improvement was observed in GI. PIDL was found to decrease with an associated MU per Gy increase, ($P < 0.0001$). A very strong positive association was found between FS and V12 ($r > 0.9$) implying an implicit inverse GI association with FS ($r < -0.7$). NTO

strictness causes fluence contraction that in turn yields normal brain sparing and betterment in dose metrics needed to obtain balance in plan goals. In summary, it was seen that the plan metric enhancements saturate with the application of stricter NTO function variations. That is, reduction of further plan improvement implies achievement of optimal plan results.
Keywords: Stereotactic radiosurgery, Brain sparing, Objective function.

Role of rare earth ytterbium on the structural and magnetic properties of cobalt ferrite nanoparticles

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In this article, we report the role of Yb^{3+} on the crystal structure, cation distribution, infrared, room temperature magnetization properties of cobalt ferrite. The samples of $CoFe_{2-x}Yb_xO_4$ (x = 0.00, 0.05 and 0.10) nanoparticles were successfully prepared in single phase using sol-gel auto-combustion method. X-ray diffraction technique was employed to obtain the various structural properties. The crystallite size was obtained by using Scherrer's equation which is around 23 nm. The lattice constant increases from 8.383 Å to 8.386 Å with Yb^{3+} doping. The X-ray diffraction method was used to determine the cation distribution. The results suggests that Yb^{3+} occupy predominantly octahedral site where as Fe^{3+} ions occupy both tetrahedral (A) and octahedral [B] site. The other structural parameters like dislocation density, lattice strain etc. shows string influence of Yb^{3+} doping. The magnetization measurements performed using VSM technique shows deceasing nature with Yb^{3+} doping. Saturation magnetization decreases from 77.91 emu/g to 65.12 emu/g. Neel's model was employed to understand the magnetic behaviour of the present samples.
Keywords: Yb^{3+} doped cobalt ferrite, XRD, Cation Distribution, VSM.

Fabrication and characterization of $Ba_{1-x}La_xTiO_3$ nanomaterials: Insights into optical, fluorescence, and structural properties

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Barium titanate ($BaTiO_3$) is a critical oxide material used in electronics. Some of the most important uses of these materials are in high-frequency energy reservoirs, waveguides, modulators, resonators, filters, memory systems, microwave transducers, and photonic switching technologies. Doping lanthanum (La) into its structure increases its energy storage capabilities and alters its optical features, thereby affecting the operational efficiency of

devices. The structural characterization of $BaTiO_3$ was conducted utilizing X-ray diffraction (XRD) alongside Raman spectroscopy, thereby offering additional insights into its structural attributes. The analysis of absorption and bandgap was executed employing UV-Vis. spectroscopy measurements. Furthermore, fluorescence spectroscopy highlighted the emission aspects connected to defect states and La doping. The morphology was studied via scanning electron microscopy (SEM) image analyses. These results indicate that the synthesized materials have great potential for use in light-emitting devices and optical sensor systems. In conclusion, the results of this study indicate that La-infused $BaTiO_3$ exhibits potential consideration for integration into electronic and photonic applications.

Keywords: energy storage, dielectric material, Barium titanate, oxide materials.

Investigating impact of polypyrrole substitution on hopping length and on the formation of tetrahedral and octahedral sites in gallium nitride doped ferrite nanocomposites

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The present communication aims to investigate the impact of Polypyrrole substitution as a filler in Gallium Nitride ferrite nanocomposites. For the composition of $Ga_3NFe_{97}O_3$ synthesized by Sol-Gel method three different weight percentages of Polypyrrole 3%,10%,30% mixed with 97%, 90%, 70% by weight of Gallium Nitride ferrite and reported elsewhere by corresponding author. The analysis was done in terms of hopping length, tetrahedral bond, octahedral bond, tetrahedral edge, shared octahedral edge, unshared octahedral edge values. The lattice parameter 'a' calculated from X-ray diffraction analysis was around 6 A^o both for ferrite and Polypyrrole nano composites. For the addition of 3%, 10% Polypyrrole the hopping length, tetrahedral bond, octahedral bond tetrahedral edge, shared octahedral edge, unshared octahedral edge values are increased and for 30% Polypyrrole there is a slight decrement. This is due to change in ionic radii, different crystal structures of GaN and Fe_2O_3 surrounded by Polypyrrole. Also, non-magnetic GaN occupying strongly tetrahedral A-site.

Keywords: Gallium Nitride ferrite, Polypyrrole, Hopping length, Octahedral bond.

Environmental stability of quantum materials under thermal, mechanical, and radiation stress: A systematic review for aerospace applications

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Quantum materials, including graphene, transition-metal dichalcogenides (TMDCs), topological insulators, correlated oxides, and spin–orbit coupled heterostructures, exhibit electronic and magnetic responses governed by topological protection, strong electron correlation, and low-dimensional quantum confinement. These characteristics underpin ultra-sensitive detection, high-efficiency communication components, robust navigation architectures, and emergent spintronic and thermoelectric functionalities. Consequently, quantum materials are increasingly considered for aerospace systems that require high performance under severe environmental constraints. Yet their operational viability remains uncertain because the behaviour of these quantum states under extreme thermal, mechanical, and radiation conditions is not systematically understood. Aerospace environments expose materials to rapid thermal excursions, high-frequency mechanical vibration, shock loading, high-g acceleration, and substantial ionising-radiation flux. For quantum materials whose functionalities depend critically on defect density, interfacial bonding, crystallographic order, and subtle band-structure features, these stressors can induce chalcogen vacancies, modify spin textures, disrupt surface-state conduction, suppress carrier mobility, alter magnetoresistance, or destabilise structural phases. Existing studies report such effects, but the evidence is dispersed across physics, materials science, and engineering, with inconsistent test conditions and non-standardised metrics. This study proposes a Systematic Literature Review (SLR) supported by a quantitative bibliometric analysis to consolidate and critically evaluate the experimental evidence on the stability of quantum materials under aerospace-relevant stressors. A structured search strategy was implemented in Scopus and Web of Science for the period from 2010 to 2025. The search design was grounded in three pillars: (i) experimentally validated quantum-material families exhibiting non-classical transport; (ii) environmental stressors aligned with MIL-STD-810H and NASA GEVS standards (thermal cycling, thermal shock, cryogenic exposure, strain, vibration, shock, proton/electron/gamma irradiation, total ionising dose); and (iii) degradation-related outcomes including electronic drift, optical attenuation, structural transformation, interface degradation, and device-level failure. High-volume but irrelevant research domains such as batteries, catalysis, and electrochemistry were excluded to avoid conceptual noise. Retrieved records underwent deduplication and PRISMA-based eligibility screening. Based on preliminary evidence and domain trends, the bibliometric component is expected to reveal an expanding but uneven research landscape, characterised by dense activity in TMDC radiation studies and strain-dependent transport in topological insulators, in contrast to limited investigation of multi-stressor or synergistic degradation phenomena. The thematic synthesis is anticipated to highlight recurrent degradation mechanisms, namely displacement-damage accumulation, chalcogen vacancy formation, surface-state scattering, interfacial decohesion, and thermally driven electronic or structural phase transitions. A cross-material comparison is likely to reveal significant heterogeneity in environmental resilience, underscoring the need for material-specific reliability frameworks. A methodological quality appraisal is expected to expose deficiencies such as inconsistent stress protocols, inadequate environmental control, limited ageing studies, insufficient replication, and weak statistical reporting. By integrating disparate studies into a coherent analytical structure, this review aims to produce the first rigorous comparative assessment of the environmental robustness of quantum materials. The findings will inform material selection, reliability-conscious device engineering, and aerospace qualification strategies, enabling the rational transition of quantum materials from laboratory-scale demonstrations to aerospace technologies.
Keywords: Quantum materials; Radiation and thermal stress; Aerospace reliability.

Raman scattering, photoluminescence and photo detection properties of hydrophobic Al doped ZnO nanoarrays

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Zinc oxide (ZnO) and Aluminum-doped zinc oxide nanorod arrays are deposited on glass/ITO substrate by a modified sol gel process. The as-grown samples are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, photoluminescence (PL) spectroscopy and photo-electrochemical analysis. The SEM micrographs show that the undoped, 1 at. % and 2 at% Al doped films are composed of nanorods and the concentration of 3 at. % Al doping hinders the rod-like structures growth. The investigations of XRD reveal that the synthesized undoped and Al doped ZnO nanorods possess a perfect hexagonal growth habit of wurtzite zinc oxide, along the (002) direction of preference. The Raman spectra demonstrate that the vibrational mode of E1(LO), which is very weak in undoped, 1at% and 2 at% Al doped ZnO, is strongly enhanced with 3 at. % Al doping into ZnO lattice. PL spectra show that strong UV emission in pure, 1 at. % and 2 at. % Al doped ZnO, while there is dominant green emission in 3 at. %Al doped ZnO. The contact angle of the ZnO nanostructures varied between 91° and 110° depending upon the Al content. Moreover, all the samples are photo electrochemically active and exhibit the highest photocurrent of 20 µA for the 2 at. %Al doped ZnO nanorod arrays.

Keywords: ZnO, Nano arrays, Contact angle, Raman Scattering, Photo sensing.

Studies of porous structure and its impact on hydrogen adsorption in activated carbons using different models

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Understanding the impact of pore structure on hydrogen (H_2) adsorption is of importance for H_2 storage applications. Here we report our investigation on porous structure- surface area, pore volume and pore size distribution (PSD) in three different kinds of activated carbons- granular activated carbon (GAC), activated carbon fibre (ACF) and activated carbon cloth (ACC). Then we study the impact of porous structure on the adsorption of H_2. To understand the porous structure and H_2 adsorption, different models were employed. The PSD was determined using different kinds of DFT models. It was found that the amount of H_2 adsorbed was highest for ACF. This was attributed to the high surface area and pore volume in ACF. Moreover, it was found that the amount of H_2 adsorbed was higher in GAC in compared to

that in ACC, although GAC and ACC possess similar surface area and pore volume. This was explained by the micropore dominating structure in GAC. Further to understand the interaction of H_2 with the pore walls, isosteric heat of adsorption was calculated.
Keywords: Hydrogen; Adsorption; Activated carbons; Models.

High-performance supercapacitor electrodes: Hydrothermal synthesis of spherical MoS_2 with enhanced capacitive efficiency

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In this study, MoS_2 nanostructures were successfully synthesized through a simple one-pot hydrothermal method using ammonium heptamolybdate and thiourea as precursors. Structural analysis via X-ray diffraction confirmed the formation of MoS_2 with randomly stacked layers, which is attributed to ammonia intercalation during synthesis. Field-emission scanning electron microscopy revealed that the product consists of sphere-like, porous MoS_2 assemblies formed from ultrathin nanosheets—a morphology highly favourable for electrochemical applications because it increases accessible surface area for charge storage. The electrochemical performance of these MoS_2 nanostructures was systematically evaluated. Cyclic voltammetry displayed nearly rectangular CV curves, indicating a dominant electric double-layer capacitance mechanism and efficient ion transport. A maximum specific capacitance of 106 F/g at 5 mV/s was achieved. Galvanostatic charge–discharge tests further confirmed good capacitive behaviour, giving a maximum specific capacitance of 92.85 F/g at 0.5 mA/cm². The material also demonstrated excellent cycling stability, retaining 93.8% of its initial capacitance after 1000 cycles, highlighting its long-term durability. Electrochemical impedance spectroscopy revealed a low charge-transfer resistance and ideal capacitive characteristics, suggesting fast interfacial kinetics. Overall, the study confirms that hydrothermally synthesized sphere-like MoS_2 nanostructures possess electrochemical properties, making them suitable for future high-performance supercapacitor electrodes.
Keywords: MoS_2 nanostructures; Hydrothermal; Supercapacitor electrodes; Electrochemical.

Comprehensive characterization of $Mg_{1-x}Co_xFe_2O_4$ spinel nanoparticles: Effects of cobalt doping on structural and optical properties

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Cobalt-doped magnesium ferrite nanoparticles $Mg_{1-x}Co_xFe_2O_4$ (x = 0.2–0.8) were successfully synthesized via the hydrothermal route, and their structural, optical, and microstructural characteristics were systematically investigated. X-ray diffraction (XRD) confirmed the

formation of a cubic spinel structure without secondary phases, with lattice parameters decreasing from 8.452 Å to 8.382 Å as Co^{2+} concentration increased, consistent with the substitution of smaller Co^{2+} ions at octahedral sites. The crystallite size reduced from 8.55 to 7.57 nm, accompanied by an increase in dislocation density, indicating enhanced lattice strain induced by Co incorporation. FTIR spectra displayed the two-characteristic metal–oxygen vibrational bands (ν_a and ν_b) around ~580–400 cm^{-1}, verifying the occupancy of cations at tetrahedral and octahedral sites, with slight shifts reflecting local structural distortion. UV–Vis. absorption measurements revealed strong absorption in the UV region, while PL spectra exhibited intense emission peaks in the 350–450 nm region attributed to oxygen-vacancy-related recombination, with emission intensity increasing with Co content. FESEM images showed agglomerate, nearly spherical nanoparticles, and EDAX confirmed the presence of Mg, Co, Fe, and O elements, validating the successful substitution of Co into the $MgFe_2O_4$ lattice. Overall, the results demonstrate that Co doping significantly tailors the microstructural and optical properties of $MgFe_2O_4$ nanoparticles, making them suitable for magnetic, optoelectronic, and catalytic applications.

Keywords: Co-doped $MgFe_2O_4$, Spinel ferrite, XRD analysis, Optoelectronic applications.

Flow description of Casson nanofluid in a conducting field with inclination effects: An artificial neural network approach

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This paper aims to examine the convective heat and mass transfer flow of Casson hybrid nanofluid with nanoparticles of Silica and Tin Oxide and Engine Oil as base fluid (EO/SnO_2-SiO_2), through a permeable medium bounded by a semi-infinite flat plate in the presence of chemical reaction, Dufour, Lorentz force, thermal radiation, and radiation absorption. In this study, the governing equations of the flow model are transformed into a dimensionless form, and the regular perturbation method is utilized to determine the solutions for the rate of fluid flow, temperature, and species diffusion. The skin friction coefficient, Nusselt number, and Sherwood number are used to represent the shear stress, rate of heat transfer, and rate of mass transfer at the plate, respectively. The effects of different parameters, such as the suction parameter, magnetic parameter, radiation absorption parameter, Casson parameter and Dufour number on the flow are analyzed using graphs and tables. The results indicate that the rate of heat transfer in the Casson nanofluid is higher than that in the nanofluid. Additionally, to strengthen prediction accuracy and validate the analytical results, an Artificial Neural Network (ANN) model is developed using the generated dataset of flow, thermal, and concentration profiles. The ANN is trained to predict key performance indicators such as skin friction, Nusselt number, and Sherwood number under varying physical parameters.

Keywords: Casson nanofluid, Heat and mass transfer, Thermal radiation, Dufour effect.

Power-dependent photoluminescence in graphene/ MoS_2 Van der Waals heterostructure at room temperature

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Quantum materials exhibit a broad class of robust phenomena governed by subtle quantum effects. The rich interplay among diverse internal degrees of freedom, including spin, orbital and charge, can give rise to multiple coexisting and competing quantum phases. In particular, the family of transition metal dichalcogenides has attracted significant attention as a promising material for addressing the unique electronic properties of quantum materials. Additionally, this family has been extensively studied using optical spectroscopy to explore its exotic quantum phases. However, despite immense studies on exploring multiple features, particularly using optical responses, the deep understanding of intricate electronic phenomena remains unclear. Here, in order to strengthen our understanding of such properties, we study room temperature PL emission spectra of MoS2 underneath Gr, by shining the laser of wavelength 532 nm. Our study unlocks the anomalous behavior in the PL emission of the underlying MoS2/Gr heterostructure on the Si substrate. Our study also highlights the linear power dependence of the PL peak, strongly indicating the biexciton formation in MoS2-Gr heterostructures. The fact here is that such an anomaly is being reported for the first time to the best of our knowledge, and this study requires further theoretical and experimental investigation to gain a better understanding of our work.
Keywords: Quantum materials; Graphene; MoS_2, PL.

Enhanced antibacterial performance of Sol-Gel synthesized nickel ferrite nanoparticles

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Nickel ferrite ($NiFe_2O_4$) nanoparticles were successfully synthesized using the sol-gel method. XRD analysis confirmed the formation of a single-phase cubic spinel structure with crystallite size 21 nm. FTIR spectroscopy revealed characteristic metal-oxygen vibrational modes corresponding to tetrahedral and octahedral sites. Raman spectroscopy analysis verified the phase purity and characteristic vibrational modes of the nickel ferrite nanoparticles. Brunauer-Emmett-Teller (BET) analysis indicating a surface area 7.45 m^2/g. UV-Vis., spectroscopy showed strong optical absorption in the visible region with a band gap energy 1.73 eV. Vibrating

sample magnetometer (VSM) measurements confirmed the ferromagnetic nature of nickel ferrite nanoparticles, exhibiting saturation magnetization and coercivity at room temperature. The Nickel ferrite nanoparticles also displayed enhanced antibacterial activity against both Gram-positive and Gram-negative bacteria, attributed to the generation of reactive oxygen species, indicating the applications in biomedical field.

Keyword: Nickel ferrite, Structure, Elastic Properties, Optical, Antibacterial application.

Synthesis, structural, magnetic and microwave absorption properties of Mn^{3+} substituted cobalt-nickel nanoferrites with composition $Co_{0.9}Ni_{0.1}Mn_xFe_{2-x}O_4$ using sol-gel combustion method

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In this work, structural, magnetic and microwave absorption properties of Mn^{3+} substituted cobalt-nickel nanoferrites with composition $Co_{0.9}Ni_{0.1}Mn_xFe_{2-x}O_4$, (where x =0.0 and 0.05) synthesized using sol-gel combustion method were reported. X-ray diffraction analysis confirmed the formation of single-phase Mn^{3+}-substituted cobalt-nickel nanoferrites. Magnetic properties estimated using Vibrating Sample Magnetometer (VSM). Saturation magnetization was found to decrease with Mn substitution. Further, simple casting technique was used to prepare flexible Co-Ni ferrite film using PVA. The EMI shielding behavior estimated for the films using vector network analyzer (VNA) in the frequency range 8-12 GHz, suggest that Mn^{3+}substituted cobalt-nickel nanoferrites exhibit microwave absorption properties.

Keywords: spinel ferrite; XRD; VSM; Microwave applications.

Structural, morphological, optical and dielectric properties of copper ferrite graphene oxide nanoparticles

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A composite material comprising copper iron oxide (Delafossite)-decorated reduced graphene oxide (RGO) was synthesized via a citrate-gel auto combustion method. Copper iron oxide (Delafossite) structured material demonstrates robust stability in aqueous conditions. Consequently, it has been explored for multiple purposes, such as Solar cell absorber layers and serving as photocathodes for CO_2 photoelectro-chemical reduction, solar water reduction, and as a cathode material in lithium batteries. Therefore, this work investigates the effect of Graphene Oxide (GO) added during synthesis on $CuFeO_2$ crystallinity, optical, morphological and electrical properties. Scanning electron microscopy (SEM) images confirmed the porosity of the materials, with average pore diameters measured at 1.76 nm

for RGO and 1.32 nm for the nanocomposite. The optical bandgap energy of the deposited material varying from 2.405 eV to 1.864 eV with increasing the concentration of GO. These results make the $CuFeO_2@GO_x$ a potential absorber material with a tuneable bandgap for solar cell application in a high energy spectrum.

Keywords: Nanoparticles: Morphology, Optical, Dielectric properties, Impedance.

Room temperature magnetoelectricity in CuO-doped $Bi_4Ti_3O_{12}$ ceramics

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In order to attain magnetoelectric (ME) multiferroic phase at room temperature, CuO has been interstitially doped in well-known lead free layered structured $Bi_4Ti_3O_{12}$ (BIT) ferroelectric ceramics, since multiferroic materials possess considerable interest in modern memory storage technologies such as spintronic devices. Addition of CuO (x = 0.25, 0.5 & 0.75 mol %) induces feeble magnetization at room temperature in BIT ceramics. The optimal saturation magnetization of 3.37 memu/g was observed in x=0.25 sample, which decreases further upon increasing the doping concentration. Magnetic field driven electric polarization effect was investigated at room temperature, which shows that remnant polarization was significantly improved upon increasing the magnetic field strength (H=0-7 kOe), which indirectly indicates the presence of ME coupling effect in CuO doped BIT ceramics. The highest remnant polarization of 9.93 $\mu C/cm^2$ was achieved for x=0.75 sample at H=7 kOe. In the direct test of ME effect, all the samples showed weak ME effect at room temperature. The highest magnetoelectric coupling coefficient of α=0.0115 $mVcm^{-1}Oe^{-1}$ was estimated in low concentration (x=0.25 mol%) CuO doped BIT ceramics. Although, the noticed ME effect weakens upon increasing the doping concentration. Additionally, investigation on magnetodielectric effect in the prepared samples also validates our present inference. As reported, the magneto-dielectric effect may arise from magnetoresistance (MR) and Maxwell-Wagner polarization effect. Our low field MR studies suggests that the observed large magnetodielectric effect in x=0.25 sample is not due to extrinsic phenomenon. Moreover, the magnetoimpedance effect study also confirms the presence of coupling mechanism between magnetic and electric phase in CuO doped BIT ceramics. The strong magnetic super exchange interaction among Cu-O ions induces feeble spontaneous magnetization, which resulted in weak magnetoelectric coupling effect at RT in $Bi_4Ti_3O_{12}$ lead free ferroelectric ceramics.

