3rd International Conference on

Recent Advancements in Material science and Nanotechnology

RAMAN-2026

NIRMA UNIVERSITY
INSTITUTE OF TECHNOLOGY
NAAC ACCREDITED 'A+' GRADE

ABSTRACT BOOK

Institute of Technology
NIRMA UNIVERSITY

About Conference

Building on the grand success of RAMAN-2020, 2022, and 2024, which attracted over 200 participants and led to indexed publications in Materials Today Proceedings (Elsevier) and the Journal Interactions (Springer Nature), the 3rd International Conference on Recent Advancements in Materials Science and Nanotechnology (RAMAN)-2026, will be held on January 30–31, 2026, at the Institute of Technology, Nirma University, Ahmedabad, Gujarat, India. The conference offers a premier platform for academicians, researchers, technocrats, and students to showcase cutting-edge research in Materials Science and Nanotechnology. With peer-reviewed presentations, keynote lectures by eminent scientists, and invited talks from global experts, RAMAN2026 aims to foster collaboration between academia and industry, driving innovation and advancing the frontiers of science and technology.

About Electronics and Communication Engineering

Department of Electronics and Communication Engineering is one of the major departments of the Institute of Technology since its inception. Its strength lies in the well-equipped laboratories, meritorious students and industrial connection. It focuses on providing the right mix of academic, technical, leadership and communication skill-set to help students transform into industry professionals.

About Faculty of Physics

The Faculty of Physics is a vibrant section engaged in theoretical and experimental condensed matter research, spanning ferrite and magnetic materials, and computational studies of 2D nanomaterials for NEMS, solar cells and sensors. holds two patents, has awarded eight PhDs, and currently guides six research scholars. also manages four funded projects from GUJCOST, GSBTM and UGC-DAE-CSR worth ₹90 L.

From the Desk of Dean

Dr. R. N. Patel

Faculty of Technology
Nirma University

Greeting to all the delegates of RAMAN 2026!

The 3rd International Conference on Recent Advancements in Materials Science and Nanotechnology (RAMAN-2026) aims to promote research-driven innovation in the rapidly evolving domains of materials science and nanotechnology. The conference provides an excellent platform for academicians, researchers, technologists, and students to interact, share knowledge, and exchange innovative ideas.

This conference is being organized at a highly opportune time, as the demand for advanced materials and nanotechnology-based solutions continues to grow across industries and research sectors. Such academic forums not only highlight emerging technological trends but also foster collaboration by enabling researchers to present their findings, validate results, and explore meaningful partnerships.

I congratulate the Department of Electronics and Communication Engineering for taking this commendable initiative in organizing an international conference on research areas of contemporary relevance. I also extend my sincere appreciation to all the committee members, contributors, reviewers, and volunteers for their dedicated efforts and support in making this event possible.

I wish RAMAN-2026 a grand success and hope that the conference proves to be intellectually stimulating, educative, and impactful in all respects.

Wishing the Conference a grand success and that it proves to be educative and effective in all respects.

From the Desk of Director

Dr. Himanshu Soni

School of Technology
Nirma University

Greetings to all the delegates of RAMAN-2026!

The 3rd International Conference on Recent Advancements in Materials Science and Nanotechnology (RAMAN-2026) aims to promote research-driven innovation in the rapidly evolving domains of materials science and nanotechnology. The conference provides an excellent platform for academicians, researchers, technologists, and students to interact, share knowledge, and exchange innovative ideas.

This conference is being organized at a highly opportune time, as the demand for advanced materials and nanotechnology-based solutions continues to grow across industries and research sectors. Such academic forums not only highlight emerging technological trends but also foster collaboration by enabling researchers to present their findings, validate results, and explore meaningful partnerships.

I congratulate the Department of Electronics and Communication Engineering for taking this commendable initiative in organizing an international conference on research areas of contemporary relevance. I also extend my sincere appreciation to all the committee members, contributors, reviewers, and volunteers for their dedicated efforts and support in making this event possible.

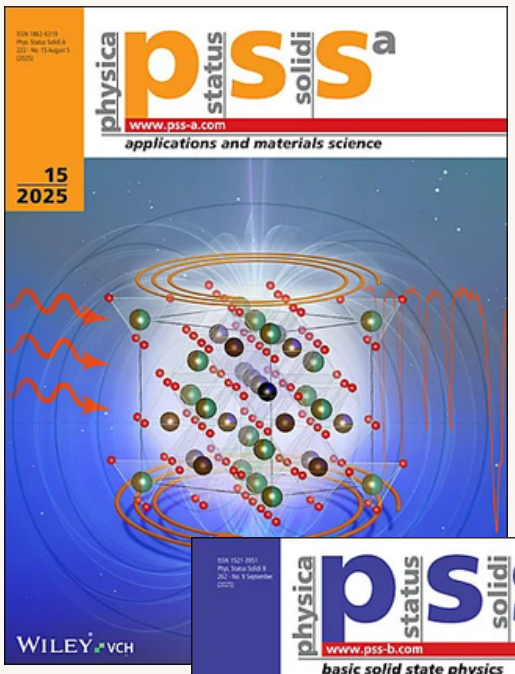
I wish RAMAN-2026 a grand success and hope that the conference proves to be intellectually stimulating, educative, and impactful in all respects.

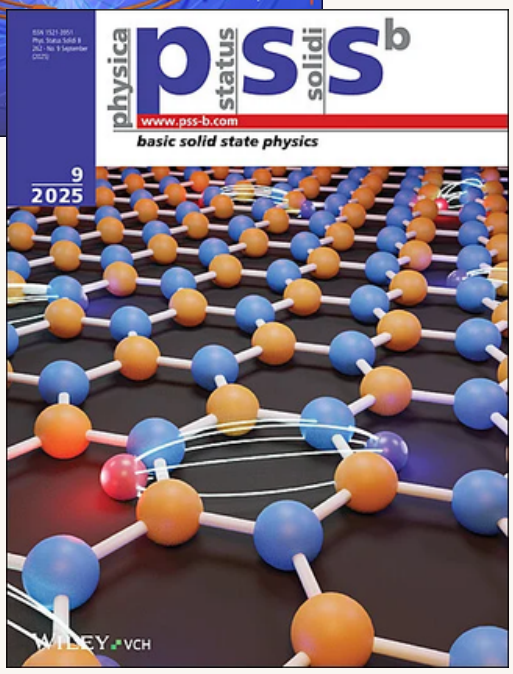
WILEY

CONFERENCE SPECIAL COLLECTION

3rd International Conference on Recent Advancements in Materials Science and Nanotechnology (RAMAN 2026)

Participating Journals





Scan the QR Code

Submission Form for RAMAN 2026 Special Collection (Wiley)

Guest Editors

Dr. Keyur Sangani
Dr. Chetna Chauhan
Dr. Ritesh Kumar Chourasia

January 30–31, 2026

Nirma University, Ahmedabad, India

Conference Organizing Committees

Core Organizing Committee

Convener

Dr. Ankur Pandya

Organizing Secretary

Dr. Tanuj Gupta

Co-Convener

Dr. Chetna Chauhan

Joint Organizing Secretary

Dr. Keyur Sangani

Local Organizing Team

Dr. R N Patel, Dean, FoTE

School of Technology

Dr. Himanshu Soni, Director

Dr. N P Gajjar, Head (EC Department)

Dr. N M Devashrayee, Professor

Dr. Harsh Vyas, Assistant Professor

Mr. Hemal Khatri, Assistant Professor

Mr. Gaurav Darji, Lab. Assistant

School of Engineering

Dr. Shibu Pillai, Assistant Professor

Dr. Neha Patni, Assistant Professor

Dr. Ankur Dwivedi, Assistant Professor

Advisory Board

Dr. Mohamed Ellouze, SFAX, (Tunisia)

Dr. Martin Desimone, Universidad de Beunos Aires, (Argentina)

Robert C. Pullar,Ca' Foscari Uni of Venice (Italy)

Dr. Sami Mahmood, University of Jordan, (Jordan)

Dr. Hasitha Mahabaduge, Georgia College and State University (USA)

Dr. Sundhindra Rayaprol, CSR, BARC, Mumbai (India)

Dr. Anurag Srivastava, IIITM, Gwalior (India)

Dr. Nandu Chaure, Pune University, Pune (India)

Dr. Prafulla K Jha, MSU Baroda, (India)

Dr. Rajshree B Jotania, Gujarat University, Ahmedabad (India)

Dr. Nikesh Shah, Saurashtra University, Rajkot (India)

Dr Brajesh Tiwari, IITRAM, Ahmedabad (India)

Dr. Ritesh Kumar Chourasia, LNMU, Darbhanga (India)

Invited Talk

Journal Trends & Editorial Insights on Scientific Publishing

Dr. Jayita Patwari

Deputy Editor, Physical Sciences, Wiley

Email: jpatwari@wiley.com

In today's rapidly evolving research landscape, understanding the academic publishing process is more important than ever for advancing careers, increasing research visibility, and contributing meaningfully to the global scientific dialogue. In this talk, I will try to shed some light on the often opaque "editorial black box" by unfolding the intricacies behind editorial decisions and the importance of understanding how to make your paper stand out in a competitive environment. This talk will highlight Wiley's Material Sciences and Physics portfolio, our ongoing award and recognition initiatives, and collaboration opportunities such as conference sponsorships and special collections. Attendees will gain insights into Wiley's editorial processes, including peer review, editorial checks, manuscript writing tips, and ethical guidelines, particularly regarding ethical AI use in publications. The presentation will also discuss India-specific submission and acceptance trends and invite feedback on Wiley journals and development plans. Additionally, the session will shed light on editorial career paths, with a special emphasis on Wiley's growing presence in India. This talk aims to provide a clearer understanding of the academic publishing landscape and practical strategies for enhancing research visibility and success.

Mechanical and Transport Properties of Ca-Based Binary Bulk Metallic Glasses: (Dental) Bone Grafting

N. K. Bhatt*[a]

[a] Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar – 364001, Gujarat

Corresponding author: [a]bhattnisarg@hotmail.com, nkb@mmkbhavuni.edu.in

ABSTRACT

Atomic mass transport in Ca-based bulk metallic glasses (BMGs) plays a decisive role in governing their thermodynamic and mechanical response in view to their dental bone grafting application. In this study, interdiffusion behavior in binary Mg_2Ca, Al_2Ca, and Al_4Ca BMGs is analyzed using MD simulations in conjunction with the non-equilibrium thermodynamic Darken–Manning framework. Composition-dependent interdiffusion coefficients reveal pronounced deviations from ideal Darken behavior, arising from strong chemical short-range order and correlated atomic motion inherent to the glassy phase. The Manning correction factor is found to be significant, indicating non-random atomic jumps and enhanced collective diffusion mechanisms. Diffusion is dominated by non-phononic modes and localized rearrangements. These diffusion characteristics directly correlate with enhanced mechanical stability and thermophysical performance of Ca-based BMGs. The present analysis establishes DM theory as an effective framework for interpreting diffusion in Ca-based BMGs and provides fundamental insights into the coupling between atomic transport and glassy structure, where Stochastic forces ignite the diffusion process in the glassy state. The free-volume theory-based analysis proposes that in the glass-phase, holes behave as vacancies where migration is controlled by the nature of interatomic forces, while for the liquid-phase holes are fluctuating cavities with very short life-time.

Illuminating Structure and Function: Neutron Diffraction and Scattering Techniques in Advanced Materials Research and Industrial Applications

Sudhindra Rayaprol

UGC-DAE Consortium for Scientific Research Mumbai Centre, CFB, BARC Campus, Trombay, Mumbai - 400085, INDIA

Email: sudhindra@csr.res.in; rayaprol@gmail.com

Neutron diffraction and allied scattering techniques have emerged as indispensable tools for unraveling the structural, magnetic, and dynamic properties of materials across diverse domains. Unlike conventional probes, neutrons offer unique advantages: deep penetration, sensitivity to light elements, and direct coupling to magnetic moments. These attributes enable comprehensive insights into crystalline order, local distortions, and magnetic ground states, complementing synchrotron X-ray and electron-based methods.

This talk will highlight recent advances in applying neutron diffraction and scattering to multi-functional materials, including high-entropy oxides, double perovskites, and energy-relevant compounds. Case studies will demonstrate how academic research leverages these techniques to design and understand emergent phenomena, while industrial applications exploit them for alloy development, residual stress mapping, and quality assurance in engineering components.

By integrating examples from collaborative experiments at international neutron sources with modeling approaches such as pair distribution function analysis and relaxation dynamics, the presentation will emphasize the synergy between fundamental science and technological innovation. The discussion will also address challenges in accessibility, data interpretation, and the growing role of computational tools in maximizing the impact of scattering techniques.

Ultimately, neutron diffraction and scattering provide a bridge between academic curiosity and industrial necessity, offering a powerful lens to engineer the next generation of functional materials.

Ultra-light-weight sustainable carbon-based microwave absorbing / shielding material made from sustainable pyrolysed cork wastes

Robert C. Pullar [1*], Rui M. Novais [2], Ana. P. F. Caetano [2], Kuzhichalil P. Surendran [3]

[1] Department of Molecular Sciences and Nanosystems (DSMN), Ca' Foscari University of Venice, 30172 Venezia Mestre, Italy

[2] Department of Engineering of Materials and Ceramics / CICECO – Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, 3810–193 Aveiro, Portugal

[3] Materials Science and Technology Division, CSIR-NIIST, Industrial Estate, Trivandrum 695019, India

[*]*Corresponding author: robertcarlyle.pullar@unive.it*

ABSTRACT

Carbon is well-known to be an effective microwave absorber, suitable for EMI shielding and radar-absorbing materials (RAM) for stealth technologies, from the high MHz to millimetre wave frequencies. However, it is usually produced from environmentally unsustainable precursors in the form of a nanomaterial (nanopowders, CNTs, graphene) or carbon fibre, with expensive processing and often used as a composite with other materials. Cork is a renewable and sustainable material extracted from the outer bark of the cork oak tree, and it is a fully sustainable / renewable resource. The bark is harvested every 10 years, without harming the tree, which continues to live on as a carbon sink, with a productive lifetime of >200 years. Cork is highly porous and lightweight in nature, due to its microstructure of honeycomb-like ~20 mm hexagonal cells with 1 mm thick cell walls. This makes it an exceptional thermal, acoustic and vibrational insulator. Cork powder is the main cork industry waste from fabrication, producing over 50,000 t / year of this low economic value waste and, hence, its valorisation would be of great benefit. Here we present the capabilities of pyrolysed cork wastes (cork-carbon) as an economic and sustainable microwave absorber over the X-band (8-12 GHz), used without a binder or other additives. Furthermore, it has an exceptionally low density (0.03 g/cm^3) comparable to aerogels, which gives it the lowest ever reported specific shielding effectiveness (SEE) of up to 1200 dB cm^3 g^{-1} over the entire X-band range, depending on thickness. The high SSE is also partly due to multiple reflections of the EM wave per unit volume within the ultra-porous cork microstructure. It has also been shown that the pyrolysed cork-carbon is thermally stable up to 400 ºC, making it an excellent ultra-light-weight microwave / EMI shielding material.

Impedance Spectroscopy for Next-Generation Photovoltaics

Ritesh Kumar Chourasia*

Post-Graduate Department of Physics, Samastipur College, Samastipur-848134, (A constituent unit of L.N.M.U., Darbahnga-8460004), Bihar, India

Corresponding Author: riteshphyzics@gmail.com; dr.riteshchaurasia@gmail.com

ABSTRACT

Impedance spectroscopy has long been a powerful tool for investigating electrochemical systems and solid-state devices. In recent years, it has become increasingly important for studying emerging photovoltaic technologies, where unusual material properties and complex device architectures introduce new experimental and interpretational challenges. In this invited talk at RAMAN-2026, I will provide a practical introduction to impedance spectroscopy for researchers working on modern photovoltaic devices and related fields. I will begin by outlining key guidelines for performing reliable measurements and for avoiding common experimental artifacts. I will then briefly review the essential mathematical framework and introduce the circuit elements most relevant for photovoltaic systems. Next, I will discuss strategies for collecting high-quality impedance spectra and highlight frequent sources of misinterpretation. Finally, I will survey widely used analysis approaches, including equivalent circuit modelling, capacitance–frequency analysis, and mobility extraction methods, emphasizing their underlying assumptions, advantages, and limitations. By combining practical advice with physical interpretation, this talk aims to help researchers use impedance spectroscopy more effectively to extract meaningful insights from next-generation photovoltaic devices.