Keywords: Multiferroics; Ferroelectrics; Magnetization; Ceramics; Magnetoelectric materials.

Cerium single atom anchored cobalt molybdenum oxide nanorods: Experimental synthesis, characterization and DFT mechanistic insights for high performance electrodes

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The increasing demand for high performance energy storage devices necessitates electrode materials with fast diffusion kinetics, good electrochemical activity and long-term structural stability. However, conventional transition metal oxides suffer from the limited active sites, volume changing, low conductivity and sluggish electron transport. Nano structuring offers partial mitigation by increasing surface area and improving electrolyte interaction, yet achieving complete utilization of metal centers remains a challenge. In this regard, integrating singe atom catalytic concepts into nanostructured hosts provides an effective strategy to maximize atomic efficiency while preventing structural destruction. Here, we report the synthesis of cerium anchored cobalt molybdenum oxide (Ce-Co-Mo-O) nanorods using simple hydrothermal route combined with controlled defect engineering. The one-dimensional nanorods morphology provides continuous electron pathways, while cerium anchoring introduces localized electronic modulation within Co-Mo-O lattice structure. X-ray diffraction (XRD) confirms the formation of a phase-pure mixed-metal oxide structure without secondary cerium-related phases, indicating successful atomic-level incorporation. UV–Vis. spectroscopy reveals enhanced light absorption and a reduced band gap, attributed to Ce-induced electronic-state modification. Density functional theory calculations further demonstrate that cerium anchoring increases electronic density near Fermi level and lowers surface adsorption energies, which leads to enhanced electrochemical properties. This combined effects of nanorods geometry and cerium induced activation makes them for energy storage devices.
Keywords: Cerium anchoring; Nanorods; Hydrothermal synthesis; Band gap; Energy storage.

Optimized rice straw ash as a sustainable pozzolanic precursor for high-performance geopolymer mortars

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This study investigates the potential of rice straw ash (RSA), an agricultural by-product, as a sustainable precursor for geopolymer mortars in response to the declining availability of fly ash (FA). RSA was synthesized through controlled combustion at different temperatures followed by mechanical grinding, and the optimized sample (RSA650-20) exhibited high amorphous silica content, fine particle size, and stable thermal characteristics.

Characterization confirmed enhanced reactivity and minimal unburnt carbon under these processing conditions. Incorporating RSA650-20 as a 25% replacement for FA in geopolymer mortar resulted in compressive strength comparable to conventional FA–GGBFS systems while maintaining satisfactory workability. Microstructural observations revealed a dense and cohesive matrix with well-developed aluminosilicate and calcium-rich gels, confirming efficient geo-polymerization. These results demonstrate that optimally processed RSA can serve as a viable supplementary cementitious material, promoting the valorisation of agricultural residues, reducing dependence on FA, and advancing the development of eco-efficient, low-carbon construction materials.

Keywords: Rice straw ash; Pozzolanic material; Controlled burning; Agricultural by-product.

Experimental and machine learning-aided prediction of compressive strength of geopolymer mortar using processed rice straw ash

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One of the primary challenges confronting cement production today is its significant environmental impact. To advance sustainable construction, this study investigates alkali-activated mortars prepared with fly ash, ground granulated blast furnace slag, and alkaline activators, with and without rice straw ash as a partial replacement for FA. Specimens were designed with NaOH molarities of 7.5, 10, 12, and 14, and paste volumes ranging from 26% to 36%. Compressive strength was measured at 3, 7, and 28 days, while XRD, EDX, and SEM analyses were conducted for microstructural characterization. Results show that RSA incorporation consistently enhanced matrix densification, reduced porosity, and improved particle binding, with improvements becoming more pronounced at higher NaOH molarities. Compared to control mixes, RSA-incorporated mortars exhibited denser microstructures and achieved higher compressive strength across all curing ages. Machine learning techniques including support vector machine, cascade forward neural network, random forest, and transformer model were applied to predict compressive strength, with CFNN achieving the highest accuracy. These findings highlight RSA as a viable and sustainable additive that enhances mechanical and microstructural performance while supporting CO_2 reduction and waste valorisation in construction.

Keywords: Geopolymer mortar; Rice straw ash; Artificial neural network; Microstructure.

Low-temperature chemical bath deposition of MoO_3 thin films: Structural and electrochemical evaluation

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The molybdenum trioxide (MoO_3) thin films were deposited using a chemical bath deposition (CBD) approach with ammonium molybdate at 60°C, 80°C, and 100°C for two hours in order to investigate the effect of temperature on film growth. The samples were deposited on Nickel (Ni) foil, stainless-steel (SS) foil, and Nickel (Ni) foam, allowing for the assessment of surface coverage and substrate-dependent adherence. At higher temperatures, X-ray diffraction verified the development of crystalline orthorhombic MoO_3 with enhanced crystallinity, and FTIR analysis revealed distinctive Mo=O and Mo–O–Mo vibrations that indicated successful phase formation. SEM images showed how the morphology changed, especially on Ni foam, from fine grains at lower temperatures to well-developed. Electrochemical investigations revealed distinct pseudocapacitive behaviour with symmetric charge-discharge patterns and steady redox activity. Because of improved ion transport and increased crystallinity, Ni foam-supported electrodes performed better due to their increased electrolyte accessibility and large surface area. Additionally, overall, the favourable structure, morphology, and electrochemical properties of CBD-grown MoO_3 thin films indicate great promise for high-performance supercapacitor applications.
Keywords: Chemical bath deposition, Temperature, Specific Capacitance, Morphology.

Application-driven first-principles and Ab initio molecular dynamics study of rare-earth mononitrides (REN)

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Rare-earth mononitrides (REN) constitute an important class of functional ceramic materials due to their structural robustness and potential applicability in high-temperature electronic environments. In this work, a comprehensive first-principles investigation is carried out on NdN, PmN, SmN, EuN, and GdN to understand their structural stability and finite-temperature behavior. Density Functional Theory (DFT) calculations are carried out using the Quantum ESPRESSO package to determine the ground-state structural characteristics in the rocksalt (Fm–3m) and Pm–3m crystal phases, followed by ab initio molecular dynamics (AIMD) simulations within the Born–Oppenheimer framework. The AIMD simulations are primarily performed in the canonical (NVT) ensemble to examine thermal stability, atomic mobility, and lattice fluctuations at finite temperatures relevant to ceramic applications. The time evolution of total energy, temperature, and atomic trajectories is analyzed to assess the dynamical stability of both crystal phases. In addition, variable-cell molecular dynamics calculations are used to qualitatively explore pressure-induced structural responses and volume fluctuations. The results indicate that the rocksalt (Fm–3m) phase exhibits superior thermal stability across the REN series, maintaining structural integrity with small atomic displacements around equilibrium positions. In contrast, the Pm–3m phase shows enhanced sensitivity to temperature, manifested through larger lattice distortions and increased anharmonic atomic motion. These findings highlight the critical role of finite-temperature effects in determining the structural robustness of rare-earth nitride ceramics. Overall, the combined DFT and AIMD approach provides valuable insights into the thermal and dynamical stability of REN compounds, offering a reliable theoretical framework for assessing their suitability in

advanced ceramic and electronic applications operating under realistic temperature conditions.

Keywords: Rare-Earth Nitrides (REN), Ceramic Materials, Ab Initio Molecular Dynamics.

Enhancement of thermal, UV, DC and AC electrical characteristics of rare-earth Er^{3+} doped Cd-Mg ferrites

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The work highlights thermo-electric, UV, frequency dependent AC di-electric, impedance, conductivity and temperature dependent DC conductivity properties of Er^{3+} doped Cd-Mg ferrites for x=0.000-0.025 with chemical composition $Cd_{0.2}Mg_{0.8}Er_xFe_{2-x}O_4$ [*x*= 0,0.005,0.010,0.015,0.020 and 0.025] prepared with citrate-gel technique. Thermo-electric power studies related to See beck coefficient(S) and carrier concentration (η) are observed from room temperature to well beyond curie temperature. The value of 'S' is negative for all undoped and doped samples confirming that ferrites resemble the behavior of N-type semi-conductors. Curie temperature ranges between 503 to 593 K, observed values of S range between -2.023 µV/K to -6.883 µV/K and carrier concentration(η) range between $7.124x10^{22}$ $/m^3$ to 7.537×10^{22} $/m^3$. UV-Vis absorptance data was recorded with UV-Vis., spectrometer in a wavelength range of 200nm-900nm. Energy band gap was recorded to lie in the range of 2.0000 to 2.0156 eV. DC resistivity of CMEF-compounds has been computed as a function of their dopants (CMEF-0 to CMEF-5) between 300K to 750K. DC dielectric resistivity of CMEF-compounds was determined and found to be in the range of 6.352×10^4 Ω-m to 1.563×10^5 Ω-m. Activation energy was found to lie between 0.6372eV-0. 8995eV. It was observed that the curie temperature first decreased and then increased with increasing Er^{3+} substitution from 511 to 567K. LCR meter was used between 4Hz-8MHz. AC conductivity(σ_{ac}) and log(σ_{ac}) values are recorded at 8MHz frequency. The observed values of log(σ_{ac}) ranged from -2.8831 to -2.9509. With increase in dopant log(σ_{ac}) values increased and then decreased. The higher dopant (CMEF-5) exhibited high conductivity. Dielectric loss tangent (tanδ) values are found to be in the range of 0.0859-0.1515.

Keywords: Thermo-electric, UV-Vis, DC resistivity, AC conductivity, LCR meter.

Interchannel delay mitigation in PPG-based pulse wave velocity estimation using low-cost analog filtering

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Pulse Wave Velocity (PWV) is a widely accepted indicator of arterial stiffness and an important marker of cardiovascular health. Traditional PWV measurement techniques rely on pressure-based sensors such as applanation tonometry or invasive catheterization, limiting their suitability for continuous and wearable monitoring. Optical sensing approaches, particularly

photoplethysmography (PPG), offer a low-cost and non-invasive alternative for PWV estimation. In a typical PPG sensor, an LED–photodiode pair detects pulsatile blood volume changes in tissue, with the photodiode generating a small photocurrent that is converted to a voltage using a transimpedance amplifier (TIA). The acquired signal requires filtering to suppress noise and baseline drift. In low-cost PPG systems, this filtering is commonly implemented using capacitive analog filters, which introduce channel-dependent phase delays. While such delays are acceptable for heart rate estimation, they significantly degrade timing accuracy in PWV analysis, leading to erroneous velocity estimates. This work proposes a method to compensate for interchannel delay while retaining the simplicity and low hardware cost of capacitive filtering, enabling more reliable PPG-based PWV estimation for wearable and resource-constrained applications.
Keywords: Pulse wave velocity, Interchannel delay, Photoplethysmography, Analog filtering.

Synthesis and characterization of chitosan based silver nanocomposite using neem extract

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This work reports the green synthesis of a chitosan-based silver nanocomposite, where neem powder extract served as an eco-friendly bio reductant for the formation of silver nanoparticles. The samples were characterized through multiple techniques, including, Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDX), and X-ray Diffraction (XRD) techniques. EDX results shows that the investigated compound contains silver. This result shows that the formation of silver nanoparticles and neem extract will act as a capping and reducing agent. The synthesized chitosan based silver nanocomposite can be used as an antioxidant, antidiabetic and anticancer substances.
Keywords: Chitosan, Silver nanocomposite, Neem powder extract Ecofriendly.

Light-matter interaction: An in-vitro and theoretical studies in characterizing the interaction of antihistamine drug bilastine with carrier protein human serum albumin

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Light-matter interactions are very intricating process in biological systems in providing a plethora of information and leverages on how the properties are changed when molecules absorb, emit, scatter light energy. Biomolecular interactions with small molecules play a crucial role in the biological process multiplicity including drug development and disease cure. Spectroscopic techniques like UV-Visible, fluorescence and circular dichroism provide a wealth of information based on the principle of light-matter interactions. The therapeutic action of drug is exhibited when binds to specific receptors which are biological macromolecules. The present work shows the findings of the interaction of antihistamine drug bilastine (BLS) with carrier protein human serum albumin (HSA). The key findings from UV-Visible, fluorescence, circular dichroism and docking studies shows that bilastine binds at site-2 in subdomain IIIA within the hydrophobic pocket of human serum albumin with a binding constant of 10^4 M^{-1} order. The interaction is spontaneous and an entropy-driven process. Interaction-induced structural changes in human serum albumin were observed from circular dichroism studies. Molecular docking studies envisaged the preferential binding of bilastine in subdomain IIIA of human serum albumin matching to the observation of marker displacement studies. The involvement of the residues in the binding was analyzed from the 2-dimensional diagram and the ligplot of the complexes.

Keywords: Light-matter interaction, Human Serum Albumin, Molecular docking.

Structural and luminescence properties of Nd^{3+}-doped strontium-boro-tellurite glasses integrated with ZnO and Bi_2O_3

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This study details the synthesis and detailed characterization of a complex glass system. The glass samples were successfully produced through the conventional melt-quenching method within 1000 °C, resulting in clear, high-quality specimens. X-ray diffraction (XRD) confirmed the amorphous structure of the samples by showing broad humps without crystalline peaks, indicating a disordered structure characteristic of the glassy nature of the fabricated samples. Physical parameters such as density and molar volume were measured to assess the structural integrity and compactness of the glass network. Results revealed that adding ZnO and Bi_2O_3 significantly boosts density, owing to Bismuth's high molecular weight, while also altering molar volume. Fourier Transform Infrared (FTIR) spectroscopy provided insights into the glass structure, identifying components such as TeO_4 trigonal bipyramids, TeO_3 trigonal pyramids, and BO_3/BO_4 units. The presence of ZnO and Bi_2O_3 as network modifiers was confirmed by shifts in vibrational bands, indicating a transition of bridging oxygens to non-bridging oxygens (NBOs). Optical absorption spectra in the UV-Vis-NIR range showed sharp bands from Nd^{3+} ions transitioning from the $^4I_{9/2}$ ground state to various excited states, with spectral positions remaining stable despite host modifications. Photoluminescence studies under 582 nm excitation revealed three emission bands in the near-infrared region corresponding to the $^4F_{3/2} \rightarrow {}^4I_{9/2}$, $^4F_{3/2} \rightarrow {}^4I_{11/2}$, and $^4F_{3/2} \rightarrow {}^4I_{13/2}$ transitions. The strongest emission at approximately 1060 nm highlights the potential of these glasses for solid-state laser applications. Decay curve analysis of the $^4F_{3/2}$ level indicated a primarily single-exponential decay, although the addition of heavy metal oxides affected non-radiative relaxation rates. The overall integration of heavy

metal oxides in strontium-boro-tellurite glasses is well explored to observe their potential applications in Photonics.

Keywords: Luminescence at 1060 nm; Boro-Tellurite glass; Structural, Heavy metal oxide.

Effect of microwave heating on phase evolution and optical bandgap tuning of Na doped iron oxide nanoparticles

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The sodium doped iron oxide nanoparticles were synthesized via hydrothermal (HT), and citrate-gel auto-combustion (CGA) methods. Further, they were subjected to microwave heating at different temperatures, viz., 500 and 700°C/20 min., respectively. The samples obtained were analyzed using the X-ray Diffractometer (XRD), Fourier Transform Infrared Spectrometer (FT-IR), and UV-Visible spectrophotometer. It was found that the samples prepared by the CGA method exhibited the single-phase cubic spinel structure upon microwave heating at 500°C pertaining to a minute secondary phase of monoclinic kind. On the other hand, the HT method revealed the monoclinic phase structure on microwave heating at 500, and 700°C. Interestingly, the optical bandgap (E_g) tuning was observed in the case of as-synthesized and microwave heated samples.

Keywords: Nanoparticles; Hydrothermal; Citrate-gel; Microwave heating; Bandgap.

Studies of porous structure and its impact on hydrogen adsorption in activated carbons using different models

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Understanding the impact of pore structure on hydrogen (H_2) adsorption is of importance for H_2 storage applications. Here we report our investigation on porous structure- surface area, pore volume and pore size distribution (PSD) in three different kinds of activated carbons- granular activated carbon (GAC), activated carbon fibre (ACF) and activated carbon cloth (ACC). Then we study the impact of porous structure on the adsorption of H_2. To understand the porous structure and H_2 adsorption, different models were employed. The PSD was determined using different kinds of DFT models. It was found that the amount of H_2 adsorbed was highest for ACF. This was attributed to the high surface area and pore volume in ACF. Moreover, it was found that the amount of H_2 adsorbed was higher in GAC in compared to that in ACC, although GAC and ACC possess similar surface area and pore volume. This was

explained by the micropore dominating structure in GAC. Further to understand the interaction of H_2 with the pore walls, isosteric heat of adsorption was calculated.
Keywords: Hydrogen; Adsorption; Activated carbons; Models.

Impact of thermal treatment on the photovoltaic performance of SnO_2 nanoparticle-based dye-sensitized solar cell

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Sonochemically synthesized SnO_2 nanoparticles were investigated as alternative photoanode materials for dye-sensitized solar cells (DSSCs), with particular emphasis on how thermal treatment modulates their key physicochemical characteristics. Systematic post-calcination revealed a strong interplay between particle size, isoelectric point (IEP), and dye-loading capability-factors that critically govern device performance. Structural and spectroscopic analyses confirmed crystal growth and agglomeration at higher temperatures, accompanied by a notable reduction in IEP, which collectively diminished sensitization efficiency. In contrast, SnO_2 treated at lower calcination temperatures preserved an optimal surface environment for enhanced dye adsorption, leading to significantly improved photocurrent and overall cell performance. The study establishes a clear correlation between thermal tuning, surface chemistry, and photovoltaic behavior, highlighting a simple yet effective strategy to improve SnO_2-based DSSCs without altering composition or device architecture.
Keywords: Sonochemical Method; Nanoparticles; Photovoltaic; Isoelectric point.

Unlocking the electrochemical sensing potential of Cu/ZnO- for precise simultaneous detection of tyrosine, dopamine and ascorbic acid

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Across the globe, a silent storm brews as diabetes, diabetic foot ulcers, and neurological maladies like Schizophrenia and Parkinson's disease rise with alarming frequency. Amidst this complex landscape, the intricate interplay of tyrosine, dopamine, and ascorbic acid emerges as telltale analytes, revealing the hidden struggles taking place within. In this study, an abiotic sensor adorned with the dynamic duo of Cu/ZnO was unveiled, which enhances the electrochemical analysis of L-tyrosine, dopamine, and ascorbic acid. Cu/ZnO nanoparticles were characterized using FT-IR, Raman, XRD, SEM, TEM, and XPS. HRTEM's inverse FFT showed d-spacing values of 0.23, 0.29, and 0.317 nm corresponding to Miller indices 101, 100, and

011, with ZnO and Cu presence on the surface. SEM, TEM, and XPS analyses confirmed the presence of Cu(I) and Cu (II). CV, DPV, and CA studies showed simultaneous detection of DA, AA, and Tyr, with CV revealing oxidation peak separations of 193 mV for AA-DA, 444 mV for DA-Tyr, and 637 mV for AA-Tyr. The designed CZMG electrode exhibits remarkable sensitivity to DA, AA, and Tyr, with its stability and reproducibility being commendably consistent.

Keywords: Copper-doped ZnO modified graphite electrode; Dopamine; Tyrosine; Ascorbic Acid; Cyclic voltammetry.

Effect of sintering temperature on gas sensing and photocatalytic performance of pristine WO_3

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The present study systematically investigates the influence of sintering temperature on the gas-sensing and photocatalytic performance of pristine WO_3 nanostructures synthesized via a facile one-step hydrothermal route. The as-synthesized WO_3 powders were sintered at 425, 525, 625, and 725 °C to modulate their structural, morphological, optical and surface characteristics. Comprehensive characterization using XRD, FE-SEM/EDAX, TEM/HRTEM, XPS, UV–Vis spectroscopy and BET surface area analysis confirmed the formation of phase-pure monoclinic WO_3 with a well-defined nanoplate-like morphology. Among the investigated samples, WO_3 sintered at 525 °C exhibited optimized crystallinity, enhanced specific surface area, favorable pore characteristics and a higher concentration of surface oxygen species. Gas-sensing measurements demonstrated a maximum response of 85.09% toward 100 ppm acetone at an operating temperature of 300 °C, accompanied by rapid response (30 s) and recovery (90 s) times, excellent selectivity, and long-term stability. In addition, the same sample showed superior photocatalytic performance, achieving approximately 40% degradation of methylene blue under natural sunlight irradiation within 2 h. The enhanced dual functionality is attributed to the synergistic effects of optimized grain size, increased surface area, improved charge transport and enriched surface oxygen chemistry, all governed by the sintering temperature. These findings establish sintering temperature as a critical parameter for tailoring pristine WO_3 nanostructures for efficient acetone gas sensing and photocatalytic wastewater remediation applications.