Solid-state supercapacitors based on fast ionic ceramics

Anshuman Dalvi

Department of Physics, Birla Institute of Technology and Science, Pilani (RJ) India-333031
[*]Corresponding author: [a]adalvi@pilani.bits-pilani.ac.in

ABSTRACT

Batteries and supercapacitors are two widely used energy storage devices. Batteries offer high energy density, whereas supercapacitors deliver high power density. Therefore, supercapacitors are used in applications requiring rapid charge-discharge cycling, e.g., in electric vehicles. There has been considerable attention to developing supercapacitors with a 'solid-state electrolyte.' This is because the use of liquids or gels limits mechanical and thermal stability and device flexibility. Fast-ionic ceramics have been explored for solid-state batteries; therefore, for a hybrid device, it is inevitable to develop supercapacitors using fast-ionic ceramics. We have been consistently working on this new generation of liquid-free, solid-state supercapacitors (SSCs) for more than a decade. Using composites of NASICON, Garnet and perovskite-structured Li^+/Na^+ ion conductors combined with ionic liquids or solid polymer electrolytes, our group has developed various fast-ionic hybrid composites for electrolytic applications in these ceramic ASSCs. Using these composite electrolytes, we have assembled supercapacitors using (i) high-surface-area activated carbon and (ii) carbon aerogels. These SSCs demonstrate excellent thermal stability, long cycling, low ESR, and are useful for high-power applications. The interface was modified successfully using a microgel layer approach. Their performance parameters are comparable to those of the liquid electrolyte-based supercapacitors. Fundamentals and recent exciting results relevant to the topic will be presented.

Electronic Structure and Chemical State Determination in Oxides through X-ray & Ultraviolet Photoelectron Spectroscopy

Amish G. Joshi

CSIR-Central Glass & Ceramic Research Institute, Naroda Centre, 168-169 GIDC Industrial Estate, Naroda, Ahmedabad – 382 330

Email: amish.cgcri@csir.res.in

ABSTRACT

Oxide materials exhibit diverse electronic and chemical functionalities that arise from mixed valence cations, defect chemistry and strong coupling between lattice, charge and spin degrees of freedom. In this talk, I will present a detailed overview of how X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS) can be employed for electronic structure and chemical state determination in complex oxide systems. Emphasis is placed on methodologies for extracting quantitative and semi-quantitative information including elemental composition, oxidation state, valence charge transfer, work function and valence band density of states. Core-level peak deconvolution, atomic sensitivity factor-based quantification and 3s exchange splitting are discussed as essential tools for valence estimation in transition-metal oxides. UPS measurements are shown to reveal the Fermi level position, band tails and contributions from O 2p and transition-metal 3d states. A series of case studies involving electrochromic WO_3 films, Prussian Blue analogues, ZnO–graphene composites, (R-Go) reduced graphene oxide and mixed-valence manganites demonstrate how intercalation, reduction and thermal processing alter electronic structure and induce functional responses. The talk emphasizes methodological aspects of valence quantification and highlights the relevance of surface-sensitive spectroscopy in correlating oxide chemistry with functional properties.

INDEX

INDEX

INDEX

INDEX

INDEX

INDEX

Magnetothermoelectric correlation of $Ca_{2-x}Pr_xMnTiO_6$ (x=0.0, 0.25, 0.5, 0.75, 1.0)

Smita Borole*, Nilofar Kurawale, Rohan Kamble and Sudhindra Rayaprol
UGC-DAE Consortium for Scientific Research Mumbai Centre, BARC Campus, Mumbai 400085
Savitribai Phule Pune University, Ganeshkhind, Pune - 411007
*Corresponding Author Email: smita.borole1996@gmail.com

ABSTRACT

Double perovskites are emerging materials with fascinating physical properties, attracting growing interest from both experimentalists and theoreticians. Given that over 60% of primary energy is lost as waste heat, their potential for thermoelectric and spintronic applications has driven extensive research in recent years [1]. The double perovskite oxide system $Ca_{2-x}Pr_xMnTiO_6$ ($0 \leq x \leq 1.0$) has been investigated to explore the correlation between its magnetic behavior and thermoelectric response, particularly the Seebeck coefficient. Structural analysis confirms that all compositions crystallize in an orthorhombic structure, with Pr substitution inducing subtle lattice distortions that influence electronic transport and magnetic ordering. Magnetic measurements reveal a transition from complex magnetic interactions in Ca_2MnTiO_6, characterized by spin frustration and negative magnetization, to antiferromagnetic ordering with increasing Pr concentration. The Néel temperature (T_n) is found to increase systematically with Pr content, indicating enhanced magnetic exchange interactions. The Seebeck coefficient (S) exhibits negative values throughout, suggesting dominant electron type conduction, and its magnitude shows a strong dependence on temperature and magnetic ordering. The observed correlation between the magnetic transitions and anomalies in the Seebeck coefficient highlights the role of spin–charge coupling and carrier scattering mechanisms in governing thermoelectric performance. These findings demonstrate that controlled magnetic tuning through rare-earth substitution can effectively modulate thermoelectric properties, offering new insights into the design of magneto-thermoelectric materials based on double perovskite oxides.

Keywords: Double perovskite oxides, Thermoelectric materials, Mixed valent system.

References:

[1] Tohru SUGAHARA et.al, Thermoelectric Properties of Double Perovskite Oxide $Sr_{2-x}M_xFeMoO_6$ J. Ceram. Soc. Jpn **116**. (2008), 172328.
[2] Prachi Mohanty, et.al, Room temperature ferrimagnetism, magnetodielectric and exchange bias effect in Phys. Rev. Mater. **2023**, 7, 084408.

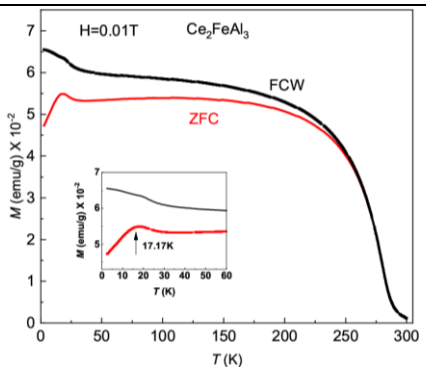
Experimental Investigations for Magnetic Properties of Ce_2FeAl_3: Dependence on Structure

Nilofar Kurawle[a,b*], Smita Borole[a,b], Sudhindra Rayaprol[a,b]
UGC-DAE Consortium for Scientific Research-Mumbai Centre, Mumbai 400085, India.
Savitribai Phule Pune University, Ganeshkhind, Pune - 452001
*Corresponding author: kurawle31@gmail.com

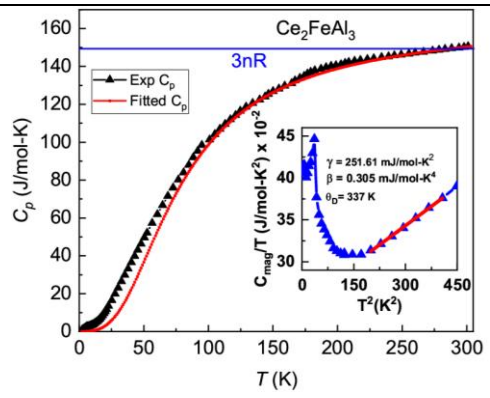
ABSTRACT

The Ce–Fe–Al intermetallic compounds are expected to exhibit fascinating properties due to strong 4*f*–3*d* electron correlations and magnetic ordering since both Ce and Fe are magnetic ions. Magnetization *M(T)* measurements of Ce_2FeAl_3 show a magnetic transition near 280 K, indicating long-range magnetic ordering with an additional transition taking place around 17 K. The magnetic irreversibility is observed in this compound below ~ 250 K. Magnetization, *M*(*H*), at various temperatures show spontaneous moment for initial fields which then increases almost linearly with increasing field showing no signatures of saturation. Specific heat measurements show a weak feature below ~ 20 K and no observable feature at high temperatures. The interesting observations made in the magnetism of this compound is that the magnetic ordering around 250 K, could be a short-range order or due to cluster dynamics. Analysis of specific heat (C_p) measurements show that, γ, the electronic contribution is ~ 250 mJ/mol K^2, which is in the range of heavy-fermion systems. Therefore, it can be summarized that Ce_2FeAl_3 exhibits complex magnetism with exotic features of heavy fermion, Kondo behavior and magnetic frustration. Results of the physical property studies will be presented and discussed in the light of influence of structural symmetry.

Keywords: Magnetization, Heat Capacity, Structure, Magnetic frustration, Intermetallics



Temperature dependence of magnetization M(T) measured in an applied magnetic field of H = 0.01 T (ZFC) and (FCW) conditions.



Heat capacity as a function of temperature in zero field. Inset shows low T fit for Cp/T vs T^2 graph.

References:

[1] Nair H S, Ghosh S K, Kumar R K, Strydom A M J. Phys. Chem. Solids **2016** 91 69.

[2] Nilofar Kurawle, Soumen Samanta, Shovit Bhattacharya, Sudhindra Rayaprol1, J. Phys.: Condens. Matter, **2025**, 37, 025606 (10pp).

Device-Level Physics-Based Multi-Objective Genetic Algorithm Optimization of PV–Wind–Biomass Hybrid Energy System

Shebaz A Memon*[a], Danish Siddiqui [a], Darshit S Upadhyay [a], Rajesh N Patel [a]
[a] Department of Mechanical Engineering, Nirma University, Ahmedabad -382481, India
*Corresponding author: shebaz.memon208@yahoo.com, shebaz.memon@nirmauni.ac.in

ABSTRACT

This study presents a device-level, physics-based multi-objective optimization framework for a PV–Wind–Biomass Hybrid Energy System designed for a semi-urban region in western India. Material- and device-dependent performance models for photovoltaic modules, wind turbine aerodynamics and biomass gasification kinetics are directly embedded into a Multi-Objective Genetic Algorithm-based optimization routine to determine the optimal sizing of the three renewable subsystems. The objectives are to minimize the Levelized Cost of Energy and to maximize the Human Development Index, thereby coupling techno-economic performance with socio-developmental impact. The algorithm explores device-interaction dynamics under hourly solar irradiance, wind-velocity and biomass-availability profiles, while enforcing a selective dispatch strategy where the biomass gasifier operates only when solar and wind generation are insufficient. The optimized configuration demonstrates significant improvements in cost effectiveness, renewable penetration and social benefit, achieving a balanced trade-off that reflects the physical behaviour of each energy-conversion device. The results highlight how material efficiencies, conversion characteristics and capacity factors influence hybrid system performance and show that incorporating device-level physics provides clearer insight into the operational synergy of multi-resource systems. This framework offers a scientifically grounded approach for designing advanced hybrid renewable systems with enhanced economic and societal value.

Keywords: renewable energy-conversion devices, evolutionary multi-objective methods, socio-techno-economic assessment, optimization trade-off analysis

Graphene-Supported Ag_4 Clusters for CH_4 Dissociation: A DFT Study

Niyati Gajjar[a,*], Sanjeev K. Gupta[b], P. N. Gajjar[a, **]
[a]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380 009, India;
[b]Computational Materials and Nanoscience Group, Department of Physics, St. Xavier's College, Ahmedabad 380 009, India
[*]Corresponding author: [*]nbgajjar9698@gmail.com, [**]pngajjar@gujaratuniversity.ac.in

ABSTRACT

In our study, based on density functional theory (DFT), we have investigated Ag_4 cluster decorated on a graphene sheet to explore their CH_4 dissociation. The study examines the structural stability and electronic characteristics of Ag_4 cluster. After confirming the stability of these clusters, they were decorated on a graphene layer, followed by an investigation of the CH_4 dissociation mechanism. The adsorption characteristics and energetics of CH_4, its intermediates (CH_X, X = 0-3), and hydrogen atoms were analyzed to understand the underlying reaction mechanism. Both adsorption and co-adsorption behaviors were explored. he transition states corresponding to each elementary C-H bond cleavage were determined using the Climbing Image Nudged Elastic Band (CI-NEB) method. Transition state calculations reveal that the dissociation of CH_4 into CH_3 and H exhibits a lower energy barrier, indicating that Ag_4 decorated graphene are promising candidates for CH_4 dissociation applications.

Ab initio Study of HfS_2 Monolayer as a Gas Sensor for CO, H_2S, and NH_3 Gases

[*]Pratik H. Mesvaniya[1], Sanjeev K. Gupta[2], P. N. Gajjar[1, **]
[1]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380 009, India;
[2]Computational Materials and Nanoscience Group, Department of Physics, St. Xavier's College, Ahmedabad 380 009, India
[*]Corresponding author: [*]pratikhm9@gmail.com, [**]pngajjar@gujaratuniversity.ac.in

ABSTRACT

In this era of industrialisation and pollution, it is essential to have sensors capable of detecting toxic and pollutant gases. In this study, density functional theory was employed to explore HfS_2 monolayer as a gas sensor for CO, H_2S and NH_3 gases. The structure of HfS_2 monolayer is confirmed to be both thermodynamically and dynamically stable using calculated cohesive energy and phonon dispersion curve with no imaginary frequencies. This monolayer is a semiconductor with indirect bandgap of 1.07 eV. The adsorption energies for CO, H_2S and NH_3 after adsorption onto the monolayer are -0.29 eV, -0.32 eV and -0.29 eV, respectively with corresponding recovery times of 83.84 ns, 220.64 ns and 79.49 ns, respectively. The optical bandgap of monolayer shifted after the adsorption of each gas. There are notable shifts in absorption coefficient spectra after adsorption of gases. Overall the results of the study suggest that HfS_2 monolayer is a promising reversible gas sensor for CO, H_2S and NH_3 gases. Moreover, this work fulfils Sustainable Development Goal 3 and 13.

Keywords: Density functional theory, Two-Dimensional monolayers, Gas sensor, SDG 3, SDG 13

Transition from Paramagnetic Behavior to Weak Ferromagnetic Ordering in Fe-Doped GeTe Bulk Alloy

Nileshkumar Parmar[1], and Mitesh Sarkar[1,*]
[1]Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India – 390002
*Corresponding author: miteshsarkar_msu@yahoo.com

ABSTRACT

Although pure GeTe is non-magnetic, doping it with magnetic ions such as Fe can induce ferromagnetism and improve its magnetic properties, making Fe-doped GeTe a promising material for spintronic applications. In this study, dilute quantity of Fe (0.05) doped GeTe bulk alloy was synthesized using a vacuum-sealed melting technique and the sample was systematically characterized to understand their structural and magnetic behavior. X-ray diffraction (XRD) confirmed a mixed crystal structure consisting of rhombohedral and orthorhombic phases of GeTe. Raman spectroscopy showed two main peaks at 116.32 cm^{-1} and 140.59 cm^{-1}, with the latter attributed to Te–Te vibrational modes [1]. Temperature-dependent magnetic measurements showed that the material behaves paramagnetic below 250 K and above 250 K there is a slight increase in the magnetization value. This indicates a ferromagnetic behavior above this temperature. Magnetization curves at 50 K, 150 K, and 300 K displayed paramagnetic characteristics, with reduced magnetic moment alignment as temperature increased. These findings indicate that Fe doping introduces a temperature-dependent magnetic ordering transition in GeTe, demonstrating the strong effect of Fe on its magnetic properties. Overall, the results will provide useful insights into the thermally sensitive magnetism of Fe-doped GeTe and support its potential use in thermomagnetic and spintronic device applications [2].