Keywords: Tungsten trioxide; Sintering; Morphology; Acetone gas sensor; Photocatalysis.

Antioxidant potential of a dicoumarol analog and unveiling its binding nature with double-stranded DNA: Spectroscopic, docking and ADMET studies

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The interaction of radiation/light with matter is a powerful tool for probing biomolecular interactions with small molecules of biological importance. The changes in optical behavior, such as absorption, emission, and scattering properties, can aid in analyzing the binding mechanism, binding-induced structural changes, pharmacodynamics, and pharmacokinetics. Since bis-coumarins are known for their biological potential, we report the synthesis of its analog 4-hydroxy-3-[(4-hydroxy-2-oxochromen-3-yl)-(3-hydroxy, 4-methoxyphenyl) methyl] chromen-2-one, followed by its antioxidant potential. The antioxidant potential of HMD was comparable to the potential of standard ascorbic acid. The IC_{50} values for superoxide radical scavenging, DPPH radical scavenging, and hydroxyl radical scavenging were found to be 27, 28, and 29 µM, respectively, compared to 25, 27, and 28 µM for standard ascorbic acid. The ADMET properties of HMD revealed its nephrotoxicity, respiratory toxicity, and cardiotoxicity. The properties like drug likeness, pharmacokinetic and oral bioavailability have been evaluated theoretically. The UV-Vis., fluorescence, and circular dichroism spectroscopies have been employed in unveiling the binding nature of HMD with DNA. The binding strength was found to be 10^3 M^{-1} order. Thermodynamic studies at 303, 308, and 318 K revealed that the binding was spontaneous with negative free energy of -28 kJ mol^{-1}. Marker displacement results confirmed the binding of HMD as a minor-groove binder and were supported by DNA denaturation and DNA viscosity studies. HMD binding in DNA did not affect the DNA structure and conformation as revealed by circular dichroism studies. Docking study at theoretical level showed the preferential location of HMD in the minor-groove of the DNA.

Keywords: Bis-coumarin, DNA, Antioxidant, ADMET, Spectroscopy.

Role of annealing ambience on the interfacial chemistry and electrical properties of HfO_2/Si stacks for MOS devices

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HfO_2 films of thickness 10 nm were deposited on chemically cleaned p-type Si wafer using pulsed DC magnetron sputtering technique. Post-deposition annealing was performed at 400 ℃ and 700 ℃ in oxygen (O_2) followed by nitrogen (N_2) ambience to investigate the interface quality depends electrical characteristics of HfO_2/Si stacks for MOS devices. The chemical composition and bonding states of the ZrO_2 films were analyzed by X-ray photoelectron spectroscopy (XPS; Kratos Analytical, UK) employing monochromatic Al Kα radiation. Narrow scan of XPS spectra of Hf 4f peak reveals that the role of oxygen annealing with respect to temperature. The stoichiometric Hf $4f^+$ doublet peak was clearly observed for the films annealed at 700 ℃ with a weak presence of non-HfO_2 peak in O1s spectra. The crystallographic structure of the annealed films was examined by X-ray diffraction (XRD; Rigaku, Japan) using Cu Kα radiation (λ = 1.5418 Å). XRD spectra confirm the amorphous nature of HfO_2 layer even after annealing at 700 ℃. Capacitance–voltage measurements were extracted from as-deposited and annealed Pt/HfO_2/Si MOS devices at 10, 100 KHz, and 1 MHz, and current–voltage (I–V) characteristics were obtained by sweeping the bias from −5 V to +5 V using an Agilent B1500A semiconductor parameter analyzer. The accumulation capacitance value of annealed devices at 400 ℃ was increased to almost 100% from the same of as-deposited devices. It might be due to the fortification of HfO_2 thickness, rather than the impetus of the native silica layer. The effective dielectric constant value was 22 for the device annealed at 400 ℃, owing to not only strengthening of HfO_2 layer with tightly bounded atoms, but reduction of oxygen vacancies in HfO_2 layer and interface at HfO_2/Si. Further, the effective dielectric constant value was slightly decreased to ~20 in the case of devices annealed at 700 °C. Current–voltage characteristics revealed that the leakage current level was decreased to nA scale after annealing at 700 ℃, whilst the same was in the scale of μA for as-deposited devices. The possible reason for this could be the strengthening of native SiO_2 layer and reduction of oxide traps in the bulk HfO_2 and interface traps at HfO_2/Si stack after annealing at 700 ℃. As-deposited and annealed devices at 400 ℃ showed both Schottky and Poole–Frenkel (P-F) conduction mechanism, whereas the P-F mechanism was dominated in the devices annealed at 700 ℃.

Keywords: Pulsed DC Sputtering, HfO_2, Dielectric constant, Interface quality, Leakage currents.

Silicon-based n-i-p heterojunction photoanode for large scale photoelectrochemical water splitting

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With the rising global demand for sustainable energy, the production of green hydrogen through the photoelectrochemical (PEC) route has emerged as a highly promising solution. Heterojunction photoelectrodes are advantageous for PEC applications due to their ability to enhance light absorption, improve charge carrier generation, and facilitate efficient charge separation and transfer while minimizing recombination losses. In this work, a high-performance silicon-based n-i-p heterojunction photoanode with an FTO/TiO_2/Si/NiO architecture has been successfully developed using earth-abundant materials, leveraging the inherent benefits of the heterostructure design. Targeting the practical application of the photoelectrodes for solar fuel production, the heterojunction was fabricated via the industry-

relevant magnetron sputtering technique, ensuring scalability and uniformity. The optimized FTO/TiO_2/Si/NiO_A configuration achieved an impressive surface photovoltage of 600 mV and delivered a photocurrent density of approximately ~0.65 mA/cm^2 at 1.23 V_{RHE} under simulated solar illumination (100 mW/cm^2), with a low onset potential of around ~0.11 V_{RHE}, attributed to the strategic selection of materials and architectural design. The photoanode also demonstrated remarkable photochemical stability, retaining over ~96% of its initial photocurrent after 10 hours of continuous operation in 1 M KOH (pH 13.5). Furthermore, the successful fabrication and demonstration of a large-area (25 cm^2) photoanode validated both the performance and the scalability of the approach, reinforcing its potential for industrial-scale PEC water splitting applications.

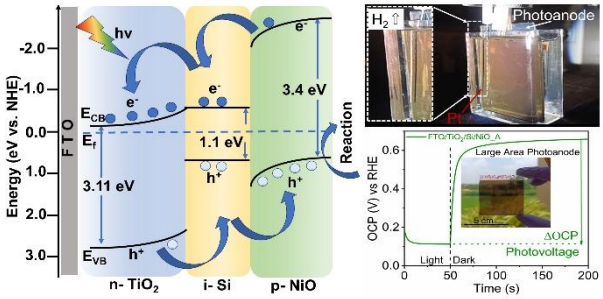

Figure 1: n-TiO_2/i-Si/p-NiO heterojunction photoanode enabling efficient water splitting with enhanced photovoltage and visible hydrogen evolution on a large-area photoanode.

Keywords: Photoelectrochemical water splitting, Si-based photoanode, *n-i-p* heterojunction, Magnetron sputtering, Large area device.

Strength–corrosion correlation of Mg-alloyed AlTiSnZr lightweight high-entropy materials

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In this paper, the light-weight high entropy alloy using the general formula $AlTiSnZrMg_x$ (x = 0, 0.5, 1.0, and 1.5 mol%, abbreviated as $ATSZM_x$) system is explored for its thermal stability, microstructure, mechanical properties, and corrosion resistance. DTA indicated thermal stability up to 525°C with endothermic peak at 652°C corresponding to the BCC matrix and $MgTi_3$ phase. The XRD patterns after post-sintering indicated the presence of dominant tetragonal BCC structures and intermetallic phases (Al_3Zr, $MgTi_3$), wherein the disorder was increased with up to 1.0 mol% Mg. SEM indicated uniform distribution of BCC phase and HR-TEM recorded 0.37 nm lattice spacing for the BCC (101) plane and nanocrystalline grains. $ATSZM_{1.0}$ HEA system is reported to exhibit the highest fracture strain (8.6%), micro-hardness (530HVN±15.48) and fracture strength (698MPa ± 19.87) due to the synergy of cocktail effect and phase homogeneity. Corrosion resistance was established by the electrochemical measurements with lower current densities and larger diameter of the Nyquist plot being achieved. Such properties of $ATSZM_{1.0}$ HEA sample make it a promising candidate in the

marine, aerospace, high-temperature structural applications involving high strength and corrosion resistance.

Keywords: High entropy alloys; Corrosion Resistance; Mechanical alloying.

Structural and electrical properties of ZrO_2/Si stacks for MOS devices

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10 nm thick ZrO_2 films were deposited on chemically cleaned p-type Si (111) wafer using pulsed DC magnetron sputtering technique. Post-deposition annealing was performed at 400, 500 and 600 ℃ in oxygen (O_2) ambience followed by nitrogen (N_2) ambience to investigate the interface quality depends electrical characteristics of ZrO_2/Si stacks for MOS devices. The chemical composition and bonding states of the ZrO_2 films were analyzed by XPS employing monochromatic Al Kα radiation. Narrow scan of XPS spectra of Zr 3d peak reveals that the role of oxygen annealing at 600℃effectively formed the stoichiometric Zr $4f^+$ doublet peak with a presence of weak non-ZrO_2 peak in O 1s spectra. The crystallographic structure of the annealed films was examined by XRD using Cu Kα radiation. XRD spectra confirm the poly-crystalline nature of ZrO_2 layer for the films annealed at greater than or equal to 500 ℃. The C–V measurements were extracted from as-deposited and annealed Pt/ZrO_2/Si MOS devices by sweeping the voltage from -5 to +5 V at 10, 100 & 1000 KHz. The accumulation capacitance value was almost doubled relatively when compare with as-deposited devices in the case annealed devices at 600 ℃, with almost negligible stretch in depletion region. The considerable increment in the oxide capacitance value could be owing to strengthening of the dielectric film and reduction in the bulk oxide and interface trap densities. The effective dielectric constant value (k) was ~ 24 for the device annealed at 600 ℃. This enhancement in 'k' is plausibly linked to a combination of film densification, reduced defect density, and phase evolution from an amorphous to crystalline phases, viz., tetragonal or orthorhombic- ZrO_2. I - V characteristics revealed that the leakage current density was decreased to μA/cm^2 from mA//cm^2 (heating at 600 °C). The reason is the reduction of oxygen-vacancy-related defect states within the ZrO_2 bulk but also to the strengthening and controlled growth of the interfacial SiO_2 layer, which reaches a thickness of approximately 1.6 nm (annealed at 600 ℃).

Keywords: Pulsed DC Sputtering, ZrO_2, Interface quality, Dielectric constant, Leakage currents.

Rare-earth engineered $CoFe_2O_4$ nanoparticles on $Ti_3C_2T_x$ MXene for enhanced triboelectric nanogenerator performance

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Triboelectric nanogenerators (TENGs) have emerged as promising energy-harvesting devices for powering next-generation self-powered electronics; however, their practical deployment is often limited by low surface charge density and inefficient charge retention in conventional polymer-based tribo-layers. To address these challenges, this study presents a rational materials-engineering strategy that integrates two-dimensional conductive MXenes with rare-earth-doped ferrite nanoparticles to construct high-performance nanocomposite tribo-layers. In this work, $Ti_3C_2T_x$ MXene was synthesized via selective HF etching of the Ti_3AlC_2 MAX phase, yielding few-layered MXene sheets with abundant surface terminations. Subsequently, cobalt ferrite ($CoFe_2O_4$) nanoparticles doped with rare-earth ions (Y^{3+} or Gd^{3+}, 1 at. %) were grown *in situ* on the MXene sheets using a hydrothermal route. The resulting MXene–ferrite hybrid nanocomposites were fabricated into flexible free-standing films and employed as one electrode in contact-mode TENG devices. Structural, morphological, and compositional analyses confirmed the successful decoration of uniformly distributed doped $CoFe_2O_4$ nanoparticles on the MXene sheets, while preserving the layered architecture of $Ti_3C_2T_x$. The incorporation of rare-earth dopants into the ferrite spinel lattice was found to significantly modify the dielectric response, leading to improved interfacial polarization and enhanced charge storage. Electrical performance measurements revealed a marked improvement in triboelectric output for the doped nanocomposites compared to the undoped counterpart. In particular, the Y^{3+}-doped MXene/$CoFe_2O_4$ composite (MX@CFO–Y) exhibited the most pronounced enhancement, suggesting that rare-earth substitution in ferrite spinels is a highly effective approach for boosting surface polarization and charge trapping. Under a contact frequency of approximately 1.7 Hz and moderate contact force, the MX@CFO–Y-based TENG generated a transferred charge of ~1.08 mC per contact cycle, outperforming both the Gd^{3+}-doped (0.77 mC) and undoped MX@CFO (0.65 mC) devices. Overall, all nanocomposite TENGs achieved transferred charges in the range of 10^{-7}–10^{-6} C per cycle, corresponding to effective surface charge densities of ~650–1080 mC m^{-2}—nearly an order of magnitude higher than those typically reported for polymer-only triboelectric systems. These results demonstrate that careful compositional engineering—specifically, the integration of high-permittivity, charge-donating rare-earth-doped ferrites within a conductive 2D MXene framework—can dramatically amplify triboelectric charge generation. The proposed MXene–ferrite nanocomposite architecture offers a promising pathway toward high-output, durable, and scalable TENGs for self-powered sensing and energy-harvesting applications.
Keywords: TENG, MXene, Cobalt Ferrite, Rare-Earth doping, Triboelectric enhancement.

Solvothermally synthesized Yb^{3+}: Cu_2SnS_3 nanostructures for supercapacitor electrodes

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Ytterbium (Yb^{3+})-doped Cu_2SnS_3 (CTS) nanostructures were successfully synthesized via a solvothermal route to explore their potential as high-performance supercapacitor electrodes. Structural and morphological properties were investigated using X-ray diffraction (XRD) and scanning electron microscopy (SEM), while optical characteristics were examined through diffuse reflectance spectroscopy (DRS). XRD analysis confirmed the well-formed crystalline CTS host structure, with a slight shift of diffraction peaks toward lower angles upon Yb^{3+}

doping at different concentrations (x=0.01, 0.03), indicating the presence of tensile lattice strain. The crystallite size was observed to increase with increasing dopant concentration. SEM images revealed a flower-like morphology for pristine CTS, which gradually diminished upon Yb incorporation, suggesting dopant-induced microstructural modification. Electrochemical investigations using Impedance spectroscopy (EIS), cyclic voltammetry (CV), and Galvanostatic charge-discharge studies demonstrated a significant enhancement in charge storage performance with Yb doping, where the specific capacitance and coulombic efficiency increased as a function of dopant concentration. Notably, the 3% Yb-doped CTS electrode delivered a maximum specific capacitance of 216 F g^{-1} at 1 A g^{-1} current density along with good rate capability. Furthermore, the electrode exhibited excellent cycling stability, retaining approximately 80% of its initial capacitance after 1000 charge-discharge cycles.

Keywords: Solvothermal synthesis, Electrochemical energy storage, Pseudocapcitor.

Photovoltaic and electronic properties of WO_3 modified n-Ge heterostructure

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The Au/n-Ge heterostructure is fabricated with a nanostructured WO_3 thin layer utilizing the economical spin coating technique. Optical absorption, morphological properties of spin coated WO_3 thin films suggest strong absorption at 328 nm in the UV region and granular morphology with 25 to 40 nm particle size. The electrical characteristics of the Au/WO_3/n-Ge heterostructure demonstrate enhancements in forward current, reduced series resistance, and an increased rectification ratio relative to the Au/n-Ge Schottky contact. The barrier height and ideality factors of the Au/n-Ge Schottky contact were determined to be 0.63 eV and 1.51, whereas those for the Au/WO_3/n-Ge heterostructure were 0.59 eV and 1.1, respectively. The capacitance-voltage measurements conducted at 1 MHz illustrate the fluctuations in accumulation and depletion regions of the heterostructure, highlighting the impact of the WO_3 layer situated between the metal and semiconductor. A transition in the transport mechanism from ohmic to TCLC is observed in the Au/WO_3/n-Ge heterostructure that may be ascribed to the exponential distribution of traps or defects at the oxide-Ge interface. The observed fluctuation in the electrical characteristics of the heterostructure may be attributed to the mitigation of Fermi level pinning at the n-Ge surface and a decrease in the density of states at the oxide-Ge interface. The experimental result indicates that the WO_3 interlayer substantially affects the transport characteristics and improves the performance of the Au/WO_3/n-Ge heterostructure, demonstrating its potential in photovoltaic and optoelectronic applications. This investigation also evidences the photovoltaic properties of heterostructures under various illumination intensities from 20 to 100 mW/cm^2 in steps of 20 mW/cm^2. The obtained photovoltaic parameters such as open circuit voltage (V_{OC}), short circuit current (I_{SC}) and fill factor (FF) were compared for different illuminations intensities. It was observed that the V_{OC} was found to be decreased and I_{SC} found to be increased significantly with increased illumination intensity. Further, the variation of photovoltaic

parameters with illumination intensity could be addressed with respect to carrier extraction losses and larger shunt resistance governed at higher optical power.
Keywords: Spin Coating; Photovoltaic; Electronic; n-Ge heterostructure.

Spectroscopic and electrical properties of MoO_3 doped lead germanate glasses

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MoO_3-doped PbO–GeO_2 glasses were prepared by the melt-quenching technique and studied for their structural, optical, and dielectric properties. X-ray diffraction patterns exhibited broad diffuse halos, confirming the amorphous nature of the glasses. Optical absorption spectra indicated the presence of Mo^{6+} ions acting as network modifiers and promoting the formation of non-bridging oxygens in the glass network. A decrease in optical band gap with increasing MoO_3 content was observed, attributed to the partial reduction of Mo^{6+} to Mo^{5+} ions, leading to the creation of localized states. FTIR analysis confirmed the presence of GeO_4, GeO_6, Ge–O–Ge, and PbO_4 structural units, indicating significant modification of the GeO_2 network. Dielectric studies showed that the dielectric constant and loss increased with temperature and MoO_3 concentration, while decreasing with frequency. AC conductivity exhibited thermally activated behavior with low activation energy, suggesting a hopping conduction mechanism. The enhanced dielectric parameters at higher MoO_3 concentrations indicate the potential of these glasses for dielectric and electronic applications.
Keywords: Optical band gap; Dielectric properties; AC conductivity; Non-bridging oxygens.

Digital twin of lithium-Ion batteries using a 2-RC thevenin equivalent circuit model

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In the physics domain, a digital twin acts as a living mathematical mirror of a physical system, where governing laws replace static data fitting. Instead of treating systems as black boxes, physics-based digital twins evolve in time according to conservation laws, constitutive relationships, and dynamic state equations. This allows the virtual model to respond causally to changes in inputs, boundary conditions, and disturbances, much like its real counterpart.

Such twins enable “what-if” experimentation that would be unsafe, expensive, or physically impossible in reality. By continuously updating internal states, physics-driven digital twins transform simulations into predictive, adaptive entities that bridge theoretical physics and real-world operation. Battery performance evaluation under diverse operating conditions is both expensive and difficult to scale using conventional experimental testing methods. In addition, the internal electrochemical states of a lithium-ion batteries such as state of charge, polarization effects, and internal resistance dynamics, cannot be directly observed during real-time operation. Although high-fidelity electrochemical models can represent these internal behaviours with high accuracy, their substantial computational complexity makes them impractical for rapid simulations, real-time analysis and large-scale digital twin deployment. To address these challenges, this work proposes a physics-based digital twin of a lithium-ion battery developed using an Equivalent Circuit Model (ECM). The ECM is based on a 2-RC Thevenin model, which captures the essential battery behavior by modelling ohmic losses and both fast and slow polarization phenomena, which allows accurate representation of transient voltage response using electrical analogue components. Compared to other detailed electrochemical models, the proposed 2-RC ECM significantly reduces computational cost while retaining sufficient physical interpretability. The proposed digital twin is based on the fundamental physical principles governing lithium-ion battery behavior, rather than relying solely on data-driven modelling. The parameters of the Equivalent Circuit Model are derived from the relationships among voltage, current, and time, which are governed by basic electrical and electrochemical laws. The terminal voltage of the battery is expressed as a function of the open-circuit voltage and internal voltage drops caused by resistive and dynamic effects. Ohmic resistance accounts for instantaneous voltage losses due to electron and ion transport, while parallel resistor–capacitor (RC) networks represent charge transfer processes and diffusion-related polarization phenomena. The proposed digital twin enables continuous virtual experimentation, allowing battery behaviour to be analysed under multiple operating conditions without the need for repeated physical testing. It supports effective evaluation of voltage response, dynamic performance, and internal state evolution under different current profiles. By using a physics-informed ECM, the digital twin preserves interpretability while remaining computationally efficient. This approach supports scalable simulation for battery packs or cells, which can help for real-time applications such as battery management systems and control design. Additionally, the digital twin framework allows flexible parameter adaptation, fault analysis, and performance evaluation without repeated physical testing, thereby reducing development cost and improving system reliability and interpretability. This research will be extended by utilizing data-driven models and the integration of Cyber Physical Systems (CPS) by using real-time data in the future.