Keywords: Alloy, Magnetization

References:

[1] Tuning of structural, band gap and optical properties through Sb substitution in Fe doped GeTe bulk alloys, Nilesh Parmar, Sitara Menon and Mitesh Sarkar, Materials Today: Proceedings, (2023). https://doi.org/10.1016/j.matpr.2023.02.014

[2] Half-metallicity and magnetism of GeTe doped with transition metals V, Cr, and Mn: A theoretical study from the viewpoint of application in spintronics, Y. Liu, S. K. Bose and J. Kudrnovsky, Journal of Applied Physics, 112, 053902 (2012). https://doi.org/10.1063/1.4750031

Solid-State Microstructural and Thermal Analysis of Cassava–PVA–Fiber Biofoam as a Sustainable Polymer Composite

Nimish Shah, Yagnik Kundaria, Dev Baraiya, Mamta Saiyad
Chemical Engineering Department, Institute of Technology, Nirma University, Ahmedabad
*Corresponding author: nimish.shah@nirmauni.ac.in

ABSTRACT

Biodegradable polymer composites have emerged as promising alternatives to expanded polystyrene (EPS), which persists in the environment due to its hydrophobicity, high crystallinity, and thermal stability. This study presents the fabrication and solid-state analysis of a sustainable biofoam derived from cassava starch, polyvinyl alcohol (PVA), sorbitol, and lignocellulosic fibers using a thermo-pressing route. The cassava–PVA matrix forms a semicrystalline polymer network, while sorbitol acts as a plasticizer enhancing chain mobility, and natural fibers provide reinforcement and porosity control. The foam was prepared at 100 °C followed by ambient aging, enabling moisture removal, pore stabilization, and partial recrystallization within the polymeric structure.Solid-state characterization focuses on crystallinity evolution, hydrogen-bonding interactions, pore architecture, and thermal transitions relevant to packaging and insulation applications. The composite is expected to exhibit reduced crystallinity relative to native starch due to PVA incorporation, with enhanced microstructural stability contributed by polymer–fiber interactions. Thermal analysis reveals multi-stage degradation typical of biopolymers, while the porous morphology facilitates low density and cushioning behavior. Biodegradation observations further indicate favorable environmental performance.Overall, the cassava-based biofoam demonstrates a balance of microstructural, mechanical, and thermal properties, supporting its potential as a biodegradable replacement for conventional thermocol in sustainable materials applications.

Keywords: Biopolymer composite, Cassava starch, Crystallinity, Porous polymer foam, PVA, Solid-state characterization, Thermal analysis.

Defect-Mediated Magnetic and Dielectric Modulation led Magneto-Dielectric Response in Pb^{2+} Substituted $PrFeO_3$ Antiferromagnetic Nano-ceramics

Jasvinder Singh[a], Shaili Rani[a], Sunil Kumar[b*], Sunil Kumar Dwivedi[a]
[a]Department of Physics, School of Applied Sciences, Om sterling Global University, Hisar, Haryana
[b]Department of Applied Sciences & Humanities, Sardar Beant Singh State University, Gurdaspur, Punjab
*Corresponding Author email: sunil_nano@yahoo.com

ABSTRACT

Investigation of oxygen vacancy modulated magnetic and dielectric characteristics led by coupling between them has been reported in this paper. Pb^{2+} tailored $PrFeO_3$ antiferromagnetic insulator ($Pb_xPr_{1-x}FeO_3$, where $x = 0.1$, 0.2 & 0.3) solid solutions have been reported for magneto-dielectric coupling. Orthorhombic crystal phase signature for successful synthesis of $Pb_xPr_{1-x}FeO_3$ magneto-dielectric ceramic synthesized via solid state reaction method. Microstructural analysis led by grain size calculation as well grain growth estimated from porosity has been carried out from scanning electron microscopy whereas elements as per according to stoichiometric formula confirmed from XPS spectroscopy. Structural modifications led formation of additional oxygen vacancies which alter Fe–O–Fe superexchange pathways resulting in strengthened spin canting and improved weak ferromagnetism. Magnetic enhancement has been studied from magnetic hysteresis recorded by Vibrating Sample Magnetometer and S-shaped curve between magnetization vs. Magnetic field shows magnetic ordering in prepared magneto-dielectric solid solutions. The existence of multivalence state of Fe (Fe^{2+} & Fe^{3+}) due to increase in concentration of oxygen vacancies led by Pb^{2+} substitution at Pr^{3+} at A-site in PrFeO3 has been confirmed from XPS spectral data. Dielectric analysis showed improved dielectric polarization, increased permittivity, and reduced dielectric loss due to vacancy-induced polaronic hopping and space-charge contributions. Notably, the Pb-substituted samples exhibited a pronounced magneto-dielectric effect, arising from the strong coupling between magnetic ordering and defect-mediated dielectric relaxation. These findings demonstrate that controlled Pb^{2+} substitution is an effective route to tailor the multifunctional magnetic and magneto-dielectric properties of $PrFeO_3$, making the material a promising candidate for spintronic, magneto-electric, and multifunctional device applications.

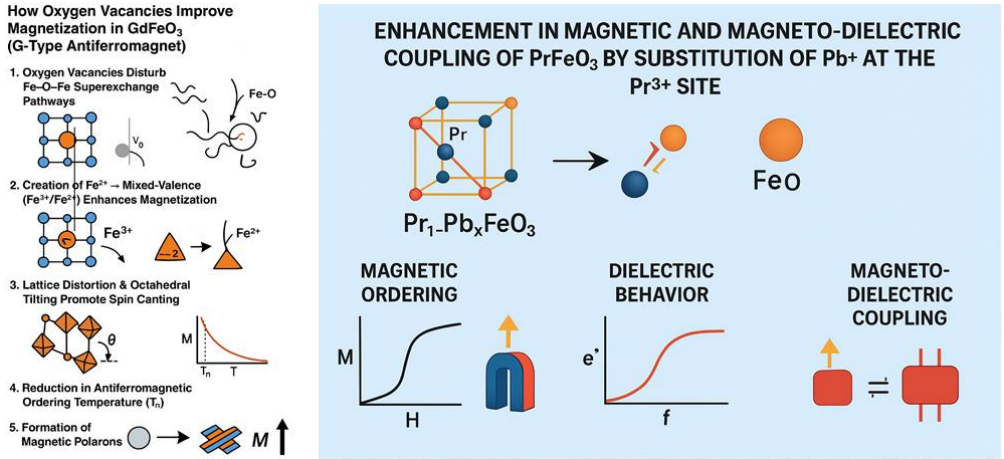


Figure: Graphical abstract shows enhancement in magnetic order due to oxygen vacancies created due to Charge Imbalance and Magneto-Dielectric Coupling

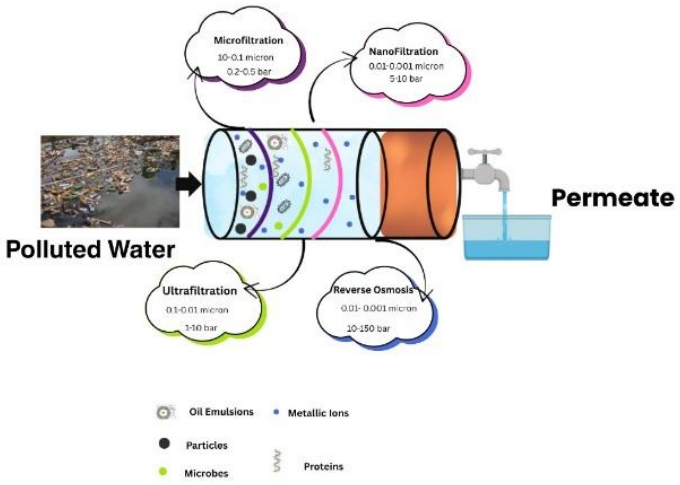
POLYMERIC NANOCOMPOSITE MEMBRANE FOR WASTEWATER TREATMENT

Manan Nahta, Prachi Modi, Nikita P. Chokshi, Nikita P. Chokshi
Chemical Engineering Department, Institute of Technology, Nirma University, Ahmedabad, Gujarat
*Corresponding author: nikita.chokshi@nirmauni.ac.in

ABSTRACT

Water scarcity and aquatic pollution from industrial and household wastewater discharge pose critical global challenges, creating a need of advanced purification solutions. While membrane filtration is highly effective in contaminant separation, conventional polymeric membranes are often limited by inherent downsides such as hydrophobicity, fouling and insufficient mechanical strength. Polymeric nanocomposite membranes (PNCMs), formed by adding various nano-entities (nanofillers) into the polymer matrix, represent a sustainable, promising and energy-efficient approach to overcome these limitations. This review examines the recent progress in PNCM technology for wastewater purification, mentioning preparation methods such as phase inversion and interfacial polymerisation. Key nanofillers discussed include carbon-based nanoparticles (like graphene oxide and carbon nanotubes) and various metal/metal oxide nanoparticles (e.g., TiO_2, Ag, ZnO). The strategic inclusion of these nanofillers enhances membrane properties, notably improving hydrophilicity, mechanical strength, water flux, selectivity, and anti-biofouling performance. PNCMs demonstrate exceptional efficacy in removing a wide spectrum of pollutants, specifically focusing on industrial dyes, organic micropollutants, and toxic heavy metal ions like Cr(VI) and Pb(II). We analyse the governing separation mechanisms and critical issues, outlining future research imperatives required for full-scale industrial implementation of these high-performance materials.

Keywords: Polymeric Nanocomposite Membranes; Wastewater Treatment; Nanofillers; Antifouling; Thin-Film Nanocomposite.



Performance of Hemp-derived Interconnected Carbon NanoSheets on Counter Electrode in DSSCs

Garima Dwivedi[a], Guncha Munjal[a], Amita Chaudhary [b, *] Ashok N. Bhaskarwar1[a]
[a]Department of Chemical Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, INDIA
[b]Department of Chemical Engineering, Nirma University, Ahmedabad, INDIA
*Corresponding Author: amita.chaudhary@nirmauni.ac.in

ABSTRACT

An alternative to the conventional platinum (Pt) counter electrode catalyst in dye-sensitized solar cells (DSSCs) has been developed by synthesizing interconnected carbon nanosheets (ICNS) derived from hemp, a common weed plant. The detailed synthesis process of ICNS is presented, with structural and morphological analysis conducted using SEM, XRD, and Raman spectroscopy to confirm the formation of the conductive carbon network. Electrochemical performance of the ICNS as the counter electrode was evaluated through electrochemical impedance spectroscopy (EIS) and cyclic voltammetry, benchmarked against Pt electrodes. Pure ICNS electrodes on fluorine-doped tin oxide (FTO) substrates showed a solar-to-electric conversion efficiency of 4.01%, significantly lower than 12.3% efficiency achieved by Pt electrodes. Incorporating Pt into ICNS at different weight ratios (12, 16, and 18 w/w%) progressively enhanced efficiency to 5.49%, 5.74%, and 6.56% respectively, attributed primarily to increases in fill factor as corroborated by J-V characteristics. Further studies emphasize the influence of counter electrode coating thickness and contact angle on performance, with non-ionic surfactants facilitating uniform film formation on FTO. This ICNS-Pt composite system demonstrates a cost-effective and environmentally friendly counter electrode alternative for DSSCs, providing a promising route to reduce Pt reliance while maintaining reasonable device efficiency.

Keywords: Dye-sensitized solar cells (DSSCs); Platinum counter electrode; Interconnected carbon nanosheets (ICNS); Hemp-derived carbon; Power conversion efficiency

References:

[1] Wu, J., et al. (2017). "Counter electrodes in dye-sensitized solar cells." Chemical Society Reviews, 46(19), 5974-6023. DOI:10.1039/C6CS00752J

[2] Ahmed, U., et al. (2018). "A comprehensive review on counter electrodes for dye sensitized solar cells." Solar Energy, 174, 1091-1115. DOI:10.1016/j.solener.2018.09.001

Integrating Band-Gap Engineering and Magnetocaloric Response in Armchair 2D Materials

Riddhi Moteria [a*], Vatsal Dagli [a], Ankur Pandya [a], Keyur Sangani [a], Prafulla K. Jha [b]
[a] Institute of Technology, Nirma University, Ahmedabad, 382481, India
[b] Department of Physics, Faculty of Science, The M.S. University of Baroda, Vadodara, 390002, India
[a*]Corresponding author: 23bec162@nirmauni.ac.in

ABSTRACT

This study examines the evolution of electronic, mechanical, and relativistic magnetothermal behavior in armchair nanoribbons of graphene and attempts to further correlate the analysis to similar two-dimensional materials such as silicene, germanene, stanene, and phosphorene. This work draws on established insights on dimer-dependent electronic and mechanical variations from tight-binding modeling, Fermi-velocity-based dispersion, and electron-phonon interaction approaches with the electrically adjustable bond-strength concepts of BOLS theory [1]. It additionally uses the magneto-thermal framework for relativistic two-dimensional systems, providing a unified, flexible approach that connects confinement-driven electronic behavior, mechano-electronic coupling, and oscillatory magnetocaloric response [2]. In conclusion, we evaluated the correlation and dependency of the attributes by revising the governing equations using common variables while maintaining coherence across materials. The main improvement is the recognition of carrier density as a universal control parameter that concurrently regulates electronic transitions, magnetocaloric operating temperature, and the magnetic field needed for thermal inversion. The findings of the current study indicate that electrical gating can simultaneously adjust several features, allowing atomically thin nanoribbons to serve as mechanically stable, electrically versatile, and thermally sensitive platforms. This broad viewpoint offers a design framework for adaptable sensors, electrically modifiable thermal modulators, and intermediate-temperature cooling apparatus via two-dimensional nanoribbons.

Keywords: 2D Nanoribbons, Magnetocaloric Effect, Band-Gap Engineering, Mechano-Electronic Coupling, Carrier-Density Tunability

References:

[1] Pandya, A., Sangani, K., & Jha, P. K., Band gap determination of graphene, h-boron nitride, phosphorene, silicene, stanene, and germanene nanoribbons, Journal of Physics D: Applied Physics, 53 (2020) 415103.

[2] Reis, M. S., Oscillating magnetocaloric effect on graphenes, Applied Physics Letters, 101 (2012)

Relative Energetic Stability of Functionalized MXenes from High-Throughput First-Principles Data Using Uncertainty-Aware Ensemble Machine Learning

Veer Shah[a], Karan Mungra[a], Shebaz A Memon*[a]
[a]Institute of Technology, Nirma University, Ahmedabad- 382481, India
*Corresponding author: shebaz.memon@nirmauni.ac.in; shebaz.memon208@gmail.com

ABSTRACT

MXenes are two-dimensional transition-metal carbides and nitrides whose experimental feasibility is governed by energetic stability. Relative energy with respect to the lowest-energy structure within a compositional family provides a direct measure of thermodynamic favorability. However, systematic evaluation of this quantity using density functional theory becomes computationally demanding when large numbers of MXene structures are involved. In this work, a machine-learning-based framework is developed to predict the relative energetic stability of functionalized MXenes using a high-throughput first-principles dataset comprising more than 4000 structures. Compositional, structural, and electronic descriptors are employed to train and evaluate multiple regression models. Tree-based ensemble models demonstrate superior accuracy, highlighting the strongly nonlinear nature of MXene stability relationships. Feature-importance analysis indicates that lattice parameters and transition-metal identity play a dominant role in governing relative energetic stability. To further improve predictive reliability, ensemble strategies based on model stacking and inverse-variance weighting are implemented. The uncertainty-weighted ensemble achieves the best overall performance, with a coefficient of determination of 0.961 on the independent test set. The proposed framework enables rapid and physically interpretable screening of energetically viable MXenes.

Keywords: MXene materials, uncertainty quantification, materials informatics, stability descriptors, data-driven materials design

Performance, Emissions, and Durability Assessment of Ethanol-Blended Flex Fuels with Emphasis on India's Transition to E20

Maunil Modi[a], Darshit S. Upadhyay[a*]
[a] Department of Mechanical Engineering, Nirma University, Ahmedabad, India
* Corresponding Author: Darshit S. Upadhyay[a*]: darshit.upadhyay@nirmauni.ac.in

ABSTRACT

The growing need for sustainable transportation fuels and reduced dependence on conventional gasoline has accelerated the adoption of ethanol–gasoline blends in spark ignition engines. Ethanol offers a high octane rating and inherent oxygen content, which significantly influence combustion characteristics, engine efficiency, emissions, and material durability. This work examines the effects of E10, E15, and E20 blends on engine performance parameters, including brake thermal efficiency, fuel consumption, and power output, as well as exhaust emissions such as carbon monoxide, hydrocarbons, nitrogen oxides, particulate matter, and carbon dioxide. Emphasis is placed on wear, corrosion, and material compatibility issues associated with higher ethanol concentrations in engine and fuel system components. Reported experimental evidence indicates that E10 ensures stable combustion and acceptable durability in existing engines. At the same time, E20 provides improved knock resistance and efficiency potential in optimized engines, accompanied by increased fuel consumption and higher wear and corrosion risks in non-adapted systems. The discussion is presented in the context of India's Ethanol Blending Programme, which targets nationwide E20 adoption, highlighting the need for engine calibration and material upgrades to ensure long-term reliability.

Keywords: Ethanol blending; E20; performance; Emissions; Wear and corrosion

Nanofluids for Solar Thermal Collectors: Performance, Challenges, Environmental Impacts and Future Prospects

Khushang Ghael[a], Darshit S. Upadhyay[a*]
Department of Mechanical Engineering, Nirma University, Ahmedabad, India[a]
* Corresponding Author: Darshit S. Upadhyay[a*]: darshit.upadhyay@nirmauni.ac.in

ABSTRACT

The rapid rise in global energy demand and the shift toward renewable sources have intensified research into solar energy systems. Solar thermal collectors, in particular, benefit significantly from the use of nanofluids, which enhance heat transfer performance due to their superior thermophysical and optical properties compared to conventional fluids. This work provides an in-depth examination of this technology, examining how custom-made fluids perform across all major collector types, from traditional flat-plate collectors to massive parabolic troughs. Preparation techniques, stability enhancement strategies, and comparative performance improvements of nanofluids are discussed. The study also highlights current challenges and future prospects, emphasize hybrid nanofluids, advanced stabilization methods, concentration optimization, and the need for comprehensive techno-economic and environmental assessments. Overall, nanofluids demonstrate strong potential to improve efficiency in solar thermal technologies, but commercialization requires further research on stability, cost-effectiveness, and environmental safety.

Keywords: Nanofluids, Solar Thermal Collectors, Performance, Challenges, Environmental Impacts

Novel Approaches for Investigating the Melting Curve of Zirconium Carbide (ZrC)

Shraddha Chaudhari[1,2]*, Chirag Patel[1], Dipika B. Patel[3], N. K. Bhatt[4] and Amit Patel[5]
[1]Faculty of Science and Humanities, Sankalchand Patel University, Visnagar, Gujarat, India
[2]M. N. College, Visnagar, Gujarat, India
[3]Department of Physics, Indian Institute of Teacher Education, Gandhinagar, Gujarat, India
[4]Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Gujarat, India
[5]Government Science College, Gandhinagr, Gujarat University, Gujarat, India
*Corresponding author: shraddhaphysics1@gmail.com

ABSTRACT

Zirconium carbide (ZrC), known for its high melting point and exceptional mechanical strength, plays a crucial role in various applications, including nuclear reactors and heavy machinery. In our previous study [S. Chaudhari et al., ICMTP 2024, SPPHY 311, pp. 438–444, 2025], we applied the Universal Equation of State (UEOS) in conjunction with the Mie-Grüneisen hypothesis to examine the temperature dependence of the isothermal equation of state for ZrC. Building on this, the current work explores additional thermodynamic properties of ZrC, including the Grüneisen parameter, Poisson's ratio, and the melting curve, providing a deeper understanding of its behavior under varying temperature conditions.

Keywords: ZrC, Melting curve, UEOS

First-Principles Study of La-Doped $SrNbO_3$: Structural Optimisation and Electronic Properties Using WIEN2k

Patel Maneshwar Rai[1], Ritesh Kumar Chourasia[2].
[1]University Department of Physics, Lalit Narayan Mithila University, Darbhanga-846004, Bihar, India.
[2]Post-Graduate Department of Physics, Samastipur College, Samastipur-848134,A Constituent Unit of L.N.M.U.-Darbhanga-846004), Bihar, India.

ABSTRACT

Strontium niobate ($SrNbO_3$) is a conductive perovskite oxide with significant potential in optoelectronics and energy-related device applications. In this study, we perform a first-principles investigation of La-doped $SrNbO_3$ using density functional theory (DFT) within the WIEN2k framework. The pristine $SrNbO_3$ structure was obtained from the Materials Project database, and a 2×2×2 supercell was constructed to model dilute A-site substitution. La doping was introduced by replacing a single Sr atom in the supercell, and the resulting structure was fully initialized for self-consistent field (SCF) calculations. Volume optimisation was carried out for both pristine and doped structures to determine the equilibrium lattice parameters and assess structural stability. The electronic properties were subsequently examined through band structure, total density of states (DOS), and partial DOS (PDOS) analyses. These calculations reveal the modifications in electronic behaviour induced by La substitution and provide insight into the role of dopants in tailoring the functional properties of perovskite oxides.

Keywords: $SrNbO_3$, La doping, Density Functional Theory (DFT), Electronic structure, WIEN2k

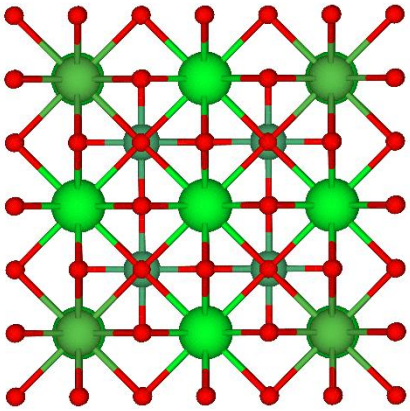


Figure: $2 \times 2 \times 2$ $SrNbO_3$ supercell with La substituted at the A-site Sr position(0,0,0) corresponding to 12.5% La doping. Green spheres represent Sr/La atoms and red spheres represent O atoms, highlighting the NbO_6 octahedral framework used for subsequent DFT structural and electronic analyses.

Experimental and Machine Learning–Based Parametric Study of Dielectric Elastomer Bending Actuators for Finger-like gripping

Aman Sanadhya[a], Reena Trivedi*[b]

[a]MINIMAX Lab, Walker Department of Mechanical Engineering, The University of Texas at Austin, 78712, Texas, United States of America

[b]Mechanical Engineering Department, Institute of Technology, Nirma University, S. G. Highway, Ahmedabad 382481, Gujarat, India

ABSTRACT

Recent advances in electro active polymers and smart material technologies have established di- electric elastomer actuators (DEAs) as a viable platform for lightweight, large-deformation soft actuation. This study presents a parametric investigation of dielectric elastomer bending actuators, focusing on the influence of actuator geometry and pre-stretch ratio (λ) on actuation performance. A series of bending actuators were designed and fabricated using 3M VHB 4905 dielectric elastomer films with varying geometric configurations and stretch conditions. Experimental testing was conducted to evaluate bending behavior and to identify practical challenges encountered during fabrication and operation.

In addition to experimental characterization, a data-driven approach was employed to assess actuation reliability. A support vector machine (SVM) model was developed to predict the success or failure of actuator bending based on geometric and material parameters. The model was trained using experimental data from around 40 fabricated actuators and incorporated nine key geometric features as inputs. The proposed framework achieved a prediction accuracy of approximately 83%, demonstrating its ability to capture nonlinear relationships governing actuation outcomes. The combined experimental and machine learning approach provides practical guidance for the design of dielectric elastomer bending actuators in applications such as soft grippers and prosthetic devices.

Keywords: Dielectric Elastomer Actuators (DEAs), Bending Actuators, Soft Robotics, Support Vector Machine (SVM).

Free Stading Carbon/TiO_2 composite film Based NO_2 Sensor

Vanaraj Solanki*[a], Anita Patel[a], Vishwa Padia[a], Mitesh H Patel[a], A. K. Dasadia[b], D. K. Dhruv*[c], Sejal Purvang Dalal[d], Shikha Varma[e]

[a] Dr. K C Patel R and D Centre, Charotar University of Science and Technology (CHARUSAT), Changa, 388421, Anand, India.

[b] Faculty of Science, A. D. Patel Institute of Technology, The C.V.M University, New Vallabh Vidhyanagar, 388121, Gujarat, India.

[c] Natubhai V. Patel College of Pure and Applied Sciences, The Charutar Vidya Mandal (CVM) University,
Vallabh Vidyanagar 388120, Gujarat, India.

[d] Civil Engineering Department, SVIT, Vasad, Gujarat, India

[e] Institute of Physics, Sachivalaya Marg, Bhubaneswar, 751005, India

*Corresponding author: [a] vanarajsolanki.rnd@charusat.ac.in , [c] dhananjay.dhruv@cvmu.edu.in

ABSTRACT

Gas sensors are essential for safety, environmental surveillance, and industrial process regulation. In this work, carbon nanostructures synthesized from waste garlic peels, through a sustainable carbonization approach, were used to synthesize free-standing Carbon/TiO_2 composite thin films via a hydrothermal route. This provides a sustainable and environmentally friendly strategy for gas-sensing applications. The material exhibits formation of carbon nanostructures and pores like morphology. Carbon nanostructures are formed with a low degree of graphitization and have structural defects and disorder as displayed by X-ray diffraction and Raman study. The fabricated carbon nanostructure-based sensor is responsive to the NO_2 gas in the concentration range of 100 ppb to 100 ppm. Sensor exhibited a high sensitivity of 109% for a 10 ppm NO_2 concentration with a reversible response. Over all the study advocate the potential of the fabricated sensor for NO2 sensing applications.

Keywords: TiO_2, Carbon, nanoflower, Composite

Study of Physiochemical Properties and application of nanomaterial in detection of Adulteration in Edible Oils

Narasimha Reddy Ravuru[a*], Leena V Bora[a],
[a] Chemical Engineering Department, Nirma University, Ahmedabad 382481, India
narasimhareddy.ravuru@nirmauni.ac.in*

ABSTRACT

A basic human diet surely consists of edible oils. We all use different types of market oil and as a key part of our diet we should examine the quality of these oils. The physiochemical characteristics of oils include acid value, saponification value, iodine value and peroxide value. This study shows the comparison between the physiochemical properties of different oils such as peanut, almond, coconut and sunflower oil brought from market and pure oil extracted from machines. Due to its crucial importance in our day-to-day life, it has been easily prone to various kind of adulterants. The prime cause of the adulteration is the plain price variations and economic gain. Adulterants like argemone oil, rice bran oil, palm oil, linseed oil etc., are frequently used to adulterate the edible oils. The use of nanoparticles has significantly improved the detection of adulterants in edible oil. In the current study simple, rapid and reliable color test such as improved nitric acid, azo dye test, baudouin test, halpen's test and solvent separation techniques have been used for detection of different adulterants. Nanoparticle-based sensors are better for detecting food adulteration, and offer high sensitivity compared with conventional methods of detecting adulteration in edible oils.

Keywords: saponification value, iodine value, nanoparticles, Baudouin test, Halpen's test

References:

[1] A. Sudhakar, S. K. Chakraborty, N. K. Mahanti and C. Varghese, "Advanced techniques in edible oil authentication: A systematic review andcritical analysis," Critical Reviews in Food Science and Nutrition, vol. 63, no. 7, pp. 873-901, 2021.

[2] E. Christopoulou, M. Lazaraki, M. Komaitis and K. Kaselimis, "Effectiveness of determinations of fatty acids and triglycerides for the detection of adulteration of olive oils with vegetable oils," Food Chemistry", vol. 84, no. 3, pp. 463-474, 2004.

First Principles Study of Structural Electronic and Photovoltaic Properties of 2D $CsPbBr_3$ Perovskite Solar Cell

Shailesh Motirale , Maulesh D Vala*, Prasann Kshatriya, Parth Zadafiya, Trilokchand Kumavat, Rahulkumar P. Jadav, Yogesh Sonvane
Affiliation: Advanced Materials Lab, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India.
*Corresponding author: mauleshphy@gmail.com

ABSTRACT

This work presents a first-principles investigation of the all-inorganic two-dimensional (2D) $CsPbBr_3$ perovskite, as it's 3D counterpart is already known to possess quite great optoelectronic properties [1] highlighting its potential for photovoltaic and optoelectronic applications. We have hence chosen to study it's 2D counterpart. Using Density Functional Theory (DFT), we systematically analyze its structural, electronic, and optical properties. Compared with conventional hybrid perovskites, $CsPbBr_3$'s all- inorganic composition provides superior thermal and moisture stability[2], effectively addressing one of the most critical challenges in perovskite solar cell development. Our calculations demonstrate that this system possesses a direct bandgap suitable for efficient light absorption. The direct Bandgap of this $CsPbBr_3$ Material is 2.49. There is a clear energy gap between the valence and conduction bands indicating semiconducting behaviour. Furthermore, electronic band alignment analysis demonstrates that 2D Heterostructures incorporating $CsPbBr_3$ can facilitate effective charge separation, which is essential for enhancing device efficiency. After measuring the electronic properties of $CsPbBr_3$ which is consistent with theoretical predictions. These findings suggest that 2D $CsPbBr_3$ combines long-term stability with strong optoelectronic performance, making it an attractive candidate for next-generation solar cells and related devices.

Keywords: Density Functional Theory, $CsPbBr_3$, hybrid perovskites, stability, structural character.

References:

[1] Ullah, S., Wang, J., Yang, P., Liu, L., Yang, S.-E., Xia, T., Guo, H., & Chen, Y. (2021). All-inorganic $CsPbBr_3$ perovskite: a promising choice for photovoltaics. Materials Advances, 2(2), 202–211.

[2]Yang, L., Gao, Y., Yan, Z., Wang, H., & Sun, J. (2019). High water resistance of monoclinic $CsPbBr_3$ nanocrystals derived from zero-dimensional cesium lead halide perovskites. ACS Omega, 4(3), 6084–6091.

Relaxation Processes and Intermolecular Interactions in Bromopropane–Methanol Binary Mixtures: A Dielectric and DFT Approach

K. J. Agheda[a], N. A. Chaudhary[b], V. S. Patel[c], A. K. Patel[c], B. S. Chakrabarty[a], A. N. Prajapati[c*]
[a] Department of Applied Physics, The M. S. University of Baroda, Vadodara - 390001, Gujarat, India
[b] Department of Applied Physics, Polytechnic, The M. S. University of Baroda, Vadodara - 390002, Gujarat, India
[c] Department of Physics, Sardar Patel University, V. V. Nagar - 388120, Gujarat, India
[*]Corresponding author: canprajapati-phy@spuvvn.edu

ABSTRACT

This work investigates the dielectric and electronic behaviour of bromopropane (BRP)–methanol (MeOH) binary mixtures, together with density functional theory (DFT) and thermodynamic analyses, to assess their relevance for electronic and energy-related material systems. Broadband dielectric spectroscopy (BDS) measurements were performed over the frequency range 20 Hz–2 MHz at a constant temperature of 293.15 K to examine the influence of composition on dielectric permittivity (ε′), relaxation time (τ), electrical modulus (M′), electrical conductivity (σ′), impedance (Z′), and loss tangent (tan δ). The tan δ spectra reveal electrode polarisation loss peaks, from which the electrode polarisation relaxation frequency (fEP) and corresponding relaxation time (τEP) were determined, providing insight into ion build-up and interfacial polarisation effects. Increasing BRP concentration weakens the hydrogen-bonded network of MeOH, resulting in reduced ε′ and enhanced M′, indicative of nonlinear intermolecular interactions such as solvation and self-association. To understand molecular-level interactions, DFT calculations were employed to obtain optimised geometries, interaction energies, electron density distributions, molecular electrostatic potential (MEP) maps, and Mulliken charge distribution (MCD) analyses. Thermodynamic parameters were also evaluated using the DFT framework. The combined experimental and theoretical approach offers a comprehensive understanding of relaxation dynamics, intermolecular interactions, and charge-transport mechanisms in BRP–MeOH mixtures, underscoring their potential applicability in dielectric devices, electronic materials, and solvent-engineered functional systems.

Keywords: Broadband dielectric spectroscopy; Dielectric relaxation; Electrode polarisation; Density functional theory (DFT); Charge transport; Thermodynamic properties

Enhancement of performance of In_2O_3/Cu based thin-film thermocouple on flexible substrate

Nirali Patel[a*], Anil Pandya[a], Anup V. Sanchela[a*]
[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Raisan, Gandhinagar 382007, India.
[*]Corresponding author: niralipatel6224@gmail.com, anup.sanchela@sot.pdpu.ac.in

ABSTRACT

A thermocouple is a type of temperature sensor that measures temperature. Thin-film thermocouples, fabricated in flexible substrates, have advantages such as small size, light weight and flexibility [1]. In this study indium oxide and copper are used to make a thin-film thermocouple on a flexible PET substrate. Thin film of both indium oxide and copper is synthesized using RF magnetron sputtering. Thermoelectric properties of indium oxide thin film have been optimized by variation in deposition pressure and heat treatment. When the deposition pressure is increased from 3×10^{-3} mbar to 3×10^{-2} mbar, the thermopower of the In_2O_3 thin film increases significantly from -47 µV/K to -151 µV/K. After the heat treatment of In_2O_3 thin film, thermopower improve to -196 µV/K. Using these parameters, various thin-film thermocouples were fabricated, and increasing the deposition pressure enhanced their sensitivity from 36 µV/K to 77 µV/K. Subsequent heat treatment of the In_2O_3 leg further improves sensitivity from 77 µV/K to 121 µV/K.