Keywords: Digital Twin; Lithium-Ion Batteries; Transient Voltage Response.

Thickness-tuned interference engineering for efficient SHG in subwavelength χ(2) films

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We introduce an ultra-minimal optical geometry for highly efficient second-harmonic generation (SHG), based on a single subwavelength-thick χ(2) film deposited on an optically thick substrate and driven at normal incidence. In contrast to conventional resonant cavity or nanostructured platforms, our approach exploits Interference Engineering to establish phase-matching-like conditions through a single geometric degree of freedom: the film thickness. By tuning this thickness to enforce constructive interference between the distributed nonlinear polarization and the radiating second-harmonic mode, the structure is tailored to maximize spatial and phase overlap across fundamental and harmonic fields. This mechanism elevates thickness from a passive geometric parameter to an active interference-control "knob''. To quantify the spatial and phase correlation between the driving source and the radiating mode, we introduce the Cauchy-Schwarz normalized Overlap Coefficient as a predictive figure of merit. This coefficient directly captures how effectively the nonlinear polarization profile projects onto the eigenmode $E_2\omega(z)$ responsible for out-coupling. Efficient SHG emerges only when these quantities oscillate in-phase across the depth of the film: regions where $E\omega^2(z)$ and $E_2\omega(z)$ align contributes constructively to the radiated harmonic field, while out-of-phase regions cancel and squander intrinsic nonlinearity. Thus, beyond conventional Fabry–Perot field enhancements, conversion efficiency is fundamentally governed by the mutual spatial correlation of the interacting modes within the nonlinear slab. Our framework provides a compact and fabrication-friendly pathway toward maximizing classical SHG efficiency using a single nonlinear layer, compatible with a wide array of materials and platforms. More broadly, controlling double resonance and spatial-mode overlap through the precise tuning of the film thickness is naturally suited to emerging nanophotonic and quantum-photonic applications.
Keywords: Second harmonic generation; Phase matching; Fabry–Pérot cavities; Thin films.

Noble metal modified TiO_2 nanostructures with improved Visible-light photoactivity

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Enhancing the visible-light photoactivity of titania-based photocatalysts via noble metal modification is of significant interest for environmental remediation. This study investigates the effect of silver (Ag) and palladium (Pd) incorporation into nanosized TiO_2 matrices on photocatalytic performance. Ag- and Pd-modified TiO_2 ($MTiO_2$) nanocomposites with nanoparticle and nanotube morphologies were synthesized using facile in-situ and ex-situ methods. Structural and phase analyses using X-ray diffraction (XRD) and Raman spectroscopy confirmed the formation of phase-pure anatase TiO_2. Distinct Pd reflections were observed at higher Pd loadings (>3%), while the absence of Ag-related peaks suggests homogeneous dispersion of silver within the TiO_2 matrix. Raman spectra revealed enhanced TiO_2 vibrational

modes, indicating surface-enhanced Raman scattering (SERS) effects due to noble metal incorporation. Transmission electron microscopy (TEM) confirmed uniform Ag distribution, except for localized Ag-rich regions in $AgTiO_2$ nanotubes, whereas Pd nanoparticles were clearly present in all Pd-containing samples. Optical and electronic properties were probed using UV–visible diffuse reflectance spectroscopy (UV-DRS) and X-ray photoelectron spectroscopy (XPS). UV-DRS showed a red shift in absorption onset upon metal modification. $AgTiO_2$ exhibited a characteristic surface plasmon resonance band at ~420–426 nm, while $PdTiO_2$ displayed a featureless absorption in the 300–500 nm regions. XPS confirmed Ag predominantly in the metallic state (Ag^0), whereas Pd existed in both metallic and ionic (Pd^{2+}) states. Photocatalytic performance was evaluated via visible-light-driven degradation of the wastewater pollutant 2-mercaptobenzothiazole (2-MBT) under artificial solar irradiation ($\lambda >$ 400 nm). Reaction kinetics was monitored by UV–visible spectroscopy. Complete photodegradation of the pollutant was confirmed with High-Performance Liquid Chromatography (HPLC) study. The $MTiO_2$ photocatalysts showed markedly enhanced activity compared to undoped TiO_2 and commercial Degussa P25, with $AgTiO_2$ outperforming $PdTiO_2$. Theoretical calculations for Ag- and Pd-modified TiO_2 photocatalysts are conducted using density functional theory (DFT) to investigate the influence of metal modifications on the electronic, optical, and structural properties, thereby elucidating the underlying rationale for enhanced photocatalytic activity. The noble metal–modified TiO_2 nanostructures were further investigated for their potential application in photocatalytic water splitting. The improved performance is attributed to surface plasmon sensitization and enhanced charge separation, highlighting Ag-modified TiO_2 as an efficient photocatalyst for visible light.

Keywords: TiO_2, Nanotubes, Visible light, Photocatalysis, Silver, Palladium.

Crystal structure, magnetic properties, and magnetoelectricity in $CoFe_2O_4/Cr_2O_3$ nanocomposite

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Attaining room temperature and above magnetoelectricity (ME) is a prerequisite for the ME-based device applications. On this account, the present work focuses on the usability of Cr_2O_3 (CRO) above the room temperature, in association with $CoFe_2O_4$ (CFO), by drawing a comprehensive picture of their crystal structure, magnetic, electrical, and ME properties. The CFO/CRO nanocomposite is synthesized by the sol-gel auto-combustion route, following a two-step process. A careful study of Rietveld refined X-ray diffraction patterns, complemented by Raman spectroscopy, authenticates the presence of both CFO and CRO phases. The field

emission scanning electron micrograph (FESEM) illustrates a uniform distribution of particles with an average size of ~128 nm. The thermal dependence of saturation magnetization is well described by Bloch law. The impedance-based Havriliak-Negami model effectively captures the frequency-dependent impedance behavior, confirming the presence of a single non-Debye-like relaxation. The resistivity data suggests the semiconducting-like nature of the sample and found to obey the Mott-variable range hopping mechanism. Interestingly, the ME measurements display a substantial increase in the ME operating temperature as high as 360 K for the sample. These findings may pave a novel path towards magnetically control of voltage for ME devices.

Keywords: Nanocomposites; Sol-Gel; Magnetic; Magnetoelectric.

Gas sensing functionalities of Li-Gd co-substituted ($K_{0.5}$, $Na_{0.5}$) NbO_3 ceramics derived from molten salt synthesis

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The work provides a detailed analysis of the gas-sensing properties of lithium- and gadolinium-co-substituted sodium potassium niobate ($K_{0.5}$, $Na_{0.5}$) NbO_3 ceramics prepared by the molten salt method, a high-performance and scalable process for producing high-performance piezoceramics. The X-ray diffraction with Rietveld refinement was used to determine the crystallographic phase formation and structural changes. The crystallite size was calculated using both Scherrer and Williamson-Hall analysis, which enabled the determination of lattice parameters and micro strain. Scanning electron microscopy was used to analyze the surface morphology and particle size distribution, whereas Fourier-transform infrared spectroscopy was used to determine the characteristic chemical bonding. The optical studies were determined from UV–visible spectroscopy. Understanding of the charge transport behaviour was done through electrical characterization, which involved dielectric response, impedance spectroscopy, and analysis of the activation energy. Moreover, the sensitivity, selectivity, and dynamic responsiveness of the gas-sensing properties of the synthesized ceramic were investigated systematically for a wide range of target gases. Polarization-electric field (P-E) hysteresis data also supported the fact that it is a ferroelectric material with multifunctional applications in sensing and electro-functional devices.

Keywords: Lead-free ceramics, Molten-salt synthesis, Optical bandgap, Gas sensing.

Ni^{2+} substituted Co ferrites with enhanced electrical resistivity and magnetic properties for high-frequency applications

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To examine the impact of Ni^{2+} substitution on structural, dc electrical resistivity, and magnetic characteristics, Ni-substituted cobalt ferrites of composition $Co_{2-x}Ni_xFe_2O_4$ (x = 0.0–0.5) were created using the traditional solid-state reaction method. For every composition, X-ray diffraction verified that a single-phase cubic spinel structure was formed. As the Ni content increased, the crystallite size shrank from 66 nm to 44 nm and the lattice parameter slightly reduced from 8.385 Å (x = 0.0) to 8.359 Å (x = 0.5). Grain size was systematically reduced from 5 µm to 2 µm, according to SEM analysis. Tetrahedral and octahedral metal-oxygen vibration bands with a steady shift toward lower wavenumbers were visible in the FTIR spectra. All samples showed semiconducting behavior according to DC electrical resistivity studies; when Ni content rose, resistivity increased and activation energy increased from 0.32 eV to 0.47 eV, which is compatible with a tiny polaron hopping conduction mechanism. According to magnetic studies, coercivity increased from 188.25 Oe to 356.14 Oe while saturation magnetization decreased from 80.23 emu/g to 51.22 emu/g. The findings show that Ni substitution successfully adjusts $CoFe_2O_4$ ferrites' electrical and magnetic characteristics, making them appropriate for high-frequency and high-coercivity magnetic applications.

Keywords: Ferrites; Spinel ferrite; DC electrical resistivity; Magnetic properties.

Conductance fluctuations in organo-metallic CuTCNQ single nanowire (diameter ~10 nm)

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Understanding electrical noise and conductance fluctuations in nanoscale systems is central to both fundamental mesoscopic physics and the reliable operation of nano-electronic devices. When the characteristic dimensions of a conductor approach the electronic Fermi wavelength, charge transport is no longer self-averaging and becomes dominated by quantum interference and microscopic disorder. In this work, we investigate such quantum transport phenomena in an individual organometallic charge-transfer nanowire based on Cu: TCNQ (TCNQ-7, 7, 8, 8-tetracyanoquinodimethane), with a diameter of ~10 nm, comparable to the electron Fermi wavelength (λ_F). The nanowire was deterministically fabricated by physical vapor deposition, directly bridging predefined electrodes, enabling the study of the intrinsic transport properties of a single quasi-one-dimensional nanoobject. Low-frequency voltage-noise measurements were performed in the electrically switched low-resistance state over a range of temperatures (100 – 300K). The nanowire exhibits pronounced time-dependent conductance fluctuations with a characteristic $(1/f)$ noise spectrum. Notably, the normalized noise spectral density remains nearly temperature independent, despite the dc conductance being essentially constant in this state. This behavior rules out conventional thermal or phonon-mediated noise mechanisms and points to a mesoscopic origin of the fluctuations. The results are consistent with universal conductance fluctuation–like noise arising from dynamic scattering centers, fluctuating localized states, or time-dependent quantum interference effects. Our findings establish low-frequency noise spectroscopy as a sensitive

probe of quantum transport in molecular-scale nanostructures, highlighting the intrinsic limits to transport stability in nanoscale charge-transfer systems.
Keywords: Nanowires; Electrical noise; Conductance fluctuations; Transport stability.

Structural and optical properties of vanadium oxide–CNT nanocomposites

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Vanadium Oxide is a promising thermochromic material, but its practical application is limited by modest electrical conductivity and microstructural instability. In this work, Vanadium-Oxide integrated carbon nanotube (CNT) composites at different mass ratios were synthesized via a simple solution-based route. For the obtained composites structural, chemical and morphological characteristics were systematically examined by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), and energy-dispersive X-ray analysis (EDAX). XRD analysis confirms the integration of CNT by not disrupting the host lattice positions. FTIR spectra exhibited characteristics V=O and V–O–V vibrations in the 500–1000 cm^{-1} range, along with additional bands associated with C=C vibrations in the composites, verifying successful integration of CNTs and interfacial interaction between oxide and carbon phases. Morphological analysis using FESEM revealed that tubular structures corresponding to the carbon nanotubes are embedded within the Vanadium-Oxide matrix, giving the impression that CNTs are integrated with, and locally wrapped by, the oxide phase. The integration was more pronounced with higher CNT concentration, resulting in the development of a more continuous and interconnected network. The elemental composition and purity of the composites were validated by EDAX, which confirmed the presence of Vanadium, Oxygen, and Carbon elements with no detectable impurities. Optical bandgap analysis via Tauc's plots showed a systematic reduction to lower values with increasing CNT concentration. These results demonstrate that the simple solution method yields Vanadium-Oxide integrated CNT composites with improved microstructural connectivity, providing a promising platform for tunable thermochromic applications.
Keywords: Vanadium Oxide, Carbon Nanotubes (CNTs), Nanocomposite, Optical Bandgap.

OSL characteristics and trap dynamics in Mn-activated $SrAl_2O_4$ phosphors

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Aluminates have emerged as leading candidates because they exhibit superior and persistent luminescent properties. $SrAl_2O_4$-based materials, among aluminate systems, demonstrate

notably high efficiency and structural stability. The present work explores the impact of Mn doping in $SrAl_2O_4$ on its structural features as well as its optically stimulated luminescence (OSL) and thermoluminescence (TL) responses. $Sr_{(1-x)}Mn_xAl_2O_4$ (x = 0, 0.1, 0.3, 0.5, 1, 2 and 3 wt %) were synthesized using the solution combustion method. The samples underwent annealing at 1200 °C for two hours in a muffle furnace before all characterization measurements. The formation of the material in a single-phase monoclinic structure with space group P_{21} was confirmed by X-ray diffraction analysis (XRD). No additional XRD peak was detected in the measured limit and confirmed by the energy dispersive spectroscopy (EDS) technique. The SEM images reveal that the particles possess irregular morphology and nanoscale dimensions. The samples were irradiated with $^{90}Sr/^{90}Y$ beta particles at various doses under room-temperature conditions. OSL measurements were carried out under blue light (470 nm) stimulation. High TL and OSL response were observed for 1 wt% of Mn-doped $SrAl_2O_4$. The TL glow curve exhibits a broad peak spanning 30–250 °C, which is composed of four individual components, as determined through general-order kinetic analysis using Computerized Glow Curve Deconvolution (CGCD). Both TL and OSL responses increase with the dose. Preheating the sample before OSL measurements and residual TL response suggests the existence of multiple trapping levels with different trapping/detrapping probabilities for the OSL emissions. CW-OSL decays were best fitted with three components. The work provides a detailed understanding of the multiple traps in 1 wt% Mn-doped $SrAl_2O_4$.

Keywords: $SrAl_2O_4$: Mn, Beta particles, Optically stimulated luminescence, Kinetic parameters.

Chemical synthesis route-driven structural transformation and luminescent behavior of Eu^{3+}-activated $Zn_4B_6O_{13}$ phosphors

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The choice of synthesis methods significantly influences the luminescence properties of nanomaterials intended for use in solid-state lighting device applications. In our study, zinc borate nanophosphors doped with 1 mol% europium ($Zn_4B_6O_{13}$: Eu^{3+}) were synthesized using a variety of methods such as the sol-gel, combustion, and solid-state reaction methods. The impact of these methods on the structural and photoluminescence properties of the material is thoroughly investigated. The prepared zinc-borate nanophosphors were successfully annealed at 800°C to produce nanocrystalline materials. XRD results confirmed the formation of cubic crystalline structures for all samples. All the synthesized $Zn_4B_6O_{13}$: Eu^{3+} phosphor materials showed a 95 % matching score with the JCPDS file (No. 01-076-0917) of the host material. The calculated crystallite sizes are very small relative to those reported in the literature. Various morphologies were observed through scanning electron microscopy (SEM):

polyhedron-like, hexagonal-like, and irregular morphologies for the sol-gel, the combustion, and the solid-state reaction methods, respectively. Upon excitation at 248 nm, the photoluminescence emissions followed hierarchy trends of: sol-gel > solid state > combustion reaction methods. The highest emission peak was assigned to the europium electric dipole transition, namely Eu^{3+}:$^5D_0 \rightarrow {}^7F_2$ emission peak at 615 nm. The CIE chromaticity diagram revealed a reddish colour emission for all the synthesized phosphor materials. The $Zn_4B_6O_{13}$:Eu^{3+}phosphor materials synthesized through the sol-gel technique could be potential candidates for red light-emitting diode (LED) applications.

Keywords: $Zn_4B_6O_{13}$:Eu^{3+}, photoluminescence, synthesis technique and LED applications.

Comparative analysis and ergonomic evaluation of illumination intensity in open cast mines haul roads as per directorate general of mine safety statutory guidelines

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Mechanization and technological innovation in mining operation have led today and night production which requires effective illumination for ensuring safety, improved visibility, visual acuity and reduced visual fatigue for miners working in mine environment. Directorate General of Mine Safety (DGMS) Circular 3, 2017, statutory guidelines were followed for assessment of haul road illumination in Mines. The luminaire used in Mine 1 white LED 70 watts, Mine II Sodium vapour 250 watts and Mine III Sodium vapour SVL 200 watts. The pole heights were 9m, 7m and 9m respectively with light bracket angle 110^0 in Mine I, II and III. In Mine I, pit haul road and main haul road horizontal illumination intensity in Lux was (N=21) 7.99±6.51 range 0.44–22.41; (N=6), 3.81±2.7, range 1.03-8.65, vertical left 5.26±2.66, range 1.5-10.8; 79±0.71, range 1.01-2.6, vertical right 6.10±7.38, range 0.17-27.69; 1.87±1.48, range 0.72-4.68 respectively. In Mine II the horizontal illumination intensity (N=21), 3.30±2.12, range 0.51-7.6, vertical left 4.50±4.02, range 1.18-14.85, vertical right 6.19±8.50, range 0.51-28.45. In Mine III the horizontal illumination intensity (N=10), 13.40±14.88, range 1.4-43.7, vertical left 6.43±4.79, range 1.15-15.71, vertical right 6.66±5.95, range 1.14-17.16. The mean horizontal illumination criterion intensity of 10 Lux as per DGMS Circular 3, 2017 is not fulfilled in Mine I, II haul road. However, Mine III haul road horizontal illumination intensity criterion was fulfilled as per DGMS Circular 3, 2017. Further the illumination intensity was not uniform in all the surveyed haul roads of Mine I, II and III. In some areas of haul road, the illumination was too high whereas in some parts it was inadequate.

Keywords: Illumination, Lux, Haul Road, DGMS.

Facile construction of carbon nanotubes anchored ZnS/Ag_2S nanocomposites for efficient photocatalytic hydrogen evolution

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The study shows a simple and cost-effective synthesis method for CNTs-anchored ZnS/Ag_2S nanocomposites for photocatalytic hydrogen evolution under sunlight irradiation. Results show that the integration of CNTs, ZnS and Ag_2S in a single nanocomposite structure is the one of the most promising materials for efficient photocatalysis for hydrogen production through water splitting (515 µmol/g/h). We found that CNTs anchored the well-defined microsphere-like structure of the nanocomposites, acting as a support matrix for the ZnS and Ag_2S nanoparticles, which are the active sites in photocatalysis. Based on the FESEM, XRD, XPS, UV-DRS, and PL spectra, the experimental results demonstrate that the combination of ZnS/Ag_2S/CNTs greatly increased absorption and extended it into the visible light region and also reducing recombination rate of photo charge carriers. Under solar radiation, robust stability has been achieved in the production of photocatalytic hydrogen evolution.
Keywords: Photocatalyst; Hydrogen Fuel; Nanocomposites; Solar Energy Conversion.

Remote sensing of total column ozone and tropospheric NO_2 and model observations over semi-arid region in southern India

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Since there are few ground-based continuous measurements of total ozone (O_3) and NO_2, satellite data is being used in modelling to estimate source characteristics and urban pollution. Tropospheric NO_2 from SCIAMACHY and the Total Ozone Mapping Spectrometer (TOMS) algorithm (version 8.5) are used to derive total column ozone from OMI. Results of the monthly variation of tropospheric NO_2 and total column ozone over a rural site (Anantapur) have been reported. Additionally, the NCAR-MM Chemical Box Model and Radiative Transfer Model were used to study the impact of Total column ozone effect on J (O_3). The sensitivity of photolysis rate of ozone and ozone variations to changes in total column ozone and aerosols loading was investigated in this study using a model simulation.
Keywords: Total column ozone, Topospheric NO_2, Chemical box & Radiative transfer model.

Laser shock peening of various metal alloys and its effect on microstructure and mechanical properties

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Laser Shock Peening (LSP) has revolutionized the structural integrity of high-performance metal alloys by utilizing high-intensity laser pulses (GW/cm^2) to induce deep-seated compressive residual stresses. Unlike traditional mechanical methods, LSP employs plasma-driven shock waves to generate a "compressive skin" that extends significantly deeper into the substrate - often exceeding 1 mm in depth. This work explores the fundamental physics of laser-matter interaction and the resulting microstructural evolution, including dislocation cell formation and grain refinement. These changes yield superior mechanical enhancements: specifically, a dramatic increase in fatigue life, resistance to stress corrosion cracking (SCC), and improved surface hardness. By analyzing the relationship between shock wave parameters and material response, we highlight LSP as a critical technology for life-extension in aerospace, automotive, and medical sectors. The work concludes with a comparative analysis of LSP versus conventional shot peening, emphasizing its role in the future of precision manufacturing.
Keywords: Laser Shock Peening; Compressive Stress; Hardness; Microstructure; Fatigue life.