Key words: Thermocouple, Flexible, Sensitivity

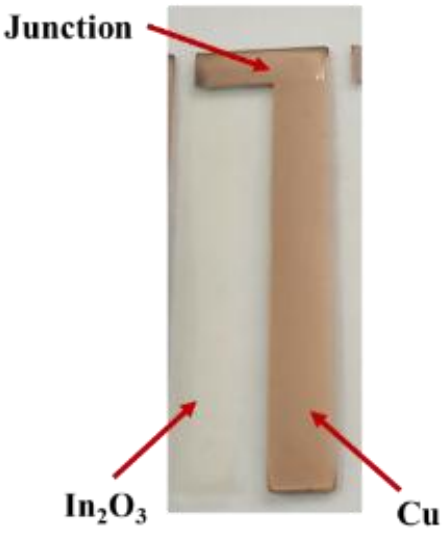


Fig.1: Real Photograph of In_2O_3/Cu based thin-film thermocouple on PET substrate.

Emerging Janus TiVC MXene for Thermoelectric applications

Bhargav K. Darji[1], Sanjeev K. Gupta[2], P. N. Gajjar[1, *]
[1]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad, 380009, India.
[2]Computational Materials and Nanoscience Group, Department of Physics-Electronics,
St. Xavier's College, Ahmedabad, 380009, India
[*]Corresponding author email: pngajjar@gujaratuniversity.ac.in

ABSTRACT

Recent work, we present a comprehensive first-principles investigation of a Janus TiVC MXene monolayer to elucidate its electronic, mechanical, and thermoelectric performance. The Janus TiVC exhibits a metallic character, while absence of imaginary frequency in phonon modes and the negative cohesive energy indicating robust dynamic stability. The thermal stability of the material was evaluated through ab-initio molecular dynamics (AIMD) at 300 K, which inherently account for anharmonic vibrational effects. Mechanical characterization, obtained through elastic-constant analysis and strain-energy fitting, reveals high in-plane stiffness, moderate Poisson's ratio, and robust structural stability, confirming the ability of TiVC MXene to withstand anisotropic loading conditions. Thermoelectric transport properties, explored using the Boltzmann transport formalism, show an improved Seebeck coefficient, high electrical conductivity and a competitive power factor across a wide temperature range. Such favorable balance between seebeck coefficient and reduced total thermal conductivity boosts the figure of merit (ZT), thereby positioning the Janus TiVC MXene as a promising candidate for next-generation thermoelectric and energy-conversion applications.

Keywords: Thermoelectric performance, elastic-constant, figure of merit

References:

[1] Chen JN, Zhang RZ, Li XH, Cui HL. Probing the electronic, optical properties and quantum capacitance of Janus TiVCT2 (T = F, Cl, Br, I, O, S, Se, Te, P, H, NH, OH) MXenes through density functional theory. Mater Today Commun 2025; 48:113545. https://doi.org/10.1016/J.MTCOMM.2025.113545.

[2] Wong, Zicong Marvin and Deng, Tianqi and Shi, Wen and Wu, Gang and Tan, Teck Leong and Yang, Shuo-Wang. High performance photocatalytic and thermoelectric two-dimensional asymmetrically ordered Janus-like MXene alloys - Materials Advances (RSC Publishing), DOI:10.1039/D0MA00391C n.d.

Study of Refractometric and Volumetric Properties of n-Butanol with Benzonitrile Binary Mixtures at Various Temperatures with DFT Analysis

U. D. Raval[a], K. J. Agheda[b], N. A. Chaudhary[c], V. S. Patel[a], A. K. Patel[a], A. N. Prajapati*[a]
[a] Department of Physics, Sardar Patel University, V. V. Nagar - 388120, Gujarat, India
[b] Department of Materials Science, Sardar Patel University, V. V. Nagar - 388120, Gujarat, India
[c] Department of Applied Physics, Polytechnic, The Maharaja Sayajirao University of Baroda, Vadodara – 390002, Gujarat, India
*Corresponding author: [a]anprajapati-phy@spuvvn.edu

ABSTRACT

Density (ρ) and Refractive index (n) of the binary mixtures of n-butanol and benzonitrile across the entire concentration range (0.0 → 1.0) were measured experimentally for temperature ranges 303.15 K to 323.15 K in the interval of 10 K. Various parameters were such as reduced free volume (V_m/R_m), molecular radii (r), polarizability (α), atomic polarization (P_A), and internal pressure (P_{int}) evaluated from the experimentally measured data. Excess parameters such as excess refractive index $(n)^E$, excess density $(\rho)^E$, excess reduced free volume $(V_m/R_m)^E$, excess molecular radii $(r)^E$ excess polarizability $(\alpha)^E$, excess atomic polarization $(P_A)^E$ and excess internal pressure $(P_{int})^E$ were also determined. These parameters were fitted to Redlich-Kister polynomial equations using the least-square fit method to obtain fitting parameters. Different mixing models for refractive index have been validated and tested. Density functional theory (DFT) method was used to determine the optimized structures, dipole moment and frontier molecular orbits (FMO) analysis of both pure compounds and their binary mixtures along with Electrochemical parameters. The study confirms the stability and reactivity of molecules. These studies were analysed to elucidate the nature of hetero-interactions, specifically interactions between, unlike molecules, within the mixtures.

Keywords: Binary mixture, Refractive Index and density, Hetero-molecular interactions, Electrochemical properties, DFT, Frontier Molecular orbitals (FMO) Analysis.

References:

[1] Prajapati A. N., Acoustic and refractometric study of binary mixtures of 1-Propanol + Benzonitrile at 313 K, Indian Journal of Pure & Applied Physics, 55(4) (2017) 297-303.
[2] Chaudhary N.A., Vaja C.R., Agheda K.J., Shah K.N., Rana V.A., Prajapati A.N., Insights into molecular interactions: Dielectric relaxation and DFT based studies on n-hexanol/N, N-dimethylformamide binary mixtures, Journal of Molecular Liquids, 418 (2024) 126675-126685.

Strain-Tuned Thermoelectric Properties of Si_2XY Janus Sheets

Priyankaben N. Thorat[1,2], Rahulkumar P. Jadav[1], Radha N. Somaiya[1,3,*], Yogesh Sonvane[1,*]
[1]Advanced Materials Lab, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India
[2]Department of Physics, Government Arts, Commerce and Science College, Khergam, Navsari 396040, India
[3]Department of Physics, Indian Institute of Technology, Bombay, Mumbai, 400076, India
*Corresponding author: somaiyaradha@gmail.com, yas@phy.svnit.ac.in

ABSTRACT

Janus two-dimensional Si_2XY (X, Y = P, As, Sb, Bi) monolayers are investigated as promising thermoelectric materials by systematically analyzing their structural, electronic, and transport properties under biaxial strain using first-principles calculations combined with Boltzmann transport theory. The optimized structures exhibit stable hexagonal lattices with pronounced Janus asymmetry and strong covalent bonding, characterized by Si–Si bond lengths of ~2.31–2.36 Å, while hybrid HSE06 calculations predict wider and more accurate band gaps than PBE, increasing consistently with the atomic mass of the group-V elements. Thermoelectric properties are evaluated over a chemical potential range of −0.2 to +0.2 eV, temperatures from 300 to 900 K, and biaxial strains between −10% and +10%. The electronic thermal conductivity (κ_e) varies from nearly zero to ~6 W m^{-1} K^{-1}, showing a pronounced minimum near the charge neutrality point ($\mu \approx 0$ eV). The Seebeck coefficient exhibits a clear sign reversal around $\mu \approx 0$ eV, reaching peak magnitudes of approximately ±150 μV K^{-1}, while the electrical conductivity increases sharply away from charge neutrality, attaining values up to ~3 × 10^5 S m^{-1}, particularly in Sb- and Bi-based systems. Consequently, the power factor reaches a maximum of ~6–8 × 10^{-4} W m^{-1} K^{-2} under moderate tensile strain (~+6% to +8%) at elevated temperatures. Overall, monolayers containing heavier elements, especially Si_2PBi, Si_2AsBi, and Si_2SbBi, demonstrate superior thermoelectric performance, highlighting the combined effects of Janus asymmetry, atomic mass contrast, and strain engineering for next-generation thermoelectric devices.

Keywords: Biaxial strain, DFT approach, Electronic Transport Properties

References:

[1] Yesim Mogulkoc,Yasin Zengin, and Gozde Enekc, "Novel Insights into Strain-Driven Modifications in Electronic, Optical, and Charge Distribution Properties of Janus $\boldsymbol{\gamma}$-Si_2XY (X/Y = S, Se, Te) Monolayers," *Advanced Theory and Simulations*, (8) (2025) e00433 1-11.

[2] Yunlai Zhu, Zihan Qu, Jishun Zhang, Xiaoteng Wang, Shuo Jiang, Zuyu Xu, Fei Yang, Zuheng Wu and Yuehua Dai, "First-principles prediction of ferroelectric Janus Si_2XY (X/Y = S/Se/Te, X≠Y) monolayers with negative Poisson's ratios," *Physical Chemistry Chemical Physics*, (26) (2024) 4555-4563.

Investigation of Dielectric Property Changes in Milk after Expiry and Water Adulteration Using LCR Meter

Jesal R. Soni[1], Deepak Gadani[1]*, Vipinchandra A. Rana[1]
[1]Department of Physics, Electronics and Space Sciences, Gujarat University, Ahmedabad, India.
*Corresponding author: [1]dhgadani@gujaratuniversity.ac.in

ABSTRACT

A study was undertaken to investigate the dielectric properties of whole cow's milk, pasteurized cow's milk, and buffalo milk in fresh form as well as after expiry, along with varying levels of water adulteration (WC). This was done using an LCR meter operating over 20 Hz - 2 MHz frequency range. The measurements were taken at a uniform temperature of 25°C with the specific goal of determining the dielectric constant (ε'), dielectric loss (ε"), and loss tangent (tanδ) for the fresh, after expiry date, and water-adulterated milk samples. It was observed that ε' exhibited a decreasing trend as frequency increased from 20 Hz up to 2 MHz, for all types of milk samples. Furthermore, the study shows that ε' demonstrated a decreasing trend with a rise of WC in milk, at any specific frequency above 2 kHz. This indicates that the dielectric constant is significantly influenced by the WC present in the milk and underscores the sensitivity of dielectric properties to variations in milk sample composition. However, at frequencies less than 2 kHz, ε" exhibited an increasing trend, and for frequencies above 5 kHz, the decreasing trend as WC in milk increased. After the expiry date of milk, ε" increases in milk samples, which shows that milk undergoes microbial fermentation, mainly by lactic acid bacteria. A linear decreasing trend of ε' and ε" with the increase of water content in the milk, for the milk samples at 100 kHz and 2 MHz, can be used to predict the % of additional water content in the milk.

Keywords: milk, water content, adulteration, dielectric constant, dielectric loss

References:

[1] Li, B.; Yang, Y.; Guo, W. Influence of added water on conductivity of fresh raw cow milk. Shipin Kexue (Food Science) 2016, 37(16), 268–271.

[2] Walstra, P.; Wouters, J. T. M.; Geurts, T. J. Dairy Science and Technology, 2nd ed.; CRC Press: Boca Raton, 2006.

Computational Approaches for Material Evaluation in H_2 Energy Systems

Krish Jigneshumar Suthar [a], Het Tusharkumar Patel*[a], Dr. Atindra Shukla [b]
[a,b] Dharmsinh Desai University
*Corresponding author: [a] 23mhuos013@ddu.ac.in

ABSTRACT

The identification of appropriate materials is a basic condition for the progress of hydrogen energy systems. The choice of materials for hydrogen storage is a complex problem that involves thermal, mechanical, and material-dependent factors, which are usually considered separately. However, recent advances in computational modeling and data-driven techniques provide possibilities for integrated approaches to material assessment. This research presents a generalized computational framework that combines physics-based modeling with machine learning concepts to facilitate the systematic exploration of hydrogen storage materials. In short, the study considers representative thermal and mechanical conditions to describe material responses under operationally relevant scenarios, and the obtained data are arranged for data-driven analysis. Instead of concentrating on particular material systems or performance benchmarks, the framework features methodological flexibility and scalability, which make it possible to be transferred to different material classes and application contexts. The purpose of this investigation is to illustrate the potential of combining simulation-based insights with data-oriented models to provide a structured material screening workflow for hydrogen storage and other energy applications.

Keywords: Hydrogen storage, Material selection, Physics-informed modeling, Finite element analysis, Machine learning.

References:

[1] Schlapbach, L., & Züttel, A., "Hydrogen-storage materials for mobile applications," Nature, vol. 414, pp. 353–358, 2001.

[2] Belytschko, T., Liu, W. K., & Moran, B., Nonlinear Finite Elements for Continua and Structures, Wiley, 2000.

Study of Dielectric Behavior of Tree Leaves with Moisture Content over 100 Hz to 2 MHz Frequency Range

Devnetra Jain, Mili Patel, Pratipal D. Chauhan, Deepak Gadani*
Department of Physics, University School of Sciences, Gujarat University,
Ahmedabad-380009, Gujarat, India.
*Corresponding author: *dhgadani@gujaratuniversity.ac.in*

ABSTRACT

The dielectric constant (ε') and dielectric loss (ε'') of orange, pomegranate, and cotton leaves were measured over 100 Hz − 2 MHz frequency range using a parallel plate capacitive solid test fixture (Agilent 16451-B) attached with a precision LCR-Meter (Agilent Make E 4980-A). It has been observed that the dielectric constant (ε') and dielectric loss (ε'') of leaves decrease with decrease in moisture content (MC) in the leaves. At given moisture content in the leaves $\varepsilon'$and ε'' both decrease with increase in frequency over the given frequency range. Further it has been observed that at 2 MHz the increase in $\varepsilon'$and $\varepsilon''$with MC for the cotton leaves is maximum, followed by pomegranate leaves, and it is least for the orange leaves. The rapid increase in the values of $\varepsilon'$and $\varepsilon''$with the increase in MC represents that there are more free water molecules per unit volume compared to bound water molecules in cotton leaves, which suggests that the internal structure of cotton leaves must be more porous, compared to the other two types of leaves. The study of dielectric properties in terms of $\varepsilon'$and $\varepsilon''$with MC of the leaves can also be useful to check the freshness of leaves.

Study of Dielectric Behavior of Wheat, Pearl, and Jawar millet flours over 1 kHz to 2 MHz Frequency Range

Minal Makvana, Renykumari Champavat, Pratipal D. Chauhan, Deepak Gadani*
Department of Physics, University School of Sciences, Gujarat University,
Ahmedabad-380009, Gujarat, India.
*Corresponding author: *dhgadani@gujaratuniversity.ac.in

ABSTRACT

In this study we have taken the Wheat, Pearl, and Jawar millet flours for the dielectric measurement. The complex permittivity ($\varepsilon^* = \varepsilon' - j\,\varepsilon''$) of Wheat, Pearl, and Jawar millet flour were measured using Precision LCR Meter (Agilent E4980A) with a parallel plate capacitive solid test fixture (Agilent 16451B) over 1 kHz to 2 MHz frequency range. It is observed that the dielectric constant (ε') and dielectric loss (ε″) of the Wheat, Pearl, and Jawar flours are found to decrease with the increase in frequency. The dielectric constant (ε') and dielectric loss (ε″) of the flours is found to increase as the density of the flour is increased, at a fixed frequency of 2 MHz. The variation of complex electric conductance, electric impedance, and electric modulus with frequency at two different densities for Wheat, Pearl, and Jawar millet were also calculated from the measured values of ε' and ε″. It has been observed that there doesn't exist any relaxation mechanism in any of the flours over the frequency range of measurements.

Low-cost graphite based thin film transistor on flexible substrate

Anmol Jaiswal [a*], Anil Pandya [a], Anup V. Sanchela [a*]
[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Raisan, Gandhinagar 382007, India.
[*]Corresponding author: 25rph002@spt.pdpu.ac.in, anup.sanchela@sot.pdpu.ac.in

ABSTRACT

In this study, graphite-based thin film transistors (TFTs) were successfully fabricated using a screen-printing technique, with graphite paint developed and synthesized in our laboratory. Several grades of graphite paint were formulated, each exhibiting distinct carrier concentration levels to investigate the influence of material properties on device performance. The TFTs produced with these various grades, along with an optimized paint composition, were systematically evaluated to understand how carrier concentration affects electrical behaviour. A detailed analysis of their transfer characteristics was conducted to assess device efficiency and field-effect mobility. For the gate dielectric layer, an insulating film of Al_2O_3 was deposited using RF sputtering. Additionally, silver was chosen as the material for the source, drain, and gate electrodes due to its excellent conductivity and compatibility with sputtering deposition. RF sputtering was employed for the electrode deposition to achieve uniform and adherent metallic contacts. The overall fabrication process highlights the integration of novel graphite paint materials with established thin-film deposition methods to advance printed electronics and optimize TFT performance.

Key words: Graphite, TFT, Screen printing, dielectric

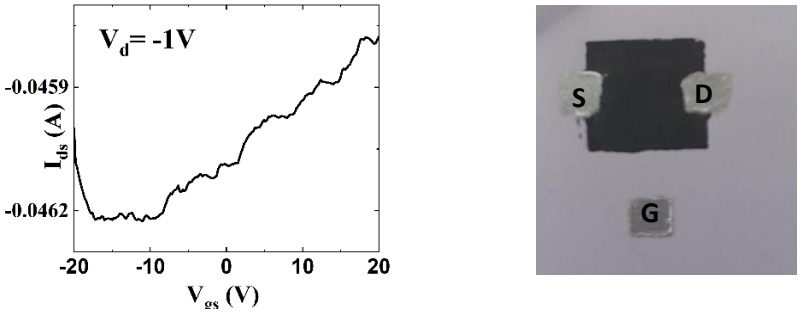


Fig.1. Real Photograph of graphite paint based thin-film transistor on paper substrate.

Effect of Mg- substitution on Structural, Morphology, Raman, Magnetic, Dielectric Properties, and Antenna Performance of Sr–Zn Hexaferrites

Dipti D. Parmara, Hina N. Chaudharib, Charmi D. Patelc, Charanjeet Singhd, Mohmed Ellouzee, Arpan Desaif, Abhishek A. Gorg, Rajshree B. Jotania*h

[a,b,c,h]Department of Physics, Electronics and Space sciences, University School of Sciences, Gujarat University, Ahmedabad, 380009, India

[d]Alliance School of Applied Engineering, Alliance University, Bengaluru, Karnataka-562106, India

[e]Faculty of Sciences of Sfax, Physics department, B. P. 1171 – 3000, Sfax, Tunisia

[f]Department of Information and Communication Technology, School of Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India

[g]Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India

*Corresponding author: hrajshree_jotania@yahoo.co.in

ABSTRACT

Mg-substituted SrZn2MgxFe16-xO27 ($0.0 \leq x \leq 1.0$) hexaferrites were synthesized through the citrate-gel technique (1300 °C for 5 h). XRD, FTIR, SEM with EDAX, Raman spectra, VSM, low (20 Hz - 2 MHz) and high frequency (0.2 -20 GHz) dielectric measurements were carried out to study the effect of Mg-substitutions on various properties of SrZn2MgxFe16-xO27. XRD analysis of x = 0.0 composition confirmed the formation of W-phase, while other samples (x = 0.2 to 1.0) showed mixed phases of W and M-type. Five active Raman phonon modes are observed between 150–800 cm−1, characteristic of W-type hexaferrites as determined by symmetry and assigned polyhedra. The surface morphology revealed formation of agglomerated grains. The EDX spectra confirm the presence of Mg, Fe, Sr, and Zn elements. The coercivity of all samples was found in between 89.73 -123.81 Oe, implying soft magnetic nature. Both high and low frequency electrical parameters revealed the same charge transport dynamics. An aperture-coupled patch antenna using the x = 0.2 as substrate and a Rogers 4003C substrate was designed and simulated using Ansys HFSS, achieving a compact patch size, resonance at 10 GHz (S11 = -27.5 dB) frequency, 1.8 dBi gain, demonstrating suitability for reconfigurable 5G antennas.

Keywords: Mg-substituted W-hexaferrites, XRD, Raman spectra, Hysteresis loops, Aperture Coupled Patch Antenna

Reference:

[1] Lee, Byungje, and Frances J. Harackiewicz. Miniature microstrip antenna with a partially filled high-permittivity substrate. IEEE Transactions on Antennas and Propagation 50, (8) (2002) 1162

Solid state structure and crystallization behavior of Polylactic acid: Influence of Microwave Assisted Synthesis

Saloni Mishra [a], Nimish Shah*[b], Shibu Pillai*[b], Mamta Saiyad [b].
[a] Institute of Science, Nirma University, Ahmedabad, Gujarat, India
[b] Chemical Engineering Department, Nirma University, Ahmedabad, Gujarat, India
*Corresponding author: [a] nimish.shah@nirmauni.ac.in, shibu.pillai@nirmauni.ac.in

ABSTRACT

Poly(lactic acid) (PLA) is a semicrystalline, biodegradable, and biobased polymer whose functional properties are strongly driven by its solid-state structure and crystallization behavior. In the present study, PLA was synthesized using two different heating modes conventional thermal melt polycondensation and microwave-assisted polycondensation to evaluate the influence of energy input mechanisms on molecular weight development and chain ordering. A detailed investigation was further carried out to examine crystal phase formation, thermal transitions, and morphological characteristics of PLA synthesized via the microwave-assisted route. Microwave heating, driven by volumetric dipole rotation, resulted in PLA with increased molecular weight and enhanced chain mobility compared to conventional surface-conductive heating, as confirmed by gel permeation chromatography (GPC). X-ray diffraction (XRD) analysis was employed to explain the effect of microwave-assisted synthesis on the crystalline behavior of the biopolymer. Differential scanning calorimetry (DSC) provided additional insights into the thermal behavior of the synthesized materials, while Fourier-transform infrared (FTIR) spectroscopy was used to analyze structural conformation. Overall, microwave-assisted synthesis significantly accelerates polymer formation and influences the molecular weight of PLA. This study highlights the critical role of heating mode in tailoring polymer structure and offers valuable insights into structure–property relationships relevant to materials physics and polymer engineering.

Keywords: Polylactic acid; Solid state stricture; Microwave Synthesis

References:

[1] Kawai, T.; Rahman, N.; Matsuba, G.; Nishida, K.; Kanaya, T.; Nakano, M.; Matsuda, M. Crystallization and Melting Behavior of Poly(L-lactic Acid). Macromolecules 2007, 40 (26), 9463–9469.

[2] Nagahata, R.; Sano, D.; Suzuki, H.; Takeuchi, K. Microwave-Assisted Single-Step Synthesis of Poly(lactic acid) by Direct Polycondensation of Lactic Acid. Macromol. Rapid Commun. 2007, 28 (4), 437–442.

Investigation of Structural, Optical and Dielectric Properties of $xBaTiO_3–(1−x)LaFeO_3$ Perovskite Composites

Heena H. Rathod [a], Manasi Raval [a, b], Manali N. Shah [c], Devang D. Shah[d], Rajshree B. Jotania [e]

[a] Department of Physics, Faculty of Science, Ganpat University, Mehsana 384012, Gujarat, India

[b] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar 382426, Gujarat, India

[c] School of Forensic Science, National Forensic Science University, Gandhinagar 382007 Gujarat, India

[d] Department of Physics, Govt. Arts and Science College, Morva Hadaf 389115, Gujarat, India

[e] Department of Physics, Electronics and Space Science, University School of Sciences, Gujarat University, Ahmedabad 380009, Gujarat, India

[*]Corresponding author: [a] rathodheena5393@gmail.com, [c] manalitrvd@yahoo.co.in

ABSTRACT

In the present study, polycrystalline fine powders of $xBaTiO_3–(1−x)LaFeO_3$ (abbreviated as xBTLF, where x= 0, 0.25, 0.5, 0.75, and 1.0) were synthesized using the solid-state reaction method. Extra-pure barium carbonate ($BaCO_3$), titanium dioxide (TiO_2), lanthanum oxide (La_2O_3), and iron oxide (Fe_2O_3) were used as starting materials. The prepared composites were characterized using X-ray diffraction (XRD), UV–visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, and dielectric spectroscopy. XRD analysis confirmed the formation of single-phase polycrystalline structures, with structural symmetry changing from orthorhombic to tetragonal as the $BaTiO_3$ concentration increased. FTIR spectroscopy confirmed the presence of characteristic metal–oxygen bonds such as Ti–O and Fe–O through their stretching and bending vibration modes. Optical properties were investigated using UV–visible spectroscopy, and the optical band gap values were estimated from the absorption. The dielectric properties were studied in the frequency range of 20 Hz to 20 MHz. The observed structural evolution, tunable optical band gap, and enhanced dielectric response suggest that the xBTLF composites are promising candidates for sensor applications and energy storage devices.

Keywords: Perovskite oxides, X-ray diffraction (XRD), UV–visible spectroscopy, Dielectric spectroscopy, Ferroelectric composites

Adsorption of Ibuprofen using Mesoporous Carbon Derived from One-Step Pyrolysis of Walnut Shells

Nilesh Mohan Khalse*[a], Narasimhareddy Ravuru[b]
[a] Department of Chemical Engineering, PRES Sir Visvesvaraya Institute of Technology, Nashik
[b] Department of Chemical Engineering, Institute of Technology, Nirma University, Ahmedabad.
*Corresponding author: [a] nilesh.khalse.vvp@gmail.com

ABSTRACT

Transforming carbon-rich biomass from forestry residues into mesoporous carbon represents an innovative and sustainable strategy for converting low-value waste into high-performance materials for environmental remediation. In the present study, walnut shells were transformed into a mesoporous carbon designed for the efficient removal of ibuprofen (IBU) from wastewater. A facile one-step carbonization route employing KOH as activators was adopted. Structural and surface analyses revealed that carbon synthesized at carbonization temperature of 700 °C showed a hierarchically porous carbon framework with an exceptionally high specific surface area of 1236 m^2/g and a pore volume of 0.843 cm^3/g. Batch adsorption studies demonstrated outstanding performance, at 40 °C removal efficiency of 92.8% was achieved. Importantly, the mesoporous carbon maintained 89% of its initial capacity after five adsorption–desorption cycles, underscoring its structural robustness and reusability. The physicochemical characterization suggests that presence of carbon matrix and different oxygen functional groups supported the π-π interactions and acid-base interactions, respectively. The adsorption process followed the Langmuir isotherm and pseudo-second-order kinetic models, indicating monolayer chemisorption-dominated behavior.

Keywords: Mesoporous Carbon, Carbonization, Walnut shells, Ibuprofen, Adsorption

References:

[1] Guo, Y., Lu, D., Wang, Z., & Wang, Q. (2025). Promising application of waste bamboo biomass-derived carbon for efficient ibuprofen removal from aqueous systems. Environmental Technology & Innovation, 37, 104025.

[2] Liu, T., Gao, C., Luan, P., Xu, D., Wang, J., Cheng, Z., ... & Chen, G. (2024). Performance evaluation of different nitrogenous biomass pyrolysis chars: Physicochemical properties and ibuprofen adsorption. Biomass and Bioenergy, 189, 107346.

Mechanical Properties of Multilayer Bio-Polymeric Films

Mrudang Shah [a], Ankur Dwivedi [b*], Mamta Saiyad [b], Nimish Shah [b]
[a] Institute of Science, Nirma University, Ahmedabad, Gujarat, India.
[b] Department of Chemical Engineering, Institute of Technology, Nirma University, Ahmedabad, Gujarat, India.
[*]Corresponding author: [b] ankur_dwivedi@nirmauni.ac.in

ABSTRACT

Multilayer polymeric films have emerged as an innovative advanced materials and have established themselves as a critical component in material science by enhancing the performance limitations of monolayer by integrating different functional advantages of multiple polymers into a single polymeric film. These multilayer polymeric films combine the layers of different polymers with distinct characteristics such as high tensile strength, low water vapor transmission, reduced gas permeability, good elongation and various other applications to achieve performance levels that can't be attained by monolayer polymeric film. The integration between polymers like polyvinyl alcohol (PVA), starch, polylactic acid and other biodegradable polymers enables films with optimized barrier behavior, improved toughness, and greater stability under environmental stress. The arrangement of hydrophilic and hydrophobic layers further enhances resistance to moisture while maintaining overall structural performance. Because of this multifunctionality, multilayer polymeric films are increasingly used across various sectors such as food packaging, pharmaceuticals, agriculture, and biomedical engineering. Here we will discuss about the film having good tensile strength and elongation property.

Keywords: Multilayer bio-polymeric films, Barrier properties, elongation, Mechanical strength, Packaging and biomedical applications.

References:

[1] Anukiruthika, T., et al., Multilayer packaging: Advances in preparation techniques and emerging food applications. 2020. 19(3): p. 1156-1186.

[2] Barletta, M., et al., Surface appearance and mechanical strength of multi-layer polymeric films. 2008. 61(2-4): p. 249-261.

DFT Study of Oxygen Electrocatalysis on Pd Decorated aza-tripheneylene based Covalent Organic Framework: Insights into OER and ORR Activity

K. Simmy Joseph [a], Brahmananda Chakraborty *[b,c,] and Shweta Dabhi *[a]
[a]Department of Physical Science, P. D. Patel Institute of Applied Sciences, Charotar University of Science and Technology, CHARUSAT Campus, Changa-388421, Gujarat, India.
[b]High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai, India
[c]Homi Bhabha National Institute, Mumbai 400085, India.
*Corresponding author: [c]shwetadabhi.phys@charusat.ac.in, [b]brahma@barc.gov.in

ABSTRACT

Creating high-performance electrocatalysts for the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) is crucial for advancing energy storage and conversion technologies. In this work, we investigate transition-metal-doped (TM = Co, Rh, Ir, Ni, Pd, and Pt) aza-triphenylene-based covalent organic frameworks (AT-COFs) as efficient bifunctional electrocatalysts using density functional theory (DFT). Among the studied systems, Pd-anchored AT-COF exhibits superior catalytic performance with low overpotentials of 0.49 V and 0.89 V for both OER and ORR. Partial density of states (PDOS) analysis reveals that Pd doping induces favorable electronic structure modulation, enhancing the adsorption of key reaction intermediates. To evaluate ORR kinetics, climbing image nudged elastic band (CI-NEB) calculations were performed for the OOH dissociation step, yielding an energy barrier of 1.62 eV, indicating kinetically accessible O-O bond cleavage under operational conditions with sufficient overpotential. Furthermore, ab-initio molecular dynamics simulations confirm the thermal and structural stability of Pd@AT-COF. These results demonstrate that Pd-doped AT-COFs are promising bifunctional electrocatalysts and provide valuable insights for the rational design of COF based catalysts for clean energy applications.

Keywords: TM@doped AT-COF, Oxygen Reduction Reaction, Oxygen Evolution Reaction, first principles simulations, Ab initio molecular dynamics.

References:

[1] Yue, S., Li, D., Zhang, A., Yan, Y., Yan, H., Feng, Z. & Wang, W., Rational design of single transition-metal atoms anchored on a $PtSe_2$ monolayer as bifunctional OER/ORR electrocatalysts: a defect chemistry and machine learning study, Journal of Materials Chemistry A, 12 (2024) 5451–5463.
[2] Hoyos-Sinchi, V., Souza, P. H. & Orellana, W., Computational insights into two-dimensional $M_3(HHTP)_2$ metal–organic frameworks as ORR/OER electrocatalysts, The Journal of Physical Chemistry C, (2025).

Exploring Dielectric Dispersion and Microwave Heating Characteristics in n-Butanol-Valeronitrile Mixtures

N. A. Chaudhary[a*], S. P. Patel[b], V. S. Patel[c], A. K. Patel[c], A. N. Prajapati[c]
[a] Department of Applied Physics, Polytechnic,
The M. S. University of Baroda, Vadodara-390001, India.
[b] Department of Applied Physics, Faculty of Technology & Engineering,
The M. S. University of Baroda, Vadodara-390001, India.
[c] Department of Physics, Sardar Patel University, Vallabh Vidyanagar - 388120, India.
[*]Corresponding author: [a] chaudharynavin2540@gmail.com

ABSTRACT

The complex permittivity spectra of binary mixtures of *n*-butanol (n-BtOH) and valeronitrile (VN) were studied over the entire concentration range (0.0–1.0 mole fraction) using a vector network analyzer in the microwave frequency region of 200 MHz–20 GHz at 313.15 K. Dielectric relaxation parameters, namely the static dielectric constant (ε_0) and relaxation time (τ_0), were extracted from the experimental data using the LEVMW-CNLS fitting program. The nonlinear concentration dependence of ε_0, τ_0 and refractive index (n) indicates the presence of heteromolecular interactions between n-BtOH and VN molecules. Excess dielectric parameters, including excess static dielectric constant $(\varepsilon_0)^E$ and excess inverse relaxation time $(1/\tau_0)^E$, were evaluated to further quantify these interactions. Kirkwood correlation factors (g^{eff}, g^F) were determined to assess dipolar orientation and molecular association. Microwave heating parameters at 2.45 GHz were also estimated. The results are relevant for microwave processing and solvent design applications.