Structural and electrochemical investigation of chromium doped $La_{0.5}Ca_{0.5}Cr_xFe_{1-x}O_3$ perovskite oxide for supercapacitor applications

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B site doping in perovskite oxides improves the supercapacitor ability by generating more oxygen vacancies, modulating redox-active states, and enhancing ionic and electronic conductivity, whereas A site doping further promotes B site cations to increase their oxidation states and facilitating rapid charge storage kinetics. Based on this dual doping strategy, a series of chromium-substituted Perovskite oxides with the composition of $La_{0.5}Ca_{0.5}Cr_xFe_{1-x}O_3$ (x = 0, 0.2, 0.4, 0.6, 0.8) were synthesized using a facile solution combustion method and investigated for supercapacitor applications. The morphology, crystalline structure, and electrochemical performance of the synthesized samples were thoroughly studied. Structural analysis confirmed the formation of a single-phase perovskite structure with successful incorporation of Cr ions at the B site. The mutual effect of Cr substitution at the B site and Ca substitution at the A site effectively modulated oxygen vacancy concentration and redox activity, leading to enhanced charge transport exhibiting pseudocapacitive behaviour. These results demonstrate

that aliovalent doping in perovskite oxides is a viable strategy for developing high-performance electrode materials for supercapacitor applications.
Keywords: Perovskites, Supercapacitors, Hybrid energy storage devices, Electrochemical.

Design, synthesis and electrochemical evaluation of nickel cerium oxide nanocomposites for nitrite detection

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Nickel–cerium oxide (Ni–Ce–O) nanocomposites have attracted significant attention for electrochemical sensing applications due to their excellent redox activity, high oxygen storage capacity, and enhanced electrical conductivity. In this work, Ni–Ce–O was synthesized through a simple and cost-effective approach to obtain a homogeneous mixed metal oxide with improved structural and electrochemical characteristics suitable for nitrite detection. The strong synergistic interaction between Ni and Ce ions facilitates rapid electron transfer, generates abundant oxygen vacancies, and provides a large number of electroactive sites, thereby enhancing the electrocatalytic oxidation of nitrite. Structural and morphological analyses confirm the successful formation of a crystalline Ni–Ce–O nanocomposite with uniform particle distribution. The reversible Ce^{3+}/Ce^{4+} redox couple, together with the catalytic activity of nickel species, significantly improves charge-transfer kinetics and promotes efficient nitrite oxidation at the electrode surface. Under optimized experimental conditions, the Ni–Ce–O-modified electrode exhibits a high sensitivity of **1.24 µA µM^{-1} cm^{-2}**, a low limit of detection (LOD) of **0.346 µM**, and a wide linear concentration range from **1 to 150 µM** for nitrite determination. In addition, the effects of scan rate, analyte concentration, pH variation, reproducibility, repeatability, and long-term stability were systematically investigated, confirming the reliable electrochemical behavior and robustness of the developed sensor. The enhanced surface activity, conductivity, and durability of the Ni–Ce–O material make it a promising electrode platform for sensitive and selective electrochemical detection of nitrite in environmental and food-related samples.
Keywords: Ni–Ce–O nanocomposites; Electrochemical; Differential pulse voltammetry.

Morphological and optical properties of cobalt doped barium hexaferrites

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Magnetic ferrites possess the remarkable ability to absorb microwave radiation with excellent efficiency, making them a beautiful material for green chemistry applications, where the selective heating of reaction mixtures can lead to reduced energy consumption and shorter reaction times. In this paper, a series of cobalt-doped Barium hexaferrites has been synthesized through a low-temperature hydrothermal method. Their morphological properties were successfully captured using Field Emission Scanning Electron Microscopy (FESEM), and elemental analysis via energy-dispersive spectroscopy revealed that no impurities were present during synthesis. In contrast, their optical properties have been studied using UV-visible spectroscopy. Morphology studies have demonstrated that the synthesized particles are characterized by a grain size of 60-70 nm with minimal agglomeration. The Tauc's plot analysis was used to calculate the energy band gap of synthesized nanoparticles. The results showed semiconducting nature with energy values of 4.95, 4.97, 4.98, and 5.02 eV
Keywords: Magnetic materials; Ferrites; FESEM; EDX; UV-visible spectroscopy.

Structure, morphology and negative dielectric behavior of (1-x) ($Al_{0.2}La_{0.8}TiO_3$) +(x) ($BiFeO_3$ /$BiZnFeO_3$) (x = 0.2 - 0.8) nanocomposites

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The (1-x) ($Al_{0.2}La_{0.8}TiO_3$) + (x) ($BiFeO_3$) (x = 0.2 - 0.8)/ALTBF and (1-x) ($Al_{0.2}La_{0.8}TiO_3$) + (x) ($BiZnFeO_3$) (x = 0.2-0.8)/ALTBZFO nanocomposites are synthesized by hydrothermal method. The present work elucidates structural, morphological, and dielectric properties of (1-x) ($Al_{0.2}La_{0.8}TiO_3$) + (x) ($BiFeO_3$) (x = 0.2, 0.4, 0.6 & 0.8)/ALTBF and (1-x) ($Al_{0.2}La_{0.8}TiO_3$) + (x) ($BiZnFeO_3$) (x = 0.2, 0.4, 0.6 & 0.8)/ALTBZFO nanocomposites. The diffraction pattern confirms the structural transformation from tetragonal to cubic. In particular, the dielectric properties such as dielectric constant (ε'), dielectric loss (ε'), ac-electrical conductivities (σ_{ac}) as a function of frequency are discussed. The impedance analysis is carried out to reveal the electrical conduction behavior. The negative dielectric behavior is observed at higher frequencies for the present nanocomposites.
Keywords: Nanocomposites; Structure; Morphology; Negative Dielectric Constant.

Structure and dielectric behavior of (1-X) ($Al_{0.2}La_{0.8}TiO_{3+\delta}$) +(X) ($BaTiO_3$ /$CuTiO_3$) (X = 0.2 - 0.8) nanocomposites

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The (1-x) ($Al_{0.2}La_{0.8}TiO_{3+\delta}$) + (x) ($BaTiO_3$) (x = 0.2, 0.4, 0.6 & 0.8)/ALTBT and (1-x) ($Al_{0.2}La_{0.8}TiO_{3+\delta}$) + (x) ($CuTiO_3$) (x = 0.2, 0.4, 0.6 & 0.8)/ALTCT nanocomposites are synthesized by hydrothermal method. The present work elucidates structural, morphological, optical bandgap, photocatalytic activity and dielectric properties of ALTBT and ALTCT nanocomposites. The diffraction pattern confirms the structural transformation from tetragonal to cubic. In particular, the dielectric properties such as dielectric constant (ε'), dielectric loss (ε"), ac-electrical conductivities (σ_{ac}) as a function of frequency are discussed. The impedance analysis is carried out to reveal the electrical conduction behavior.
Keywords: Nanocomposites; Photocatalytic; Optical Bandgap; Dielectric Constant.

Structural, optical, and electrical properties of Er–M co-doped ceria electrolytes

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Defect engineering in ceria-based oxides plays a crucial role in governing charge transport, dielectric response, and optical properties of functional ceramic materials. In this work, a series of Er–M co-doped ceria compositions, Er–M co-doped ceria (M = Sr, Ca, Mg, Na), were synthesized using a modified sol–gel process and systematically investigated for their structural, optical, and electrical properties with relevance to solid oxide fuel cell (SOFC) electrolyte applications. The incorporation of aliovalent dopants enables controlled tuning of oxygen vacancy concentration, lattice distortion, and grain boundary characteristics. Thermal decomposition behavior and phase formation were examined using TG/DTA, confirming the formation of thermally stable oxide phases. FTIR analysis verified the elimination of organic residues and the establishment of metal–oxygen bonding networks. X-ray diffraction revealed that all compositions stabilized a single-phase fluorite structure, with subtle variations in lattice parameters reflecting dopant size and charge effects. Microstructural features were

analyzed using scanning electron microscopy, while EDX and elemental color mapping confirmed homogeneous distribution of constituent elements, indicating successful dopant incorporation. Optical properties were investigated using UV–Vis spectroscopy. The absorption spectra indicate dopant-induced modifications in the optical response, with variations in the estimated optical band gap attributed to defect states and oxygen vacancy concentration introduced by Er–M co-doping. These results highlight the influence of lattice disorder and defect chemistry on the electronic structure of ceria. Electrical properties were evaluated using impedance spectroscopy over a wide temperature and frequency range. The impedance response was interpreted using an equivalent grain–grain boundary model, enabling separation of bulk and grain-boundary contributions. Porosity corrections were applied through the grain boundary model to obtain intrinsic transport parameters. Among the investigated compositions, Ca- and Sr-doped samples exhibit significantly enhanced electrical conductivity and the lowest activation energies compared to Mg- and Na-doped counterparts. This improvement is attributed to reduced dopant–vacancy association and improved grain boundary transport facilitated by favorable ionic size and valence characteristics. The present study demonstrates that Er–M co-doped ceria offers a versatile platform for tailoring the optical response and charge-transport behavior through controlled defect engineering, providing insights into structure–property relationships in advanced oxide electrolytes.

Keywords: Er-doped ceria; Impedance spectroscopy; SOFC electrolytes.

Sol–Gel synthesized polyvinyl alcohol–tantalum oxide/hydroxyapatite films for biocompatible and antimicrobial wound healing applications

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Composite films of Tantalum Oxide-Polyvinyl Alcohol-Hydroxyapatite (Ta-PVA-HAP) were prepared via a Sol-Gel method, incorporating low (LC) and high (HC) concentrations of Ta2O5 into HAP-PVA matrices. The films exhibited uniform morphology, tunable porosity, and enhanced mechanical stability which can be further explored in bio medical applications like wound healing, bone osteogenesis and osteo related cosmetic surgeries. Thickness measurements averaged 85 ± 5 µm for LC and 95 ± 7 µm for HC films. Porosity analysis revealed 42 ± 3% for LC and 48 ± 4% for HC films, while water uptake tests demonstrated swelling degrees of 120 ± 8% and 135 ± 10% for LC and HC films, respectively, highlighting improved moisture retention. X-ray powder diffraction confirmed the crystalline nature of HAP and successful incorporation of Ta2O5 without the formation of undesired phases. Electrochemical studies revealed lower corrosion current density and higher charge transfer resistance in Ta-containing films compared with placebo P-PVA films, demonstrating superior corrosion resistance. SEM analysis showed an even distribution of HAP and Ta2O5 particles within the polymer matrix. Biologically, both LC and HC films exhibited significant antibacterial activity against Escherichia coli, Staphylococcus aureus, Klebsiella pneumoniae, and Enterococcus faecalis, as well as antifungal activity against Candida albicans and Aspergillus niger. Cytotoxicity assays using MG-63 osteoblast-like cells showed over 85% viability at

concentrations up to 250 µg/mL, with minimal cell death of apoptosis or necrosis. In conclusion, Ta-PVA-HAP films demonstrated improved structural integrity, corrosion resistance, and cell compatibility, supporting their potential as multifunctional coatings for orthopedic and dental applications.

Keywords: Tantalum oxide, Sol-gel synthesis, Corrosion resistance, Anti-microbial activity.

Metal-free carbon nitride hollow spheres as artificial photosynthetic scaffolds for efficient NADH oxidation

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Natural enzymes are highly efficient and selective catalysts with broad biological and industrial relevance. Among them, oxidoreductases play a key role in redox reactions that rely on cofactors such as NAD^+/NADH. However, their large-scale application is limited by the high cost of enzymes and cofactors, necessitating the development of efficient strategies for cofactor regeneration. While enzymatic regeneration is effective, it often involves complex multicomponent systems. In contrast, heterogeneous catalysis offers a simpler and cost-effective alternative for NADH oxidation due to its high activity and relatively low cost. Here, we demonstrate a sustainable strategy for the oxidation of NADH via metal-free, photon-assisted heterogeneous catalysis. For this purpose, nitrogen- and phosphorus-rich polymeric carbon nitride nanosheets (NPCN/PPCN) were utilized as the visible light photocatalysts. A polyamine-mediated assembly route was employed to synthesize P/N-rich carbon nitride, resulting in CN-based hollow spheres (HS) using $CaCO_3$ microspheres as sacrificial templates. The NPCN/PPCN-HS catalysts were explored for photocatalytic oxidation of NADH under visible-light irradiation. Spectroscopic analyses, including UV-vis, steady-state fluorescence, and 3D fluorescence, highlighted the superior catalytic activity of the NPCN/PPCN-HS catalyst compared to the PCN catalyst. The ^1H NMR spectrum revealed no side or degradation products, demonstrating the catalyst's efficiency in NADH oxidation. This adaptable assembly strategy enables the fabrication of photocatalytic systems applicable to environmental remediation, enzymatic reactions, and artificial photosynthesis. This work presents a versatile assembly strategy for designing metal-free carbon nitride architectures that bridge artificial photosynthesis and biocatalysis. The developed photocatalytic system offers a promising platform for sustainable cofactor regeneration and holds broad potential for applications in enzymatic transformations, environmental remediation, and solar-to-chemical energy conversion.

Keywords: Carbon nitride, Photocatalysis, Cofactor, Metal-free, Layer-by-layer assembly.

Enhanced electrochemical performance of transition metal oxide composite for high energy supercapacitors

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Transition metal oxide based pseudocapacitive materials have attracted intense interest for next-generation high-energy supercapacitors, yet their practical deployment is often limited by poor electrical conductivity, inactive ion transport and structural degradation upon long-term cycling. Developing high-performance supercapacitors requires electrode materials that balance high energy and power densities. This work examines a transition metal oxide composite prepared through hydrothermal synthesis and annealed at 180°C, 320°C, 400°C, and 450°C to optimize electrochemical properties for advanced energy storage. Galvanostatic charge-discharge tests at 1 A/g delivered specific capacitances of 403.1 F/g, with energy densities of 13.9 Wh/g, respectively and a power density of 250 W/kg. The 450°C annealed sample showed the highest values, attributed to improved nanostructure that enhances charge transfer and electrolyte accessibility. These outcomes demonstrate the value of controlled annealing in hydrothermal processing for creating efficient supercapacitor electrodes, providing a pathway to superior performance in practical energy devices.
Keywords: Transition metal oxide; pseudocapacitive; specific capacitance; current densities.

Phytochemical-assisted synthesis of maghemite (γ-Fe_2O_3) nanoparticles using sphagneticola trilobata leaves: Structural and morphological analysis

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In the present study, we report the green synthesis of γ-Fe_2O_3 (maghemite) nanoparticles using the aqueous leaf extract of Sphagneticola trilobata as a natural reducing and stabilizing agent. The phytochemicals present in the plant extract facilitate the eco-friendly and cost-effective synthesis of iron oxide nanoparticles under ambient conditions, eliminating the need for toxic chemicals and harsh processing methods. The synthesized nanoparticles were characterized using a suite of analytical techniques. UV–Visible spectroscopy confirmed the optical absorption with a prominent peak around 372 nm, and the band gap energy was calculated to be approximately 2.75 eV. FTIR analysis revealed the presence of Fe–O stretching vibrations and various functional groups derived from the plant biomolecules, confirming successful capping. X-ray diffraction (XRD) patterns exhibited sharp peaks corresponding to the (220), (311), (400), (422), (511), and (440) planes, indicative of a cubic spinel structure, consistent with the standard JCPDS card for γ-Fe_2O_3. Scanning Electron Microscopy (SEM) images showed nearly spherical nanoparticles with an average particle size in the nanometer range. Energy Dispersive X-ray Spectroscopy (EDS) further confirmed the elemental composition with predominant peaks of Fe and O. These findings demonstrate that Sphagneticola trilobata leaf extract offers a green, sustainable route for synthesizing γ-Fe_2O_3

nanoparticles, which hold promise for applications in catalysis, environmental remediation, and biomedical fields.

Keywords: Green Synthesis, γ-Fe_2O_3 nanoparticles, Sphagneticola trilobata.

Optical and dielectric behavior of $Al_xNi_{1-x}TiO_{3+\delta}$ (x=0.2-0.8) nanoparticles

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The $Al_xNi_{1-x}TiO_{3+\delta}$ (x=0.2, 0.4, 0.6 & 0.8) (ANT) nanoparticles are synthesized via hydrothermal method. The X-ray diffraction patterns reveal the tetragonal structure having few secondary phase structures. The crystallite size 'D' value is varying unsystematically between 51.14±0.914 to 66.32±0.384 nm as a function of Al-content. The W-H plots are drawn to find the internal microstrain. The microstructure shows the clustered nature of ANT revealing the existence of interactions among the nanoparticles. The optical bandgap (E_g) values are determined using Tauc's plots and decreasing with an increase of Al-content. The high dielectric constant, and loss values are noted for x=0.2, and for x=0.4-0.6, a little less magnitude (as compared to x=0.2) is noted. These lossy materials may be suggested for the microwave dielectric absorber applications in the fields of electronics and energy. The electrical conduction mechanism is illustrated by means of dielectric modulus, ac-electrical conductivity and impedance analysis. The impedance analysis provides the low grain (R_g~29410.7 Ω) and the high grain boundary (R_{gb}~47065.8 Ω) resistance values for x=0.4. The bulk conductivity values (for x=0.4) are noted to be $5.411x10^{-6}$ S/cm & $3.381x10^{-6}$ S/cm as the contributions of grain and grain boundaries, respectively.

Keywords: Hydrothermal; Nanoparticles; Perovskites; Microstructure; Dielectric.

Extracting hydration signatures in cryoprotectant solutions using MCR-ALS spectral decomposition

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Hydration signatures in aqueous cryoprotectant (CP) solutions are essential for understanding ice-suppression mechanisms, yet they are often weak and strongly overlapped in infrared (IR) spectra, making conventional peak fitting unreliable. Here, we establish multivariate curve resolution with alternating least squares (MCR-ALS) as a robust, model-free approach to extract subtle hydration information from FTIR-ATR spectra of aqueous ethylene glycol (EG) mixtures across the full composition range. PCA is first used to determine the minimum number of statistically significant spectral factors, and the spectra are subsequently decomposed using MCR-ALS into chemically interpretable components corresponding to bulk-like water, bulk-like EG, and a distinct cross-molecular EG-water hydrogen-bonding motif. The concentration dependence of the MCR-ALS scores reveals a pronounced maximum of the EG-

water interaction component at intermediate compositions (X_{EG} ≈0.3-0.4), indicating the regime of strongest CP-water coupling. Independent molecular dynamics (MD) simulations support this interpretation by showing that the population of mixed water-EG hydrogen-bond (HB) configurations is maximized in the same composition window. This work demonstrates that MCR-ALS is a critical spectral analysis tool for resolving hidden hydration structures that are otherwise inaccessible, enabling quantitative identification of interaction motifs that govern cryoprotective behaviour.

Keywords: Cryopreservation; Biological Systems; Photonics; Light-Matter Interaction.

Onion peels–derived activated carbon as a sustainable electrode material for high-performance supercapacitor applications

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The growing demand for sustainable and low-cost energy storage materials has driven interest in biomass-derived carbons. In this study, activated carbon (AC) is successfully synthesized from waste onion peels and explored as an electrode material for supercapacitor (SC) applications. The onion peels are carbonized and chemically activated to develop a porous carbon structure suitable for SC application. Structural and chemical characterizations are carried out using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). XRD analysis confirms the formation of predominantly amorphous carbon with disordered graphitic domains, while FTIR spectra reveal the presence of oxygen-containing functional groups that enhance surface wettability and electrochemical activity. The electrochemical performance is evaluated using cyclic voltammetry (CV) measurements in an aqueous electrolyte. The CV curves exhibit near-rectangular shapes even at higher scan rates, indicating ideal electric double-layer capacitive behavior and good rate capability. The enhanced capacitive response is attributed to the porous structure and surface functionalities derived from the biomass precursor. Overall, the results demonstrate that onion peel waste can be effectively converted into functional AC with promising electrochemical properties. This work highlights an environmentally friendly approach to waste utilization and provides insight into the potential application of biomass-derived carbons in sustainable SC technologies.

Keywords: Activated carbon, Supercapacitor, Cyclic voltammetry, X-ray diffraction, Biomass.

Topological edge states in one-dimensional photonic crystals for optical sensing: Principles, designs, and applications

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Topological photonics has attracted strong interest in recent decades for having ability to propagate light in the robust way in the presence of structural defects. One-dimensional photonic crystals are suitable platforms for achieving topological edge states by carefully designing the refractive index variation and band structure. These edge states appear within

the photonic bandgap and are strongly localized at interfaces that makes them sensitive to changes in the surrounding refractive index. In this work, we proposed the refractive index sensor that is based on topological edge state which appears at junction of two one-dimensional photonic crystals. We further explore the emergence of topological edge state by analyzing the band structure of the two photonic crystals through the calculation of the Zak phase, which characterizes topological properties of one-dimensional photonic crystals.
Keywords: Topological photonics, 1D photonic crystals, Edge states, Zak phase.