Keywords: Dielectric Constant, Kirkwood correlation factors, Binary Mixture

References:

[1] Garad, N. P., Saknure, S. H., Gubre, A. G., & Kumbharkhane, A. C., Study of dielectric relaxation and hydrogen bonding interaction of 1,4-butanediol–1,4-dioxane mixture using TDR technique, Indian Journal of Pure and Applied Physics, 61(3) (2023) 158-164.

[2] Rana, V. A., & Pandit, T. R., Broadband dielectric relaxation spectroscopy and molecular dynamics simulation study of paracetamol–propylene glycol solutions, Journal of Molecular Liquids, 341 (2021) 117384.

Synthesis and characterization of UF PSF membrane modified with GO impregnated ZIF-11 nanohybrids for enhanced permeation and antifouling behaviors

Sapna Gawali[a], Manish Kumar Sinha[a], Balasubramanian Ragunathan[b], Lakshman Rao Jeeru[b], Surendra Sasikumar Jampa[a*]

[a] Department of Chemical Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar 382426, India

[b] Department of Petroleum Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar 382426, India

*Corresponding author. Tel: +91-7874034805. E-mail: surendra.sasikumar@sot.pdpu.ac.in

ABSTRACT

In this study, the performance of PSF ultrafiltration membranes was enhanced by incorporating ZIF-11 nanoparticles on graphene oxide (GO) sheets using an in-situ growth method. For the in-situ growth method, the reaction time is crucial because increasing it may enable the crystallized ZIF-11 to fully cover the GO sheets, thereby reducing the excess of ZIF- 11 particles and maintaining the aspect ratio of the GO sheet. The reaction time will significantly change the morphology, affecting the composite's ability to absorb selective water molecules and, in turn, affect the foulant selectivity. The present work identifies the reaction time for the in-situ growth of ZIF-11 nanoparticles on GO sheets. The composite was synthesized at different reaction times of 1, 2, 3, 4, 5 and 6 h and incorporated into the PSF matrix. Key findings include the identification of an optimal reaction time of 5 hours for the in-situ growth of ZIF-11 on GO, resulting in improved membrane characteristics. The best-performing membrane, M5ZIF-11@GO-5, demonstrated a significant increase in hydrophilicity, enhanced permeation flux (197.78 L/m².h), and notable oil-water rejection (97.9%). Furthermore, this membrane showed excellent antifouling properties with a flux recovery ratio of 96%, compared to 67% for the neat membrane.

Keywords: Ultrafiltration, Membranes, ZIF-11, GO, PSF

References:

[1] J. Ma, X. Guo, Y. Ying, D. Liu, C. Zhong, Composite ultrafiltration membrane tailored by MOF@GO with highly improved water purification performance, Chem. Eng. J. 313 (2017) 890–898. https://doi.org/https://doi.org/10.1016/j.cej.2016.10.127.

[2] A. V Gawali, S.S. Jampa, M.K. Sinha, Synthesis and characterization of mixed matrix membranes with graphene oxide-impregnated zeolitic imidazolate framework-8 for enhanced CO2/CH4 separation, Asia-Pacific J. Chem. Eng. 19 (2024) e3094. https://doi.org/https://doi.org/10.1002/apj.3094.

Influence of support materials on the activity of nickel based nano catalysts for hydrogen production via steam reforming

Narasimha Reddy Ravuru[a*], Sanjay Patel[a], Nilesh Mohan Khalse[b]
[a]Chemical Engineering Department, Nirma University, Ahmedabad 382481, India
[b]Department of Chemical Engineering, PRES Sir Visvesvaraya Institute of Technology, Nashik
Corresponding author: [a*]narasimhareddy.ravuru@nirmauni.ac.in

ABSTRACT

The by-product glycerol obtained in biodiesel production adds economic value to the overall biodiesel industry by converting it in to renewable hydrogen. This study focuses on synthesis of nickel based nano catalysts for hydrogen production from glycerol by steam reforming process using supports like alumina oxide, cerium oxide and silicon oxide. The steam reforming reaction is used in hydrogen synthesis because of low pressure and very endothermic in nature. By utilizing hydrogen as a clean fuel, the carbon dioxide emissions can be reduced which result in global warming reduction. Glycerol is a potential renewable feed stock to produce hydrogen since it contains higher hydrogen content and cheapest raw material. The catalysts were prepared by wet impregnation and coprecipitation methods. The prepared nano catalysts physio- chemical properties were investigated by SEM, BET, XRD, TGA techniques. Gas-solid atmospheric fixed-bed catalytic reactor was used to evaluate the performance of catalysts. Various operating conditions like temperature, contact time, metal loading, steam to glycerol ratio, were investigated. The Nickel catalyst supported with γ- Al_2O_3 showed superior performance in terms of glycerol conversion, hydrogen yield, catalytic stability and better resistance to carbon formation which is due to higher surface area, strong metal support interactions and anticoking ability.

Keywords: Biodiesel, Hydrogen, Nano catalyst, Steam Reforming, Wet Impregnation.

References:

[1] M. Silva, M. A. Soria, and L. M. Madeira, “Challenges and strategies for optimization of glycerol steam reforming process,” *Renewable and Sustainable Energy Reviews*, vol. 42, pp. 1187–1213, (2015).

[2] Quan, C., Gao, Z., Liu, X., Miskolczi, N.: Ethanol steam reforming for hydrogen production under Ni/Ce catalysts. J. Energy Inst. 112 (2024).

Coupled Atomistic–Continuum Modeling of Graphene–Germanene Bilayer Nanoresonators with Position-Dependent Mass Sensitivity

Saumil Desai [a], Ankur Pandya*[b], Vipul Bhojawala [a]
[a] Department of Mechanical Engineering, Institute of Technology, Nirma University, Ahmedabad - 382481.
[b] Faculty of Physics under Department of Electronics and Communication Engineering, Institute of Technology, Nirma University, Ahmedabad - 382481.
*Corresponding author: [b] ankur.pandya@nirmauni.ac.in

ABSTRACT

A coupled atomistic–continuum modeling framework is developed to investigate the vibrational behavior and mass sensing performance of a graphene–germanene bilayer nano-resonator in a doubly clamped configuration. The effective Young's modulus of the bilayer heterostructure is first evaluated using the atomic finite element method (AFEM), wherein interatomic interactions are explicitly accounted for to capture the intrinsic elastic response at the atomistic scale [1, 2]. The AFEM-derived elastic properties are subsequently incorporated into a continuum-based resonator model to analyze natural frequencies and mode shapes. Mass sensing characteristics are examined by introducing a concentrated mass at various locations along the resonator length, and the resulting resonance frequency shifts are quantified. The results reveal a pronounced position-dependent sensitivity governed by modal deformation characteristics, with maximum frequency shifts occurring when the added mass is located near vibration antinodes. Compared to monolayer resonators, the graphene–germanene bilayer exhibits enhanced mass detection capability due to the coupled effects of stiffness and mass density. The proposed multiscale framework provides a rigorous theoretical basis for the design and optimization of two-dimensional heterostructure-based nano resonant mass sensors.

Keywords: Graphene–germanene bilayer heterostructure, Atomistic–continuum coupling, Atomic finite element method (AFEM), Nano resonator vibration characteristics, Position-dependent mass sensitivity

References:

[1] Bafekry, A., Karbasizadeh, S., Faraji, M., Khatibani, A. B., Sarsari, I. A., Gogova, D., & Ghergherehchi, M. (2021). Van der Waals heterostructure of graphene and germanane: tuning the ohmic contact by electrostatic gating and mechanical strain. Physical Chemistry Chemical Physics, 23(37), 21196–21206. https://doi.org/10.1039/d1cp03632g

[2] Hamid, M. a. B., Chan, K. T., Ooi, C. H. R., Zainuddin, H., Shah, N. M., & Nidzam, N. N. S. (2021). Structural stability and electronic properties of graphene/germanene heterobilayer. Results in Physics, 28, 104545. https://doi.org/10.1016/j.rinp.2021.104545

Hexaferrite-Based Memristor Device for Neuromorphic and Magnetically Tunable Applications

Adwani Jayshree Ravikumar[1], Abhishek Atulbhai Gor[2], Niranjan Devashrayee[1] Chetna Chauhan[1]*
[1]Institute of Technology, Nirma University, S. G. Highway, Ahmedabad, Gujarat 382 481, India
[2]Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar, Gujarat 382 426, India
*Corresponding author: chetna.chauhan@nirmauni.ac.in

ABSTRACT

The rapid growth of data-centric technologies and the saturation of Moore's Law have accelerated the pursuit of next-generation memory architectures. In this work, a memristor device based on M-type hexaferrite thin films was fabricated via RF sputtering, using Barium ($BaFe_{12}O_{19}$) as the active switching materials. The device employed an ITO-coated PET substrate and silver top electrode in a Metal–Insulator–Metal configuration. Structural analysis confirmed the formation of highly crystalline hexaferrite phases through X-ray Diffraction (XRD), while current-voltage (I–V) characterization demonstrated stable bipolar resistive switching behavior with ON/OFF ratios in the range of 10^2–10^3 achieved under ±1.2 V sweeps. The device transitions from High Resistance State (depression) to Low Resistance State (potentiation) during positive bias (+1.2 V), and resets under negative bias (–1.2 V), enabling synaptic emulation. The influence of intrinsic magnetic properties on switching dynamics was also evaluated, suggesting potential for multifunctional operation. These findings position sputtered hexaferrite-based memristors as promising candidates for low-power, magnetically tunable memory and neuromorphic computing applications.

Keywords: Memristor, hexaferrite, sputtering, neuromorphic computing, characterization.

References:

[1] Abhishek A. Gor, Ankita Singh, Niranjan M. Devashrayee, Rajshree B. Jotania, and Chetna C. Chauhan; J. Mater. Sci. Mater. Electron, vol. 35, 2024.

[2] Abhishek A. Gor, Mrunali Jani, Anup V. Sanchela, N.M. Devashrayee, Rajshree B. Jotania, and Chetna C. Chauhan; Asian J. Chem, vol. 35, 2023.

Investigation of Mechanoelectrical Parameters in Lead-Free Piezoelectric Materials

Nisarg Vashi a, Ankur Pandya*b
[a] Department of Computer Science and Engineering, Institute of Technology, Nirma University, Ahmedabad – 382481, India.
[b] Department of Physics, Institute of Technology, Nirma University, Ahmedabad – 382481, India.
*Corresponding author: ankur.pandya@nirmauni.ac.in

ABSTRACT

The escalating global energy demand and environmental degradation necessitate sustainable energy harvesting technologies. This study presents a comprehensive investigation of lead-free piezoelectric materials for noise-to-electricity conversion. Through theoretical modeling and experimental validation, the mechanoelectrical characteristics of Bismuth Sodium Titanate (BNT), Potassium Sodium Niobate (KNN), and Barium Titanate ($BaTiO_3$) are analyzed to develop efficient energy harvesters. The optimized BT–BT system achieved a peak efficiency of 42% and an output of 5.3 V, surpassing conventional PZT-based systems while eliminating lead toxicity. The frequency-distance model predicts exponential power decay from acoustic sources, with optimal conversion near resonance frequencies (750–1200 Hz). These findings highlight lead-free ceramics as eco-friendly alternatives for harvesting urban acoustic energy, enabling sustainable powering of low-power IoT devices and smart infrastructure. This work advances green nanomaterials for next-generation energy systems aligned with environmental safety and renewable-energy goals.

Keywords: Lead-free piezoelectrics; noise-to-electricity; energy harvesting; BNT; BT–BT.

References:

[1] Rödel, J., Jo, W., Seifert, K.T.P., Anton, E.M., Granzow, T., & Damjanovic, D., Perspective on the development of lead-free piezoceramics, Journal of the American Ceramic Society, 92(6) (2009) 1153–1177.

[2] Erturk, A., & Inman, D.J., Piezoelectric Energy Harvesting, John Wiley & Sons, Chichester, UK (2011).

Electron Transport investigation in Carburized and Fluorinated h-Boron Nitride nanoribbons

Ankur Dwivedi[a*], Ankur Pandya[a], Keyur Sangani[a], Prafulla K. Jha[b]
[a]Institute of Technology, Nirma University, Ahmedabad-382481, India
[b]Department of Physics, Faculty of Science, The M.S.University of Baroda, Vadodara-390002, India.
[*]Corresponding author: [a]ankur_dwivedi@nirmauni.ac.in

ABSTRACT

Hexagonal boron nitride nanosheets (h-BNNS) have gained significant attention in recent years due to their close structural resemblance to the wonder material graphene, in which alternating boron and nitrogen atoms replace carbon atoms in a hexagonal lattice. Unlike graphene, bulk hexagonal boron nitride is an electrical insulator, which limits its direct application in micro- and nanoelectronic devices. However, when thinned to nanosheets and appropriately doped, h-BN exhibits promising semiconducting behavior. For instance, fluorine-doped h-BN nanosheets show markedly enhanced electrical properties. This has stimulated recent efforts toward controlled and constructive synthesis routes that enable the development of devices based on such advanced materials. These materials find potential applications in nitrogen fixation, gas adsorption, hydrogen storage, polymer composites, printable electronics, biosensors, water filtration, and gas sensing. In this context, the present study investigates the electronic transport properties, specifically electron mobility and effective mass, of carbon- and fluorine-doped h-BN nanoribbons. Calculations are performed considering electron–acoustical phonon interactions through deformation potential and polar acoustical phonon scattering mechanisms under low applied electric fields. The dependence of electron mobility and effective mass on carbon doping concentration is analyzed over a wide temperature range at a constant electric field of approximately 1 μV/nm. The results indicate that the acoustical phonon-limited electron mobility remains nearly independent of carbon doping concentration in carburized boron nitride nanoribbons.

Keywords: Boron nitride nanoribbon, Acoustical Phonon interaction, electron mobility

References:

[1] A Aldalbahi, A F Zhou, P Feng, Variations in Crystalline Structures and Electrical Properties of Single Crystalline Boron Nitride Nanosheets, Scientific reports, 5, 16703 (2015). doi:10.1038/srep16703.

[2] Zhao J, Chen Z, Single Mo atom on defective boron nitride monolayer as an efficient electrocatalyst for nitrogen fixation: A computational study, J. Am. Chem. Soc., doi: 10.1021/jacs.7b05213. (2017).

Electronic Structure and Magnetism in $MgZnX_2$ (X = Co, Rh, Ir): A First-Principles Comparative Study

Adwait Mevada*[a], N.Y. Pandya[b] , P.N. Gajjar[c]
[a] Jeel Goswami College of Science and Research, Monark University, Vahelal, Gujarat, India
[b] Government Commerce and Science College, Dahej, Bharuch, Gujarat, India
[c] Department of Physics, University School of Sciences, Gujarat University, Ahmedabad-380009, Gujarat, India.
*Corresponding author: [a] adwait.mevada.fos@monarkuni.ac.in

ABSTRACT

MgZn ternary alloys have attracted interest due to their lightweight character and tunable electronic properties. Our current work presents a density functional theory (DFT) study of $MgZnX_2$ compounds, where X = Co, Rh, and Ir. Electronic band structures, electronic density of states, electronic charge density plots and Fermi surface of $MgZnX_2$ (X = Co, Rh, Ir) have been computed using Density Functional Theory (DFT). The $MgZnX_2$ (X = Co, Rh, Ir) display metallic character as shown and exhibits highly dispersive conduction bands. The present study demonstrates that $MgZnRh_2$ and $MgZnIr_2$ are non-magnetic, in contrast to $MgZnCo_2$, which exhibits spin-polarized states. Electronic charge density plot reveals that Zn-X bonding dominates the electronic structure while Mg acts as an electron donor in the $MgZnX_2$ (X = Co, Rh, Ir). Fermi surfaces grow in complexity with the increasing atomic number of the substituent element. Our results demonstrate that group-IX substitution effectively controls the magnetic and electronic properties of Mg–Zn–based ternary alloys, highlighting their potential for metallic and spin-dependent applications.