DFT and QTAIM investigation of hydrogen-bonding interactions in quaternary ammonium–polyol deep eutectic solvents

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Deep eutectic solvents composed of quaternary ammonium salts and polyol hydrogen-bond donors are promising sustainable solvents. This work presents a computational investigation of DESs formed from benzyl trimethyl ammonium chloride and benzyl tributyl ammonium chloride with ethylene glycol, diethylene glycol, triethylene glycol, and glycerol at a 1:2 HBA–HBD ratio. All complexes were optimized at the B3LYP-D3/6-311++G(d,p) level using the vacuum model. Hydrogen-bond interactions were characterized using QTAIM and NCI analyses. The results show that increasing the HBA alkyl chain length and the number of hydroxyl groups in the HBD strengthens the hydrogen-bond network and enhances DES stability. Glycerol-based DESs exhibit the strongest interactions, indicated by shorter O–H···Cl distances, higher electron density at bond critical points, and more negative interaction energies. BTMAC-based DESs form compact structures, whereas BTBAC systems display greater geometric flexibility due to their longer butyl chains. These findings provide design guidelines for tailoring DES properties for applications in catalysis, separation, electrochemistry, and biomolecular stabilization.
Keywords: Deep eutectic solvents; Hydrogen bonding; Quaternary ammonium salts; Polyols.

Electrical conductivity and dielectric properties of saccharides coated magnetite nanoparticles

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The aim of this research was different saccharide-coated (sucrose, fructose, and glucose) magnetite nanoparticles. With the synthesis and characterization study of superparamagnetic iron oxide nanoparticles (SPION). The nanoparticles are prepared by doping. The magnetic ferrite nanoparticle into the synthesized co-precipitation method based Superparamagnetic iron oxide nanoparticles. Magnetic nanoparticles have attracted intensive attention for their

wide applications as biomaterials and energy storage devices. Superparamagnetic iron oxide nanoparticle composite is characterized by X-Ray Diffraction (XRD), high resolution transmission electron microscopy (HR-TEM) and Dielectric Measurements are performed on these composites on an LCR meter in the temperature range from 40°C to 100°C and in the frequency range 1 kHz – 10 kHz The effect of temperature and frequency variation on dielectric constant (ε'), Dielectric loss (tan δ) and a. c. conductivity (σ_{ac}) are determined. The result shows that the conductivity increases with a rise in temperature. The dielectric constant, dielectric loss, and conductivity of the Superparamagnetic iron oxide nanoparticles were compared with magnetic nanoparticles doped composite.

Keywords: SPION; saccharides; Magnetic nanoparticles; Dielectric.

Effect of interface on light-matter interaction in the MoS_2-based van der Waals heterostructure

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Molybdenum disulfide (MoS_2) is one of the widely studied two-dimensional semiconducting materials in the family of transition metal dichalcogenides (TMDs). Its high optical sensitivity, layer-dependent bandgap, and strong excitonic effect allow us to tune its electronic and optical response. MoS_2, being a van der Waals (vdW) material, allows different layers to be stacked on each other, making it easier to design devices with specific properties. In this work, we have fabricated two different heterostructure devices of mechanically exfoliated MoS_2 and Graphite to study the effect of interfaces on the optical properties of the MoS_2. The Few-layered MoS_2 has a vdW interface with a few-layered graphite. Alongside, the MoS_2 and graphite were placed in such a way that a part of them is separated by a thin layer of spacer hexagonal boron Nitride (hBN), forming a MoS_2/hBN/Graphite heterostructure. In both cases, the device was fabricated on a few-layer hBN substrate, which serves as a defect-free substrate. We perform power-dependent Raman and Photoluminescence (PL) spectroscopy measurements to understand the effect of interfaces on the characteristic Raman modes and PL emission of MoS_2.

Keywords: Two-dimensional materials, vdW heterostructures, Raman & PL spectroscopy.

Er^{3+}/Tm^{3+} co-doping and its influence on physical, optical and luminescence properties of Er^{3+} doped borate glasses

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Erbium singly doped and erbium- thulium co- doped borate glasses were fabricated by conventional melt- quench technique. The physical, optical and luminescence properties were investigated for these samples to study the role of Tm^{3+} in improving the quality of glasses for optical applications. UV-visible-NIR absorption spectra of these glasses contained many absorption bands due to the transitions between different energy levels corresponding to both the rare- earth ions. Luminescence studies involved getting emission peaks in visible and near- infra red (NIR) region of the spectrum for two different excitation wavelengths 358 and 980 nm, respectively. Decreasing intensity of prominent 453 nm emission peak was witnessed in visible region due to self-quenching or cross- relaxation process of Tm^{3+} ions. The intensity of typical broadband emission produced by Er^{3+} ions at around 1530 nm due to $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition dropped down significantly on co-doping with Tm^{3+} ions which confirmed the non-resonant energy transfer occurring between the two rare-earth ions. The emission peaks at 453, 476 and 1532 nm were considered for decay analysis and the calculated lifetime values shortened on increasing Tm_2O_3 content for all three cases. Energy transfer parameters were also calculated for 1532 nm emission with the help of Inokuti- Hirayama (I-H) model fitting for decay curves. (x, y) co- ordinate of CIE- chromaticity diagram lying in blue region for 453 nm emission pointed towards the potentiality of the present co- doped glasses in blue LED application.
Keywords: Erbium- thulium; Broadband Emission; Energy transfer.

Sustainable ZPMA-modified red mud catalyst for multi-component synthesis of benzothiazole derivatives: Characterisation, solvatochromism, and Cu^{2+} sensing

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Red mud, a major waste by-product of the aluminium industry, was transformed into a functional ceramic-based catalyst. The initially basic red mud was converted into an acidic catalyst by incorporating heteropoly acids. Structural and compositional analyses using IR, XRD, SEM, TEM, and eZAF Quant confirmed the presence of Fe, Al, Ti, and Si oxides, along with heteropoly acids, which collectively enhanced catalytic activity. The catalyst was applied to the multi-component synthesis of benzothiazole derivatives under mild conditions, and IR, ^1H,

^{13}C NMR, and mass spectrometry characterised the products. Photophysical studies revealed solvatochromic behaviour of ligands (L1a–L5a), with absorption and emission intensities correlating with solvent polarity, supported by theoretical calculations using Dimroth–Reichardt and Kamlet–Taft parameters. Among the derivatives, ligand L5a exhibited selective Cu^{2+} binding, with a detection limit of 8.19×10^{-6} M, highlighting the system's sensitivity. This study demonstrates the dual advantage of transforming industrial red mud waste into a high-performance ceramic catalyst while generating benzothiazole derivatives with potential applications in solvatochromism and metal ion sensing.

Keywords: ZPMA red mud catalyst, Benzothiazole derivatives, Solvatochromism, MI sensing.

Improving the magnetic, electrical and their coupling through nickel substitution in strontium hexaferrite

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Now a days, enhancement of magnetoelectric (ME) coupling has become an essential parameter for the next generation ME-devices. For this purpose, the present work based on improving the functional properties and ME coupling though the nickel substitution. The single phase $SrFe_{(12-x)}Ni_xO_{19}$ (x =0, 0.30, and x = 0.60) polycrystalline compound has been prepared by sol-gel auto-combustion method. The Rietveld refinement with $P6_3/mmc$ space group show marginal change in lattice parameter with hexagonal structure. The same is again confirmed through field emission scanning electron microscope (FESEM) with average particle size is around micrometre range. The lattice strain observed in X- ray diffraction has been confirmed through Raman spectra and the lattice distortion created at 12k octahedral site is the most. The variation of magnetization as a function of temperature shows spin blocking near ~ 50 K for the compounds. The saturation magnetization (M_s) value increases with the nickel substitution whereas drastic reduction in coercivity (H_c) is observed. The temperature dependence of "M_s" value follows the Bloch law and the "H_c" value show nonlinear increase from low temperature to room temperature (RT). The impedance behavior with the frequency validates the Havriliak-Negami model and the semiconducting-like nature of the sample. It shows non-Debye-like relaxation for both grain and grain boundary. The resistivity and the capacitance value have increased with the nickel substitution. Again, this enhancement followed by the improved impedance value and distortion at 12k crystallographic site uplifted the ME coupling value increased by several orders at RT.

Keywords: Structural study, Magnetism, Impedance, Magnetoelectric coupling.

Optical properties of few-layer MoS_2 on h-BN and SiO_2 substrates

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When different 2D materials are stacked on top of each other, van der Waals (vdW) heterostructures are formed, in which the layers are held together by weak van der Waals forces instead of chemical bonds. This type of structure provides clean interface and is useful for studying material properties. In this study, we fabricated a few-layered Molybdenum disulphide (MoS_2) based vdW heterostructure device with hexagonal boron nitride (hBN); as a defect free insulating substrate. Molybdenum disulphide (MoS_2) is a van der Waal crystal, whose atomic layers are widely studied due to its tuneable bandgap in the visible region and strong light-matter interaction, making it useful in optoelectronic applications. We studied the photoluminescence emission spectroscopy and Raman spectroscopy of MoS_2 at room temperature under two different substrates (hBN and SiO_2). We further extended our measurements for various incident power. Our interest is to study the effect of the interface on the light-matter interaction of few-layered MoS_2.

Keywords: Van der Waals forces; Molybdenum disulphide; PL emission & Raman spectroscopy.

Fabrication and characterization of ZnO-$NiCo_2S_4$ S-scheme heterojunction for the photocatalytic degradation of an organic dye

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ZnO is extensively used in the field of photocatalysis, but its large bandgap and rapid recombination of charge carriers hinder their widespread applications. Thus, integrating ZnO with narrow gap metal sulphides gains considerable interest from the prospect of forming S-scheme heterojunction. Pure ZnO and $NiCo_2S_4$ were obtained by solution combustion route and hydrothermal method respectively, while the heterojunction formation between them were achieved through a facile ultrasonic approach. The samples were characterized by various analytical techniques. The XRD confirmed the presence of both the crystal phases, while shift in the optical response to the longer wavelength region is validated by UV-visible absorption spectroscopic technique. The photocatalytic experiments concluded the faster degradation of organic dye compared to the pure phase counterparts. The high performance was attributed to the formation of S-scheme heterojunction, which facilitated the participation of energetic CB electrons and VB holes of $NiCo_2S_4$ and ZnO respectively in the degradation mechanism.

Keywords: Zinc oxide, S-scheme heterojunction, Dye degradation, Photocatalysis.

Investigation on structural and optical properties of alkali and alkaline earth fluorophosphate glasses doped with Sm^{3+} ions for reddish-orange lighting applications

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In this study, the structural and optical properties of quenched alkali and alkaline earth fluorophosphate glasses with the composition (60-x) P_2O_5+10MgO+10ZnO+10BiF_3+10KF were investigated for potential applications in reddish-orange lighting. These glasses were doped with varying concentrations (0.5, 1.0, 1.5, and 2.0 mol%) of Sm_2O_3. Optical properties were evaluated through absorption, excitation, and emission analyses, while structural properties were examined using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR), and Raman spectroscopy. The amorphous nature of the quenched glass samples was confirmed using XRD and SEM. Raman and FTIR analyses identified the presence of phosphate and fluorine functional groups. The absorption spectra of the fluorophosphate glasses exhibited several peaks across the UV, VIS, and NIR regions. The Judd-Ofelt (JO) theory was applied to analyze the peak intensities. The absorption spectra were utilized to determine the Judd-Ofelt (J-O) intensity parameters (Ω_2, Ω_4, and Ω_6), which followed the trend $\Omega_4>\Omega_6>\Omega_2$. The radiative parameters (A_T and τ_R) for various excited states were derived from the J-O parameters obtained. When excited at 403 nm, photoluminescence analysis revealed four emission bands corresponding to the $^4G_{5/2}\rightarrow{}^6H_{P/2}$ (P=5,7,9, and 11) transitions of Sm^{3+} ions, with a prominent reddish-orange emission at 599 nm. The emission spectra were used to calculate the stimulated emission cross-sections (σ_P). It was confirmed that fluorophosphate glasses doped with Sm^{3+} ions exhibit reddish-orange luminescence, rendering them suitable for potential reddish-orange lighting applications because the chromaticity colour coordinates fall within the reddish-orange region.
Keywords: Fluorophosphate glass; Judd-Ofelt Parameters; Emission Properties.

Synthesis and characterization of $Co_xNi_{(1-x)}MoS_4$ nanopowders as electrode materials for supercapacitor applications

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In this study, a hydrothermal synthesis method was utilized to produce $Co_xNi_{(1-x)}MoS_4$ (x = 0.2, 0.4, 0.6, and 0.8) nano powders, which were subsequently assessed as electrode materials for supercapacitor applications. In a Teflon-lined stainless-steel autoclave, precise quantities of molybdenum (IV) sulfide, nickel (II) sulfate hexahydrate, and cobalt (II) sulfate heptahydrate were dissolved in deionized water and subjected to hydrothermal treatment at 200 °C for six hours. The resulting products were thoroughly washed and dried to obtain fine nanopowders, designated as CNMS0.2, CNMS0.4, CNMS0.6, and CNMS0.8, according to their cobalt content.

Structural and phase analyses confirmed the successful formation of crystalline $Co_xNi_{(1-x)}MoS_4$ nano powders, while microscopic examinations revealed uniform elemental distribution and nanoscale morphology. Spectroscopic studies verified the presence of electroactive Co and Ni species within a stable MoS_4 matrix. According to Brunauer–Emmett–Teller (BET) analysis, an increased specific surface area facilitates electrolyte diffusion and charge storage. The electrochemical performance was evaluated using cyclic voltammetry, which demonstrated distinct pseudocapacitive behavior due to the reversible faradaic redox reactions of cobalt and nickel ions. The optimized composition exhibited enhanced specific capacitance, favourable rate capability, and good electrochemical stability, highlighting the synergistic effect of mixed metal sulphides. The improved charge storage performance is attributed to the combined advantages of a large surface area, efficient charge transport, and numerous redox-active sites. These findings suggest that hydrothermally produced $Co_xNi_{(1-x)}MoS_4$ nano powders are promising electrode candidates for high-performance supercapacitor applications.

Keywords: Nanopowders; Hydrothermal method; Cyclic Voltammetry; Supercapacitors.

Data acquisition programme by laboratory virtual instrumentation engineering workbench (LabVIEW)

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The data flow based graphical programming for data acquisition, instrument control and automation uses Laboratory Virtual Instrumentation Engineering Workbench (LabVIEW). LabVIEW simplifies programming by using graphical block diagrams for faster and user friendly technique. Programs developed here is virtual Instruments (VIs) for data acquisition in science and electrical engineering applications which extends from simple data collection involving interfacing a PC with sensors, actuators, signal conditioning, data storage, pre and post processing of acquired signals for making the data meaningful to end users. These systems involve reading, converting, storing sensor signals through combination of hardware and software. It shows various configurations like visa resource name, operation mode, frequency and primary data type in different panels. Specific parameters settings correspond to hardware structure, wired software. When VI run starts in different panels the data get into Read All Measurement panel in terms of Primary and secondary indicators. Data taken into an Excel sheet manually takes a whole day in processing for estimation of dielectric properties at different frequencies from 20 Hz to 200 kHz. The Lab View code is adaptable, reusable endlessly nested. The programmer chooses respective front panel controls, indicators to receive and supply data, create icons for each VI or sub-VI. The sub-VI is set in front panel for computations. This program determined the relevant acquisition parameters of various configurations like Visa Resource Name, operation mode, Frequency, primary, secondary and general propagating clusters on multiple configurations into a single configuration like a block diagram with a single front panel. When VI is run the data comes in same panel this procedure consumes less time. Manual measuring dielectric properties at various frequencies ranging from 20 Hz to 200 kHz manually takes 45 minutes in an excel

sheet. Therefore, virtual Instrument programme has very good user friendly utility compared to manual analysis of data.

Keywords: Data Acquisition; LabVIEW; Dielectric Properties.

Structural, vibrational, and transport properties of RSn_4 (R= Pt, Pd, and Au) compounds under pressure

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Topological nodal-line semimetals (TNLS) are an emerging class of quantum materials. In the electronic structure of the TNLS materials, the conduction and valence bands intersect along continuous lines in momentum space. This gives rise to unusual electronic, vibrational, and transport properties. Among them, RSn_4 (R = Pt, Pd, Au) compounds have attracted significant attention due to their unique electronic properties, such as extremely large magnetoresistance (XMR), high carrier mobility, and, in the case of $AuSn_4$, superconductivity with possible topological character. All three compounds shared an orthorhombic crystal system with a layered structure with two Sn layers stacked between the R (Pt, Pd, and Au) atoms. We conducted a detailed experimental study of these materials, examining their structural, vibrational, and transport characteristics under different pressure conditions, with special focus on $PtSn_4$ and $PdSn_4$. The research used HPXRD, HP Raman spectroscopy, and electrical transport measurements to study how these materials behave under different pressure conditions. The orthorhombic *Ccce* structure of $PtSn_4$ remains stable up to 24 GPa. Even though the symmetry doesn't change, the material undergoes an isostructural phase transition at 7.8 GPa. The material shows two distinct pressure-related changes, including compressibility anomalies and shifts in the pressure dependence of Raman phonon modes. The transition may result from anisotropic lattice compression, suggesting a possible pressure-induced electronic topological transition (ETT), which requires further electronic band-structure calculations to confirm. On the other hand, the $PdSn_4$ structure remains stable up to ~25 GPa. We used Raman spectroscopy and density functional theory calculations and detected a possible isostructural transition at approximately 15 GPa, as evidenced by a pressure-induced anomaly in Raman modes. The research shows that $PtSn_4$, $PdSn_4$, and $AuSn_4$ follow a chemical-pressure model, and it will be interesting to examine how external pressure affects their lattice stiffness and vibrational properties. The RSn_4 compounds exhibit distinct behaviour based on transport measurements. The materials $PtSn_4$ and $PdSn_4$ show XMR and follow Fermi-liquid behaviour at low temperatures. But $AuSn_4$ forms a non-centrosymmetric structure, as reported previously, and exhibits superconductivity at 2.4 K. Its T_c decreases by -0.3 K/GPa with increasing pressure, and the superconductivity is expected to disappear above 4.7 GPa based on the trend. The combination of *s*-wave bulk pairing with *p*-wave surface pairing in $AuSn_4$ makes this material an attractive candidate for possible topological superconductivity. This research establishes vital insights into how the lattice structure affects phonons, electronic topology, and transport properties in RSn_4-type TNLS. The research results show the possible applications for spintronics and quantum technology.

Keywords: Topological nodal-line semimetals; RSn_4 compounds; Raman spectroscopy; XMR.

Thermoluminescence kinetic analysis and dosimetric features of Sm activated ZrO_2 phosphor

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This work investigates the structural and thermoluminescence (TL) characteristics of β-irradiated samarium-doped zirconium oxide (ZrO_2: Sm) as a function of Sm concentration. The dosimetric properties were evaluated for compositions exhibiting high TL response. The $Zr_{1-x}Sm_xO_2$ samples with x = 0.1, 0.4, 0.7, 1.0, 1.5, and 2.0 mol% were synthesized using the solution combustion method. X-ray diffraction analysis confirmed that all samples are in the monoclinic phase. Among the studied compositions, the sample with 0.4 mol% Sm exhibits the highest TL intensity. Glow curves recorded at a heating rate of 1 °C s^{-1} revealed two prominent peaks located at 116 ± 1 °C (peak 1) and 176 ± 1 °C (peak 2). The peak positions were reproducible over eight repeated measurements for the same dose and aliquot. The dose response of both peaks was nearly linear in the dose range of 2–120 Gy. The TL response of peak 2 exhibits sublinear behavior up to 200 Gy. The peaks 1 and 2 faded to 13% and 4%, respectively, of their initial intensities within 7200 s of irradiation. Thermal cleaning experiments indicated that the TL glow curve comprises five overlapping peaks. Qualitative analysis using the T_m–T_{stop} method suggested that each glow peak consists of first-order kinetic components. Kinetic parameters were evaluated using the initial rise, whole glow peak, peak shape, and curve-fitting methods. The order of kinetics for both major peaks was determined to be first order. Using the whole glow peak method, the activation energies of peaks 1 and 2 were estimated to be 0.56 ± 0.01 eV (order of kinetics = 1.1) and 0.86 ± 0.06 eV (order of kinetics = 1.2), respectively. This study provides a comprehensive understanding of the dosimetric properties of $Zr_{1-x}Sm_xO_2$ phosphors and demonstrates their potential for thermoluminescence dosimetry applications.
Keywords: ZrO_2: Sm; Thermoluminescence; T_m–T_{stop} analysis; Kinetic parameters.

Solution combustion synthesis of Tb-Doped $ZnFe_2O_4$/rGO nanocomposite: Structural, morphological, and dielectric characterization

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Nanocomposites comprising reduced graphene oxide (rGO) and ferrite doped with rare-earth elements are expected to provide an efficient route for electromagnetic interference (EMI) shielding because they can exploit both magnetic and dielectric synergy. In this paper, we present an extremely simple method for the fabrication of Tb^{3+}-$ZnFe_2O_4$/rGO (Tb–$ZnFe_2O_4$/rGO) by using the solution combustion process using urea as the fuel to rapidly form the composites in one step. The phase purity and structure of the nanocomposite were confirmed by using X-ray diffraction (XRD) where the nanocomposite showed a spinel crystal structure and incorporated successfully with Tb^{3+} ions and rGO sheets. The presence of

chemical interactions between the Tb– $ZnFe_2O_4$ nanoparticles and rGO sheets were established by Fourier Transform Infrared (FTIR) spectroscopy showing vibrations corresponding to metal-oxygen bonding and C=O stretching modes. The morphology of the nanocomposite was then evaluated with scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDAX). The results indicated a uniform nanoparticle distribution was obtained on the rGO nanosheets and confirmed the presence of Tb, Zn, Fe, C and O. The dielectric properties of the nanocomposite were evaluated over the frequency range and showed increases in both permittivity and dielectric loss which were associated with space charge polarization and interfacial effects at the Tb– $ZnFe_2O_4$/rGO heterojunction. Collectively, these results demonstrate the potential for Tb– $ZnFe_2O_4$/rGO to be utilized for high-performance EMI shielding applications.

Keywords: Solution combustion, Nanocomposite, Dielectric properties, EMI shielding.

Luminescence behaviour of Dy^{3+} doped strontium halophosphate phosphor

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In the present work, Dy^{3+}-doped $Sr_5(PO_4)_3F$ (strontium halophosphate) phosphors were synthesized using the auto-combustion method in a muffle furnace with controlled raising temperature (~600 °C) under a mildly reducing atmosphere. Systematic studies were conducted to characterize phosphor structural and morphological properties using X-ray diffraction (XRD) and field-emission scanning electron microscopy (FE-SEM), respectively. Further, photoluminescence (PL) studies of Dy^{3+}-doped $Sr_5(PO_4)_3F$ phosphors were carried out. Multi-wavelength excitation viz. 325 nm, 351 nm, 365 nm, and 388 nm were observed. However, PL emission spectra showed clear, distinctive and prominent peaks at 480 nm and 575 nm under the excitation of 351 nm ultraviolet (UV) radiation only. Thermoluminescence (TL) analysis were performed by exposing the phosphors to the beta (β) irradiation ($^{90}Sr/^{90}Y$ beta source) with different doses from 2 Gy to 25 Gy. The TL response with peak at 225±3 °C was observed for all the doses and maximum for 12 Gy. Studies of deconvoluted TL peaks and radiation doses versus TL response indicates the presence of several trapping centers. Hence, trap depths corresponding to these TL peaks were estimated to be 0.55 eV and 0.85 eV. These findings strongly suggest that Dy^{3+}-doped $Sr_5(PO_4)_3F$ phosphors have significant potential to be investigated for thermoluminescence dosimetry applications.

Keyword: Halophosphate; Photoluminescence; Thermoluminescence; Kinetic parameters.

Structural biology at the electron beam–matter interface: Cryo-EM of a plant cell wall enzyme

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Understanding how energetic radiation interacts with matter underpins modern imaging and spectroscopy. Cryo–electron microscopy (cryo-EM) leverages the interaction between high energy electron beams and vitrified biological specimens to determine macromolecular structures at near-atomic resolution. Owing to their short de Broglie wavelengths and strong elastic scattering cross-sections, electrons are exceptionally sensitive probes of biological matter, enabling structural analysis of radiation-sensitive proteins using minimal dose. Here, we demonstrate how controlled electron–matter interactions in cryo-EM were employed to resolve the structure of a large, membrane-embedded plant cellulose synthase (CesA), an enzyme responsible for synthesizing and exporting cellulose, the most abundant biopolymer on Earth. Purified cellulose synthase complexes were rapidly vitrified to preserve their native hydrated conformations and to suppress radiation-induced damage. Low-dose electron beams transmitted through the frozen specimens produced contrast via elastic scattering, encoding structural information as two-dimensional projection images. By collecting millions of single-particle images over a wide angular distribution and exploiting phase contrast transfer and electron scattering physics, three-dimensional Coulomb potential maps were reconstructed using computational averaging. These reconstructions achieved near-atomic resolution, resolving side chains within the cytosolic glycosyltransferase domain and individual transmembrane helices within the lipid-embedded region. Notably, electron density corresponding to nascent polysaccharide chains was observed within transmembrane channels, illustrating how subtle variations in electrostatic potential and atomic composition modulate electron scattering to reveal both protein and carbohydrate components. The cryo-EM structure reveals that cellulose synthase assembles into a defined oligomeric complex in which multiple transmembrane channels converge, spatially aligning newly synthesized glucan chains. This architecture provides a molecular basis for coupling polymer synthesis with transmembrane transport and early-stage microfibril formation. From a beam–matter interaction perspective, these findings underscore how electron scattering encodes functional states of biological macromolecules, capturing transient biosynthetic intermediates that are inaccessible to crystallographic approaches. Advances in direct electron detectors, dose fractionation, and phase-preserving imaging have further increased the efficiency with which structural information can be extracted per incident electron, minimizing radiation damage while maximizing signal. Collectively, this study highlights cryo-EM as a powerful realization of electron–matter interaction physics applied to complex biological systems, bridging fundamental imaging principles with mechanistic insights into protein function and biomaterial assembly.

Keywords: Structural biology; Electron beam matter; Cro-EM; Cell wall enzyme.

Temperature induced phase-shift in cobalt substituted $KBiFe_2O_5$

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Recently emerged $KBiFe_2O_5$ compound exists in different space groups depending on the synthesis route. In this manuscript, the transition element cobalt (Co) is substituted at the iron (Fe) site of $KBiFe_2O_5$ (KBFO), and the 5% Co-substituted KBFO ($KBiFe_{1.95}Co_{0.05}O_5$: KBFCO) is investigated with temperature. The KBFCO sample is prepared following the conventional

solid-state reaction route. The room-temperature X-ray diffraction study confirms the phase purity of the prepared sample having a monoclinic structure in the P2/c space group. Temperature-dependent dielectric and magnetic analysis (250 to 510 K) is performed to identify the observed phase transitions. Temperature-dependent Raman study is performed from 120 to 430 K to verify the observed phase transitions. However, the temperature-dependent dielectric, magnetic, and Raman properties of KBFCO reveal an anomaly near about 420 K. It shows a Raman shift of the particular modes related to Fe-tetrahedral near 420 K. It is expected that the observed anomaly near about 420 K, a phase shift for KBFCO compound.
Keywords: Phase-transition, Monoclinic, Room-temperature, Raman shift, Magnetodielectric.

Modified power law fluid model for non-Newtonian ternary nano fluid over a vertical wavy surface to analyse the effects of MHD, viscous dissipation and natural convection on heat transfer

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This study explores natural convection flow of non-Newtonian ternary nanofluid over vertical wavy surface, considering for combined impacts of magnetohydrodynamics (MHD) and viscous dissipation. The fluid behaviour was modelled utilizing modified power-law viscosity model to capture complex rheological characteristics of the non-Newtonian fluids (Ethylene glycol). Governing boundary layer equations were converted into system of dimensionless equations, that were then resolved numerically utilizing implicit finite-difference discretization and Newton-Raphson iteration for nonlinear systems using the MATLAB partial differential equation (PDE) solver. During current investigation, impact of key physical parameters, comprising Ec(Eckert number), Nu (Nusselt number), M (magnetic parameter), non-Newtonian power-law index, Pr(Prandtl number), on velocity, Cf (skin friction coefficient), temperature, was investigated. Findings are depicted through detailed graphical and tabular illustrations, providing insights into the thermophysical behaviour of the ternary hybrid nanofluid system under varying conditions.
Keywords: Magnetohydrodynamics; Finite difference method; Heat transfer.

Low temperature dielectric relaxation, magnetic glassiness, and magnetodielectric coupling in $0.8(Bi_5Ti_3FeO_{15})/0.2(La_{0.67}Sr_{0.33}MnO_3)$ composite

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This article investigates the low-temperature dielectric relaxation, magnetic glassiness, and magnetodielectric (MD) characteristics of $0.8(Bi_5Ti_3FeO_{15})/0.2(La_{0.67}Sr_{0.33}MnO_3)$ composite synthesized by the sol-gel modified method. Dual phase nature of the composite is confirmed from the room temperature Rietveld refinement of x-ray diffraction analysis. The composites having the combined orthorhombic and rhombohedral structure with '$A2_1am$+R-$3c$' space

group. Dielectric vs. temperature studies reveal three relaxation peaks at 40 K, 100 K, and 270 K, where the low-temperature relaxations originate from small-polaron hopping and defect dipole reorientation associated with mixed-valence Fe^{2+}/Fe^{3+} and Mn^{3+}/Mn^{4+} ions, while the broad anomaly near 270 K arises from diffuse or relaxor ferroelectric behavior. Frequency-dependent dielectric spectroscopy identifies a clear temperature-driven crossover in the relaxation behavior, with activation energies of 150 meV below and 1.5 meV above 200 K. This behavior is governed by thermally activated hopping of localized charge carriers arising from mixed-valence Mn and Fe ions, evolving from a strongly localized, high-barrier regime to a more mobile, low-barrier relaxation at elevated temperatures. The ac susceptibility analysis reveals a cluster glass phase at 30 K and 5 K, confirmed by Vogel-Fulcher and dynamical scaling analyses. The large relaxation time ($\tau_o \sim 10^{-4}$ s) reflects cluster glass behavior arising from competing Fe/Mn exchange interactions and Mn antisite disorder in LSMO, leading to locally disordered spin orientations. MD measurement exhibits temperature-dependent butterfly and inverted butterfly hysteresis loops. A symmetric and reversible MD response is observed under ±13 kOe, with a maximum MD value of ~0.37% at 300 K that decreases to -0.05% at 50 K due to dipole freezing and suppressed charge-carrier hopping at low temperatures. Furthermore, Ginzburg-Landau analysis confirms a biquadratic magnetoelectric coupling (P^2M^2) governed by the coupling coefficient γ, whose magnitude is strongly enhanced at low temperatures ($\gamma \sim -392.87$ and -72.98 $(emu/g)^{-2}$ at 100 K).

Keywords: Manganite; Relaxation process; Magnetodielectric; AC susceptibility; Cluster glass.

Characterization of banana inflorescence bract for biodegradable packaging material: Insights from XRD, FTIR, DSC, and SEM studies

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Banana inflorescence bracts are an ample agricultural by-product produced during banana harvesting and post-harvest processing. Despite being rich in lignocellulosic components such as cellulose, hemicellulose, and lignin, these bracts are mostly discarded as waste, contributing to environmental burden and inefficient resource utilization. The escalating global concern about environmental safety and plastic pollution has created a pressing demand for sustainable, biodegradable packaging alternatives. Accordingly, valorization of plant-based agro-residues offers an effective pathway for developing eco-friendly materials and improved waste management. The present study explores the potential of banana inflorescence bracts collected from different banana varieties as a raw material for biodegradable packaging. A comprehensive multi-technique characterization approach was employed to analyse their structural, chemical, thermal, and morphological properties. Understanding these properties is critical for envisaging the material behaviour and performance necessities for packaging applications, including mechanical strength, thermal stability, and processability. X-ray Diffraction (XRD) analysis was used to evaluate the crystalline structure and degree of crystallinity of the banana bracts. The existence of characteristic cellulose diffraction peaks confirmed the semi-crystalline nature of the bracts, which is a critical factor contributing to mechanical strength and dimensional stability in biodegradable packaging materials. Fourier Transform Infrared (FTIR) spectroscopy enabled

detailed analysis of the chemical composition and functional groups present in the bracts. The FTIR spectra exposed characteristic absorption bands corresponding to hydroxyl, carbonyl, and ether groups, confirming the presence of cellulose, hemicellulose, and lignin. These functional groups play a substantial role in intermolecular interactions during material processing. Thermal behaviour of the banana inflorescence bracts was assessed using Differential Scanning Calorimetry (DSC). The DSC thermograms showed crucial thermal transitions, for instance, glass transition and decomposition-related events, providing valuable information about thermal stability and processing temperature limits. Satisfactory thermal stability is essential for packaging materials to endure fabrication processes and storage conditions without substantial degradation. Surface morphology was examined using Field Emission Scanning Electron Microscopy (FESEM). The micrographs exposed a fibrous and porous structure, characteristic of lignocellulosic materials. Such morphology is beneficial for strengthening biodegradable composites, as it can improve interfacial bonding and mechanical performance when combined with biodegradable matrices. Overall, the results of this study validate that banana inflorescence bracts hold suitable physicochemical, thermal, and morphological properties, supporting their potential as a sustainable raw material for biodegradable packaging. By transforming an underutilized agro-residue into a value-added material, this research contributes to waste-to-resource strategies, promotes the circular economy, and the development of environmentally friendly packaging solutions.

Keywords: Banana inflorescence bract; Biodegradable; Biomass; Sustainability.

Phytogenic silver nanoparticles synthesized from dendrophthoe falcata and ocimum tenuiflorum: Applications in surface enhanced Raman spectroscopy

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We have systematically investigated the performance of Surface Enhanced Raman Spectroscopy substrate based on green synthesized silver nanoparticles. To assess the SERS activity, three dye molecules Nile blue, crystal violet (CV), and methylene blue as well as an explosive molecule, picric acid (PA), were selected as probe analytes. Two plants mediated AgNPs were synthesized in this study, among them, the AgNPs made from Dendrophthoe falcata (AgL) showed a superior SERS enhancement of 10^6 with high reproducibility. When AgL was employed as the SERS substrate, the detection limits were upto 10 nM for Nile blue. In contrast, AgNPs synthesized using Ocimum tenuiflorum extract (AgT) showed approximately one order lower SERS enhancement accompanied by reduced signal reproducibility. FTIR spectroscopy was used to investigate the difference in phytochemical composition of the plant extracts. The TEM analysis of AgL reveals nearly spherical nanoparticles with a narrow size distribution of 3–10 nm, whereas AgT comprises larger nanoparticles with a broad size range of 10–70 nm and significant shape anisotropy (aspect ratio ~0.9–2). Finite element method - based COMSOL Multiphysics simulations were carried out to elucidate the relationship between nanoparticle morphology and the resulting local electric field enhancement. Overall,

these findings underscore the critical role of plant-derived green synthesis in tailoring nanoparticle morphology and plasmonic response, thereby offering an efficient and sustainable method for improving SERS substrate performance.

Keywords: Green synthesis; Silver nanoparticles; SERS; FEM; Femtosecond Z-scan.

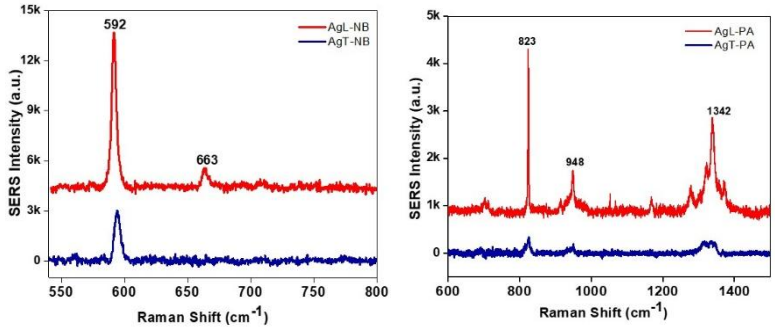

Fig.1 SERS spectra of Nile blue (10µM) and Picric Acid(500µM) using AgT and AgL substrates. AgL shows stronger enhancement in both cases due to its smaller, well-capped nanoparticles and more hotspot regions.

Statistical investigation of viscoelastic hybrid nanofluid transport over a stretching sheet in a porous medium under magnetic influence

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The present study analyzes the unsteady boundary layer flow, heat transfer, and mass transport of a viscoelastic hybrid nanofluid over a stretching sheet embedded in a porous medium under the influence of a time-dependent transverse magnetic field. The hybrid nanofluid model accounts for the combined effects of two different nanoparticles dispersed in a base fluid, and the effective thermophysical properties are incorporated into the governing equations. The flow is driven by an unsteady stretching velocity of the surface, while additional physical mechanisms such as magnetic damping, porous medium resistance, thermal radiation, Joule heating, internal heat generation or absorption, and an nth-order chemical reaction are considered. The mathematical formulation consists of the unsteady continuity equation, momentum equation in the flow direction, energy equation, and species concentration equation. By employing appropriate similarity transformations based on a time-dependent similarity variable and stream function, the governing partial differential equations are reduced to a coupled system of nonlinear ordinary differential equations. The transformed system inherently satisfies the continuity condition and is solved numerically subject to physically realistic boundary conditions. The effects of key dimensionless parameters, including the unsteadiness parameter, magnetic parameter, viscoelastic parameter, porous medium parameter, radiation parameter, Prandtl number, Schmidt number, heat source/sink parameter, and chemical reaction parameter, on the velocity,

temperature, and concentration fields are examined in detail. The results indicate that stronger magnetic and porous medium effects significantly reduce the fluid velocity, while thermal radiation and heat generation enhance the temperature distribution. An increase in the chemical reaction parameter leads to a reduction in concentration profiles and boundary layer thickness. The findings of this study provide valuable insights into unsteady hybrid nanofluid transport phenomena relevant to thermal management systems, chemical processing, and advanced energy applications.

Keywords: Visoelastic, Hybrid Nanofluid, Porous mediu, Thermal radiation.

Phytochemical - assisted synthesis of gold nanoparticles for SERS applications

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Metal nanoparticles have gained considerable attention due to its unique resonance known as the localized surface plasmon resonance (LSPR) which makes them promising candidate for all-sensing applications[1]. Surface Enhanced Raman Spectroscopy (SERS) is an exceptional analytic technique that exploits LSPR to detect the chemical and biological species at single molecular level. In particular, the amplification of the Raman signal arises from strong local electric field enhancement at the nanoparticle surface at the LSPR frequency[2]. In this study, we have prepared SERS substrate-based gold nanoparticles (AuNPs) by implementing an eco-friendly, sustainable, and low cost -green synthesis technique. Leaf extract of Psidium Guajava plant was used to synthesize Raman-active AuNPs, where the Phyto-chemicals present in the leaf extract act as reducing as well as stabilizing agent and the reaction yields highly AuNPs with narrow size and shape distributions. UV-vis absorption spectroscopy as well as Transmission electron microscopy confirmed the plasmonic and structural properties of AuNPs. The SERS performance of AuNPs were investigated using Nile Blue (NB) and Methylene Blue (MB) as probe analytes, which has shown multiple Raman peaks with enhanced intensities (Figure 1. a & b) as compared to the measurements without the substrate. An analytical enhancement factor of 10^4 and 10^3 is obtained respectively for NB and MB with good signal reproducibility and sensitivity. Our studies demonstrates that green the synthesised AuNPs are highly effective for SERS based sensing and analytical applications. The details will be discussed and presented.

Keywords: Gold nanoparticles (AuNPs), SERS, Green synthesis, Methylene Blue, Analytical enhancement factor.

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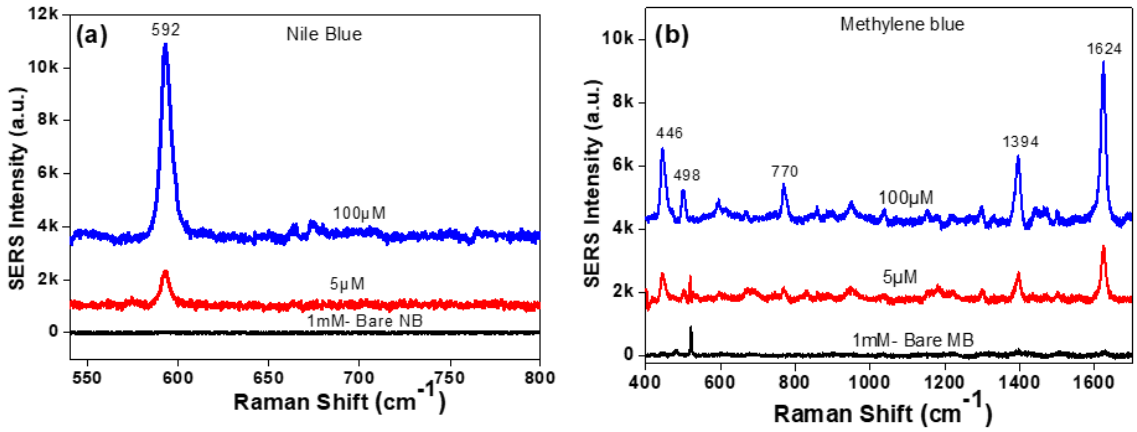

Figure 1 a. & b. SERS spectra of Nile blue and Methylene blue with different concentrations of 100µM and 5µM using AuNPs as substrate along with bare analytes of NB and MB

Optical, and dielectric properties of $AlCuTiO_{3+\delta}$ nanoparticles

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A series of $Al_{1-x}Cu_xTiO_{3+\delta}$ (x=0.2, 0.4, 0.6 & 0.8) (ACT) nanoparticles were synthesized via hydrothermal method using low operating temperatures. The diffraction patterns confirmed the presence of tetragonal structure including some secondary phases. The well-defined nanosized grains, and particles were detected in the surface morphology. The particle size distribution (PSD) showed the existence of smallest, and largest particles for x=0.2-0.8. The presence of Al, Cu, Ti, and O was confirmed from energy dispersive spectral (EDS) analysis. The wide optical bandgap was noticed for all copper concentrations. Moreover, the photocatalytic activity was observed for all samples. The frequency dependence of dielectric constant, and dielectric loss was clearly discussed. The high dielectric constant, and loss were noticed for x=0.8 sample, where the copper concentration is high. This can suggest the dielectric absorber applications. The space charge polarization mechanism, and relaxations were clearly understood using dielectric modulus, and impedance spectra. Cole-Cole plots conveyed the relaxation dynamics of x=0.2-0.8.

Keywords: Nanoparticles; Perovskites; Structure; Microscopy; Dielectric constant.

Effect of p^H on optical, and dielectric properties of $BaTiO_3$ nanoparticles

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Barium titanate nanoparticles were prepared by low temperature hydrothermal technique with varying p^H from 9 to 12. The X-ray diffraction (XRD) patterns confirmed that the barium titanate nanoparticles with pH ranging from 9 to 11 showed the existence of few small

secondary phases (*) related to tetragonal structure along with the prominent cubic phases. But for sample with p^H=12, the XRD patterns confirmed the presence of cubic phases without secondary phases. The morphology evidenced the existence of almost spherical shaped grains (FESEM-field emission scanning electron microscopy), and nanoparticles (HRTEM-high resolution transmission electron microscopy) in case of all samples. The EDS (energy dispersive spectra) confirmed the presence of Ba, Ti, and O elements among all samples. Besides, the photocatalytic activity was noticed for all samples. Using the Tauc's plots, optical band gap was determined. The dielectric constant (at p^H =12) was ~15.10 while the dielectric loss was ~1.231suggesting the sample suitable for charge stored capacitor applications. The dielectric modulus, and impedance spectra were recorded in order to evaluate the polarization, and conduction mechanism.

Keywords: Nanoparticles; Structure; Band gap; Morphology; Dielectric constant.

Alkali-controlled nanostructured γ-Al_2O_3 with high dielectric constant derived from boehmite via a microwave-assisted soft-chemical route

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Nanostructured γ-Al_2O_3 was synthesized from boehmite using a method that controls alkalinity through co-precipitation with NaOH, KOH, and LiOH·H_2O as agents, followed by microwave-assisted sintering. The effects of the alkali chemistry on phase formation, crystal structure, microstructure, optical properties, and dielectric features were carefully examined. X-ray diffraction and FTIR analyses confirmed that the NaOH-derived sample produced phase-pure γ-Al_2O_3, while the KOH- and LiOH·H_2O-derived samples exhibited some secondary aluminate phases and increased lattice distortion. Transmission electron microscopy revealed that NaOH-derived γ-Al_2O_3 had uniformly distributed, well-defined nanocrystalline grains. The KOH sample displayed moderate particle growth with some agglomeration, whereas the LiOH·H_2O sample had smaller, defect-rich, and heavily agglomerated particles. Dielectric measurements across the frequency range of 0.01Hz to 1MHz indicated stable permittivity and lower dielectric loss for the NaOH- and KOH-derived samples. In contrast, the LiOH·H_2O-derived sample had relatively higher dielectric loss. Impedance spectroscopy also revealed greater bulk and grain-boundary resistance for the NaOH-assisted γ-Al_2O_3. These results demonstrate that using alkali-controlled co-precipitation together with microwave sintering is an effective low-temperature method for producing γ-Al_2O_3 nanostructures with reliable dielectric insulating properties that are suitable for radio-frequency (RF) applications.

Keywords: Alkali-controlled synthesis; γ-Al_2O_3; Dielectric properties; Microwave sintering.

Experimental investigation of a Jatropha B20–butanol ternary blend in a ceramic-coated low heat rejection diesel engine

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The rising demand for a sustainable fuel and a curtailing emission policy has triggered many attempts to use biodiesel and alcohol mixes for diesel engines. Experimental investigations have been conducted for a most optimal mixture of Diesel, Jatropha biodiesel B20, and butanol (B20Bu10) in a ceramic-coated low heat rejection diesel engine to improve combustion efficiency. The performance and emission characteristics of the experiment were conducted with and without loads at various levels such as brake thermal efficiency, brake-specific fuel consumption (BSFC), cp-cycle pressure analysis, and prominent exhaust gases emitted during combustion. The ceramic-coated LHR diesel engine proved to be beneficial for better combustion efficiency for a mixture of B20Bu10 by increasing in-cylinder thermal performance. With respect to a standard uncoated diesel engine, B20Bu10 depicted an augmented maximum in-cylinder pressure and encouraging heat release properties with a simultaneous increment of 2.03% for brake thermal efficiency at maximum load conditions and a reduction of 3.8% for BSFC with a substantial decrease of hydrocarbons, CO, and smoke emission along with a moderate increment of NOx emission within a safe limit.
Keywords: Ceramics, Low Heat Rejection, Jatropha, Butanol, Combustion.

Tuning of emission of $SrCeO_3$ perovskite phosphors through Mn^{4+} ions activation for plant growth LED applications

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Recently, plant growth light-emitting diodes have emerged as essential light source for enhancing indoor crop yields, especially in response to adverse weather conditions. In this study, Mn^{4+}-doped $SrCeO_3$ perovskite phosphors were synthesized using a simple sol-gel method for potential application in PLEDs. The crystalline structure of the materials was characterized through XRD analysis, while their morphology was examined via SEM. Elemental and binding energy analyses were carried out by XPS studies and conforms that the existence Mn4+ ions in the prepared phosphors. The functional groups were identified via FTIR. Optical properties of samples were investigated using DRS, PLE, emission spectra, and lifetime measurements. Additionally, the chromaticity coordinates, correlated color temperature, and color rendering index were calculated for both pristine and Mn^{4+}-doped $SrCeO_3$ samples. The undoped host exhibited nearly white light emission, whereas $SrCeO_3$:xMn^{4+} (x = 0.01,0.03,0.05 and 0.07) phosphors emitted in the red region, indicating their suitability for use in plant growth LED applications.
Keywords: Metal (Mn4+) ions doped, Plant growth LEDs, phosphors.

Investigation of plasmon-exciton coupling in quantum dot-metal nanoparticle hybrid structure

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The present study investigated the plasmon-exciton coupling mechanism in Quantum Dot-Metal nanoparticle hybrid structure. The investigated hybrid structure consists of, the silver (Ag) and gold (Au) based plasmonic nanoparticles combined with a cadmium selenide (CdSe) quantum dot (QDs). In particular, two different plasmonic nano-systems were synthesized for this study**:** (i) Gold-hexagonal boron nitride nanocomposite synthesized via femtosecond laser ablation technique (Au-hBN) (iii) Silver nanoparticles (AgNPs) by green synthesis method. The hybrid system is prepared by drop-casting the nanoparticle solution on to a clean glass cover glass slip, followed by drop-casting the diluted solution of CdSe QDs. Single-particle Dark-Field scattering experiments were conducted using Dark-Field micro-spectrometer setup. The setup was based on upright optical microscope equipped with 60× objective (NA=0.65) and a halogen lamp.

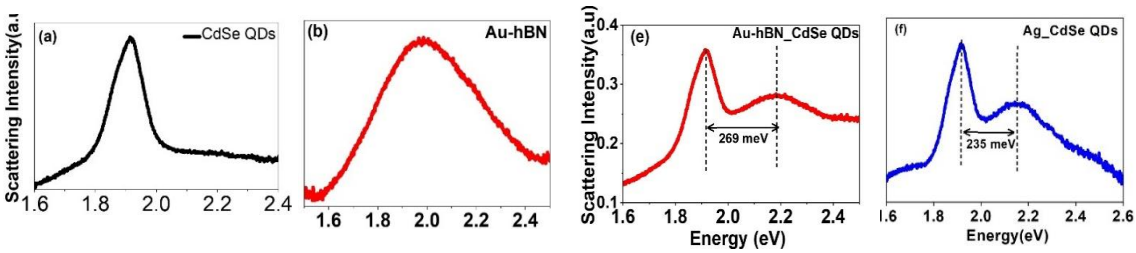

Figure1: Dark-field scattering spectra of CdSe QDs (a) Au-hBN(b) respectively. Dark field scattering spectra of Au-hBN-CdSe QDs (e) Ag-CdSe QDs (f).

Figure 1. (a), (b) depicts the dark field scattering spectra recorded from CdSe QDs, Au-hBN nanocomposites respectively. The corresponding peak position and line width are 1.91eV (0.116 eV), 1.98 eV (0.5 eV), respectively. Figure 1. (e), (f) represents the dark-field scattering spectra of hybrid systems, clearly depicting a peak splitting, particularly in Au-hBN -CdSe QDs and Ag-CdSe QD system, demonstrating a coupling between excitonic resonance in CdSe QDs and localized plasmon in metallic nanoparticles of the hybrid structure. The observed splitting is found out to be 269 meV and 235 meV in Au-hBN-QDs and Ag-QDs respectively, demonstrating a Rabi splitting mechanism. Our studies demonstrate that by tuning the plasmonic features of nanoparticles systematically, allows to manipulate the coupling strength of the plasmon-exciton interactions. The details will be presented and discussed.

Keywords: Plasmon, Exciton, Metal nanoparticles, Quantum Dots, Rabi splitting.

An optical method of analyzing petrol–ethanol fuel blends

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This study investigates the capability of near-infrared fibre-optic reflectance spectroscopy for rapid characterisation of petrol–ethanol blends. Samples of different volume percentages of petrol-ethanol mixtures (0%, 20%, 40%, 60%, 80% and 100% of petrol (v/v)) were prepared. The prepared samples were tested using the NIR reflection spectroscopy arrangement described in [1]. The spectra of the Petrol–Ethanol fuel blends at different concentrations are shown in Fig. 1. The peaks (minimum peak at 1137.24 nm and maximum peak at 1330.5 nm) where prominent changes are observed are marked in yellow in the figure. We have identified that the difference between the reflection at the minimum and maximum peaks can be used to determine the volume percentage of ethanol in petrol. The variation of the amplitude difference of these peaks with respect to the petrol concentration is given in Fig. 2. This will act as the calibration curve for determining and analyzing the petrol-ethanol blends. The present study demonstrates that using two light sources at wavelengths of 1137.24 nm and 1330.5 nm, along with light detectors, one can replace the costlier NIR spectrometer arrangement and determine ethanol concentration in petrol at a lower cost. These outcomes support the potential of our device for detecting fuel adulteration, routine quality control, and in-line industrial monitoring in a contactless, non-destructive, and rapid manner.

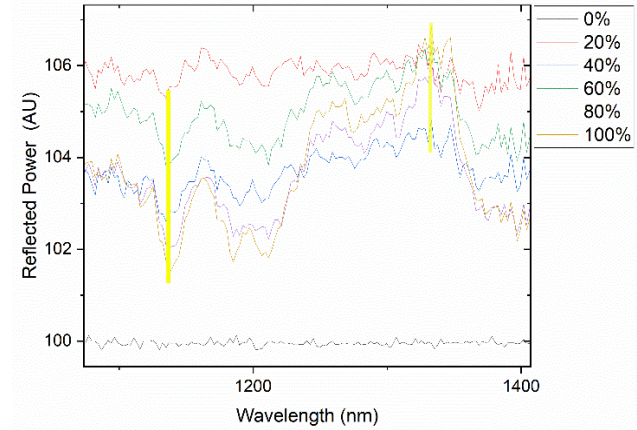

Fig. 1. NIR spectra of the Petrol–Ethanol fuel blends at different concentrations (v/v%). The peaks (minimum peak at 1137.24 nm and maximum peak at 1330.5 nm) where changes are observed are marked in yellow.

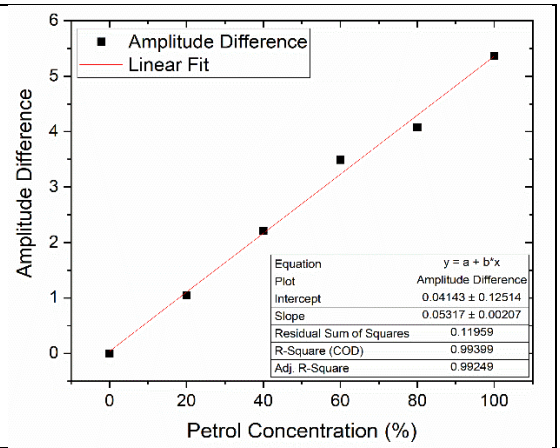

Fig. 2. Variation of the amplitude difference of peaks at 1137.24 nm and 1330.5 nm with respect to the petrol concentration.

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Angle-resolved optical properties of self-assembled colloidal monolayers: Grating diffraction, thin-film interference, and Rayleigh anomalies

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Two-dimensional photonic crystals offer a powerful platform for controlling light-matter interactions, with applications ranging from structural color engineering to optical sensing. In this work, we investigate the complex optical response of large-area, hexagonally-packed polystyrene (PS) sphere monolayers fabricated on high-index silicon substrates via surfactant-

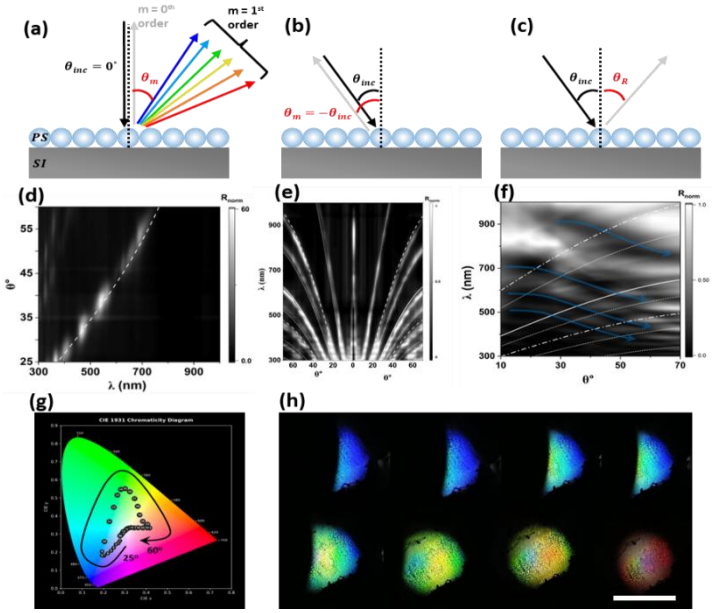

Figure : Schematic of the angle-resolved reflectance geometry setup to study (a) normal and (b) littrow diffraction (asymmetric), and (c) interference (symmetric) of the PS monolayer. (d) Diffraction plot compared with phase matching condition(dotted). € Littrow plot compared with phase matching condition (dotted). (f) Symmetric reflection plot with broad interference fringes (blue arrow) and Rayleigh anomalies (dotted and white lines). (g) Chromaticity coordinates (x, y) of the light diffracted from the PS sphere monolayer. (h) Photographs of PS monolayer observed at different angles, with incident light fixed normal to the substrate. Scale bar – 1 cm.

assisted self-assembly. To fully understand the optical phenomena at play, we performed a systematic characterization using an angle-resolved spectroscopic technique, including asymmetric diffraction, Littrow retroreflection, and symmetric specular reflection. Our findings reveal a rich interplay of three distinct optical effects. First, the grating-like nature of the monolayer was confirmed through asymmetric and Littrow diffraction measurements. The measured dispersion maps showed excellent agreement with the analytical phase-matching condition. In contrast, symmetric reflection measurements uncovered a composite spectrum. Broad, blue-shifting fringes were observed, which fit well with a thin-film interference model using an effective refractive index. These fringes are superimposed with regular discontinuities. We analytically demonstrated that these features are Rayleigh anomalies (RAs), occurring when a diffraction order becomes grazing to the surface ($\theta_m = \pm 90^{\circ}$). This work successfully deconvolves the contributions of grating diffraction, thin-film interference, and Rayleigh anomalies in a single, accessible photonic system. By identifying the clear signature of each phenomenon, our multi-modal approach provides a complete optical characterization of colloidal monolayers on high-index substrates. This detailed understanding is crucial for the rational design of large-area photonic structures for applications in structural color coatings, low-cost metasurfaces, and optical sensing platforms.

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Does EG-water hydrophilic interaction drive enhanced cryoprotection at intermediate composition? A Terahertz spectroscopic study

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Terahertz (THz) spectroscopy is highly sensitive to collective intermolecular dynamics in hydrogen-bonded liquids and therefore provides a direct probe of solvation restructuring relevant to cryopreservation. Ethylene glycol (EG) is known to exhibit maximum cryoprotective efficiency at intermediate concentrations, yet the molecular origin of this optimum remains unclear. Here, we investigate aqueous EG mixtures across the full composition range using THz time-domain spectroscopy (THz-TDS). The THz absorption shows a strongly non-ideal concentration dependence, with the largest deviation from linear mixing occurring near X_{EG} ≈0.3, indicating maximal EG-water cross-interactions in this intermediate regime. This behaviour suggests strong suppression of cooperative hydrogen-bond (HB) network fluctuations and re-orientational dynamics of water, which are key processes preceding ice nucleation. At higher EG concentrations, the dielectric response progressively approaches an EG-dominated HB-framework. These results identify a spectroscopic signature of composition-selective solvation control and provide insight into why EG is an efficient cryoprotectant in the intermediate composition range.

Keywords: Terahertz; Intermolecular interactions; Cryopreservation; Light-Matter Interaction.

Influence of Dy doped $BiFeO_3$ nanoparticles as enhanced gas sensor: An excellent acetone sensor

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Dysprosium substitution in $BiFeO_3$ significantly modulates its structural, morphological, and gas-sensing properties, as investigated in the present study. $Bi_{1-x}Dy_xFeO_3$ (x = 0.00, 0.03, 0.05, 0.07, 0.09, and 0.11) compositions were successfully synthesized via a Sol–gel auto-combustion route. X-ray diffraction analysis confirms the rhombohedral R3c phase for pristine $BiFeO_3$, while Dy incorporation induces a gradual structural transition toward

an orthorhombic phase. Dy doping also leads to notable enhancement in acetone gas-sensing performance, accompanied by a reduction in the optimal operating temperature. Among the investigated compositions, $Bi_{0.93}Dy_{0.07}FeO_3$ exhibits superior sensitivity, selectivity, and rapid response–recovery characteristics, highlighting its potential as an efficient sensor material for high-quality acetone vapor detection.

Keywords: $BiFeO_3$, Dysprosium, Gas sensing, Acetone vapours.

Lengths and sequences of nucleic acids significantly impact on conformational conversion of prion protein: Insights from molecular dynamic simulations

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Prion diseases are a group of infectious fatal neurodegenerative diseases. The conformational conversion of a cellular prion protein (PrPC) into an abnormal misfolded isoform (PrPSc) is the key event in prion diseases pathology. Under normal conditions, the high-energy barrier separates PrPC from PrPSc isoform. However, pathogenic mutations, modifications as well as some cofactors, such as glycosaminoglycans, nucleic acids, and lipids, could modulate the conformational conversion process. Understanding the mechanism of conformational conversion of prion protein is essential for the biomedical research and the treatment of prion diseases. Particularly, the characterization of cofactors interacting with prion protein might provide new diagnostic and therapeutic strategies. PrP can bind to nucleic acids with relatively high affinity. Here, we Investigate distinct DNA lengths and sequences how lead to different aggregations and their impact on the biophysical properties of PrP. We have done long simulation of prion protein with different length and different GC content of DNA and RNA. We have observed that in presence of higher GC content and length of D67 (21mer DNA) prion protein aggregates more than the other length. In that particular length Prion protein alpha helix secondary structure converts into turn structure. This visualization of the complex provides insight into how oligonucleotides bind to PrP and opens new avenues to the design of compounds against prion diseases.

Keywords: Prion protein aggregation, Abnormal misfold, Conformational conversion.

Evaluation of dose dependent antioxidant activity of quercetin loaded chitosan nanoparticles with virgin coconut oil

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Quercetin is naturally occurring polyphenolic compounds having anti-cancer potential. However, its poor aqueous solubility and bioavailability limit its clinical use. Entrapment of hydrophobic drugs into hydrophilic nanoparticles such as chitosan presents a means to deliver drug to the target site. Quercetin loaded chitosan nanoparticles with virgin coconut oil (VCO) were synthesized by ionic gelation method. Nanoparticles were stabilized by oil virgin coconut

oil. The nanoparticles were characterized for particle size, physical state of drugs and entrapment efficiency. The size of nanoparticles was found to be 203 nm. The in vitro antioxidant activity of drug loaded chitosan nanoparticles was evaluated by DPPH, nitric oxide, lipid peroxide and ferric-reducing assay. The entrapment efficiency of quercetin was found to be 83%. SEM revealed the spherical nature quercetin loaded chitosan nanoparticles with VCO. Quercetin loaded chitosan nanoparticles with VCO showed dose dependent antioxidant activity. Higher concentration of nanoparticles showed significant antioxidant activity in comparison with blank chitosan nanoparticles. It is observed that the reducing sugars can react non-enzymatically with the amino groups of proteins to form reversible Schiff bases and then Amadori products. These initial glycation products undergo further complex reactions to become irreversibly cross-linked, heterogeneous, fluorescent derivatives termed Advanced glycation end products. Antiglycation activity of nanoparticles was evaluated by incubating glucose with bovine serum albumin (BSA). Nanoparticles effectively inhibited AGEs formation, it was confirmed by spectoflurometry and SDS-PAGE.
Keywords: Quercetin, Chitosan nanoparticle, Antioxidant, Antiglycation property.