Keywords: MgZn alloys, DFT, Electronic band structure, Electronic Charge Density, Fermi surface

References:

[1] Wederni A, Daza J, Ben Mbarek W, Saurina J, Escoda L, Suñol J-J. Crystal Structure and Properties of Heusler Alloys: A Comprehensive Review. *Metals*. 2024; 14(6):688.

Multiscale Computational Investigation of Pentacyclic Triterpenoids: Structural, Electronic, and Dynamical Analyses of EGFR Inhibition and Amino Acid Interactions

Akhilesh Kumar Gupta[1*], Riddhi Sainda [1], Keyur N. Vyas[1] and Prafulla K. Jha[1]
[1]Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat – 390002, India

ABSTRACT

This study explores the intersection of computational biophysics and nanobiotechnology has opened new avenues for understanding the multifunctional activity of naturally occurring biomolecules. This study presents a comprehensive multiscale investigation into the structural, electronic, and vibrational properties of pentacyclic triterpenoids—specifically Lupeol, Morolic Acid, Hederagenin, and Quinovic Acid—focusing on their interactions with the Epidermal Growth Factor Receptor (EGFR; PDB ID: 1M17) and the amino acid Glycine. The research employs a tripartite computational protocol involving molecular docking, Density Functional Theory (DFT), and Molecular Dynamics (MD) simulations to bridge the gap between static binding predictions and time-dependent physical behavior. Detailed interaction profiling indicated that binding is predominantly governed by hydrophobic van der Waals and alkyl forces, with minimal polar contribution . Furthermore, Density Functional Theory (DFT) calculations at the B3LYP/6-31G(d) level were utilized to investigate the Lupeol-Glycine complex. Analysis of Frontier Molecular Orbitals (FMOs), Mulliken charge distributions, and Global Reactivity Parameters (GRP) provided deep insights into charge transfer mechanisms and electronic stability . The inclusion of a Polarizable Continuum Model (PCM) demonstrated the significant role of aqueous solvation on the complex's electronic structure, revealing a trend in global reactivity parameters where the solvated complex exhibited the highest softness and electrophilicity . Finally, Molecular Dynamics (MD) simulations over a 60 ns window using GROMACS confirmed the structural stability of the Lupeol-1M17 complex. Radial Distribution Function (g(r)) analysis elucidated the solvent dynamics and local structural ordering around the complex . This integrated approach provides a robust physics-based framework for the rational design of these natural triterpenoids as potential therapeutic agents.

Keywords: EGFR, Triterpenoids, Molecular Docking, DFT, Molecular Dynamics, Lupeol, Glycine

Realizing Piezoelectricity in 2D Janus Nanowire by Green's Function Approach

Sandeep Malhotra, Ankur Pandya
Institute of Technology, Nirma University, Ahmedabad-382481, India.
Corresponding Author: *ankur.pandya@nirmauni.ac.in

ABSTRACT

The concept of piezoelectricity has been realized by researchers as an electromechanical coupling between the pressure or stress applied to the active part of the electromechanical system (EMS) and the electric polarization produced thereof for more than three decades of years. Such a concept is effectively utilized by nanoelectromechanical systems (NEMS), the miniaturized counterpart of existing electromechanical systems, via which they are able to exhibit novel characteristics and applications [1-3]. The novel Green's function approach is demonstrated to investigate the induced piezoelectricity in one of the 2D Janus materials $MoSSe_2$ nanowire, by calculating the carrier transmission function of the system. Because $MoSSe_2$ nanowire, as a material, exhibits non-centrosymmetric structure, and hence it is possible to realize the piezoelectric nature under the impact of an impulse. Green's function is useful to capture the collection of impulsive responses under the impact of stimuli. Considering the shear modulus of graphene, the variation in density is investigated as a function of both compressive and elongated impulsive pressure. The results and the methodology adopted in the present work will pave the way to analyze the working and behavior of nanoelectromechanical systems (NEMS) at the nanoscale level. In the present work, Green's function-based mathematical modelling is proposed for a deeper understanding of the relation between impulse to the $MoSSe_2$ nanowire and transmission function with different deflections at different positions. These calculations are able to provide further help to understand the mechanical vibrational properties of nano-resonators made of intercalated 2D Janus materials. The findings and methods used in this study will open up ways to examine how nanoelectromechanical systems (NEMS) function and behave at the nanoscale.

Keywords: Green's function, nanoelectromechanical system (NEMS), 2D Janus materials

References:

[1] G J Verbiest, J N Kirchhof, J Sonntag, M Goldsche, T Khodkov, and C Stampfer, Detecting Ultrasound Vibrations with Graphene Resonator, ACS, 18 (2018), 5132–5137.

[2] H Craighead, Nanoelectromechanical systems, Science, 290 (2000), pp.1532-1535.

Structural, optical and antibacterial properties of chemically grown zinc oxide nanoparticles

Parth Shukla [a], Masira Pathan [a], Indrajitsinh Bihola [b], Dipika Patel [a], Piyush Solanki [b], Nikesh A. Shah [b], Keval Gadani*[a],
[a] Centre of Education, Indian Institute of Teacher Education (IITE), Gandhinagar – 382016, India
[b] Department of Physics, Saurashtra University, Rajkot – 360005, India
*Corresponding author: [a] kjgadani@gmail.com

ABSTRACT

In the present, zinc oxide nanoparticles were synthesized by chemical route sol–gel method. The XRD pattern confirms that the ZnO nanoparticles (NPs) exhibit the hexagonal structure. From XRD, crystallite size ($CS=0.9\lambda/\beta\cos\theta$) is found to be ~17.52 nm. Rietveld refinements have been performed using FULLPROF software to verify the structural phase purity for ZnO NPs. The SEM images revealed that the spherical surface morphology of ZnO NPs. Energy dispersive X-ray analysis (EDAX), carried out for elemental analysis for the studied of nanoparticles. The optical properties are investigated using UV–Visible absorption spectra. Moreover, the antibacterial activity of ZnO nanoparticles were investigated using the disk diffusion method. Frequency–dependent dielectric response, and a.c. conductivity have been carried out in the range of 20Hz to 2MHz frequency at room temperature.

Keywords: Sol–gel; ZnO; Crystallite size; Grain size; Optical bandgap.

References:

[1] Monalisa Tiwari, Vishvanath Tiwari, Neha Mishra, Keval Gadani, Piyush S. Solanki, Nikesh Shah, Mechanism of anti-bacterial activity of Zinc Oxide nanoparticle against carbapenem resistant Acinetobacter baumannii, Frontiers in Microbiology, 09 (2018) 1218.

[2] K.N. Rathod, Zalak Joshi, Davit Dhruv, Keval Gadani, Hetal Boricha, A. D. Joshi, P.S. Solanki and N. A. Shah, Size Effects on Electrical Properties of Chemically Grown Zinc Oxide Nanoparticles, Materials Research Express, 05 (2018) 035040.

Ab Initio Investigation of the Structural, Electronic, Magnetic, and Thermodynamic Characteristics of Half-Heusler CrMnGe

Arjun Rathod[a]*, A. M. Vora [b]
[a,b] Department of Physics, University School of Sciences, Gujarat University, Navrangpura, Ahmedabad – 380 009, Gujarat, India
*Corresponding author: [a] arjunnrathod@gmail.com

ABSTRACT

The structural, electronic, elastic, and thermodynamic properties of the half-Heusler alloy CrMnGe were investigated using Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) exchange correlation functional, implemented in the Quantum ESPRESSO code. Among the considered atomic configurations, the α-phase, where Cr, Mn, and Ge occupy the (0,0,0), (0.25,0.25,0.25), and (0.5,0.5,0.5) sites, respectively, is found to be the most stable. The calculated elastic constants indicate elastic anisotropy and ductile behavior, while compliance with the Born–Huang criteria confirms elastic stability. Structural stability is further supported by the negative cohesive energy, and dynamic stability is verified by the absence of imaginary phonon frequencies. Electronic band structure and total density of states analyses reveal that CrMnGe exhibits half-metallic behavior. The projected density of states shows that Cr-4s and Cr-3d states dominate the conduction band, whereas Mn-3d states mainly contribute to the valence band. The total magnetic moment is calculated to be 0.95 μB, close to 1 μB and consistent with the Slater–Pauling rule. These features suggest that CrMnGe is a promising candidate for spintronic applications.

Keywords: Half-Heusler alloy, Density Functional Theory (DFT), Quantum ESPRESSO, GGA-PBE, Half-metallicity, Spintronics.

References:

[1] Ahmed, S., Shakil, M., Zafar, M., Choudhary, M. A., & Iqbal, T., Structural, electronic, and magnetic properties of CrMnX (X = Ge, Se, Si, and Sn) compounds, Canadian Journal of Physics, 98(3) (2020) 291–296.

Temperature and Concentration Effects on Volumetric, Viscometric, and Optical Properties of p-Anisaldehyde-Methanol Mixtures

N.S. Shah [a*], H.P. Vankar[b], V.A.Rana [c]
[a] New L J Institute of Engineering and Technology, Pakwan, Ahmedabad, Gujarat, India.
[b] Department of Physics, Government Science College, Vankal 394430, Gujarat, India.
[c] Department of Physics, School of Sciences, Gujarat University, Ahmedabad 380009, Gujarat, India
[*]Corresponding author: [a] niralishah259@gmail.com

ABSTRACT

Density (ρ), viscosity (η), and refractive index (n_D) of binary mixtures of p-anisaldehyde (AN) and methanol (MeOH) were measured over the entire composition range at temperatures between 293.15 and 323.15 K. From the experimental data, molar volume (V_m), excess molar volume (V_m^E), excess viscosity (η^E), excess refractive index (n_D^E), and electronic polarizability (α_e) were evaluated. The dependence of these parameters on temperature and concentration was analyzed to examine deviations from ideal mixing behavior. The results provide information on the nature of intermolecular interactions operating in the AN-MeOH system and demonstrate the influence of temperature on volumetric, viscometric, and optical properties of the mixtures.

Keywords: p-anisaldehyde, methanol, excess parameters, molar volume, polarizability

Optical and Electrical Characterization of Zn- and Cd-Doped MnSe Thin Films Deposited by Thermal Evaporation

Darshan Jadav*[a], S M Vyas [a], A M Vora [a]
[a] Department of Physics, University School of Sciences, Gujrat University, Navarangapura, Ahmedabad – 380 009, Gujarat, India.
*Corresponding author: [a] jadavdarshaj@gmail.com

ABSTRACT

Manganese selenide (MnSe) thin films have attracted considerable attention due to their promising thermoelectric, optical, and electronic properties. In this study, pure and Zn- and Cd-doped MnSe thin films were prepared using the thermal evaporation technique and systematically characterized using SEM, EDAX, XRD, UV–VIS absorption spectroscopy, and I-V measurements. XRD analysis confirmed the formation of a hexagonal phase with good crystallinity in all deposited films. Noticeable shifts in diffraction peaks were observed upon Zn and Cd doping, indicating successful incorporation of dopant ions into the MnSe lattice. SEM images revealed uniform and homogeneous surface morphology of the thin films. EDAX analysis verified the stoichiometric presence of Mn and Se, along with the dopant elements, confirming proper film composition. UV–VIS spectroscopy showed strong absorption in the visible region, and the direct band gap was found to vary due to Zn and Cd doping. Electrical characterization through I-V measurements exhibited nonlinear and frequency independent conduction behavior for both pure and doped MnSe films. The doped films displayed modified current transport properties compared to pure MnSe, demonstrating the influence of dopants on charge carrier concentration mechanisms. These results reveal that Zn and Cd doping effectively tunes the structural, optical, and electronic properties of MnSe thin films. Consequently, the prepared films are suitable for potential applications in thermoelectric devices, optoelectronic systems, and energy storage technologies.

Keywords: Doping, Structural, Morphological, Optical, Electric

References:

[1] Jadav, D. J., Varasada, R. R., Trasadiya, M. P., Vyas, S. M., & Vora, A. M. (2024). Synthesize and Investigate Structural, Surface Morphology, Optical, and Electrical Characterization of Cu2Se Thin Films by Thermal Evaporation Technique. *Brazilian Journal of Physics*, *54*(6), 246.

Correlation between Electronic and Thermal properties of 2D materials nanoribbons

Jay Patel[a] , Ankur Pandya[b]
[a,b] Electronics and Communication Engineering Department, Nirma University, Institute of Technology, Sarkhej-Gandhinagar Highway, Ahmedabad, 382481, Gujarat, India.
[*]Corresponding author: [b]ankur.pandya@nirmauni.ac.in

ABSTRACT

Low-dimensional nanoribbons offer a tunable platform in which electronic structure, mechanical stiffness, and thermal response can be engineered simultaneously through geometry and bonding. In this work, we develop a unified correlation-based framework to connect the energy band gap (Eg) and Young's modulus (Y) and to extend this coupling to heat-capacity behaviour (Cp) through lattice-vibrational (phonon) considerations. The approach is applied consistently across five representative two-dimensional material families—graphene, silicene, germanene, stanene, and phosphorene nanoribbons—enabling cross-material comparison within a single modelling viewpoint.[1]We then introduce a thermo-mechanical extension by mapping the dimer-dependent stiffness to acoustic phonon characteristics, enabling estimation of a width-dependent Debye temperature and lattice heat capacity. This produces a parametric correlation between heat capacity and both Young's modulus and bandgap, allowing Cp – Y and Cp – Eg design maps to be constructed at fixed temperature.[2] The resulting formulation supports the construction of design maps linking electronic, mechanical, and thermal metrics, and offers a practical guide for the coupled optimization of nanoribbon-based components in flexible electronics, nanoelectromechanical systems, and thermally constrained device architectures.

Keywords: Nanoribbons, Band gap–Young's modulus correlation, Phonons, lattice vibrations, Lattice heat capacity

References:

[1]Varshni,Y. P. (1967). Temperature dependence of the energy gap in semiconductors. physica, 34(1), 149-154.

[2] Moteria, R., Pandya, A., Sangani, K., & Jha, P. K. (2025). Dimer lines-Dependent Bandgap and Mechano-Electronic Correlations in nanoribbons of 2D materials. Physica B: Condensed Matter, 417372.

Acetone Detection Mechanism on Pristine and F-Terminated Y_2C MXenes: A First-Principles Study

Disha M. Bambhaniya[1, *], Suresh V. Chaudhary[1], Sanjeev K. Gupta[2, *] and P. N. Gajjar[1, *]
[1]Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380009, India
[2]Computational Materials and Nanoscience Group, Department of Physics,
St. Xavier's College, Ahmedabad 380 009, India
[*]Corresponding author: pngajjar@gujaratuniversity.ac.in
sanjeev.gupta@sxca.edu.in and dishambambhaniya@gmail.com

ABSTRACT

Two dimensional (2D) MXenes have attracted considerable interest for gas sensing applications due to their large surface area and tunable surface terminations. Motivated by the experimental realization of Y_2CF_2, this work employs density functional theory (DFT) to evaluate acetone sensing on pristine and fluorine terminated Y_2C MXenes for diabetes biomarker detection. The optimized pristine Y_2C exhibits metallic behavior, whereas Y_2CF_2 displays semiconducting characteristics with a direct band gap of 1.12 eV. Acetone adsorption was studied in horizontal and vertical orientations on both structures, with most negative adsorption energies of −2.59 eV on Y_2C and −0.40 eV on Y_2CF_2, respectively, indicating strong chemisorption on pristine and weaker physisorption on F-terminated surfaces. Also, charge transfer analysis reveals that acetone acts as an electron acceptor on pristine Y_2C but as a donor on Y_2CF_2. Further, desorption time, work function, and projected density of states (PDOS) have been investigated to understand the sensing mechanism and surface interactions of acetone on both structures. These results indicate that Y_2C and Y_2CF_2 MXenes are promising candidates for acetone biomarker detection, with tunable interaction strengths and favorable sensing properties.

Keywords: Density functional theory (DFT), Sensing, MXenes, Projected density of states (PDOS)

References:

[1] Liu X, Zhou Q, Shen J, Ju W, Chai Z, Zhao Z. H2S sensitivity of transition metal-doped Y2CF2 with F-vacancies: A DFT study. Vacuum 2024;226:113334. https://doi.org/10.1016/J.VACUUM.2024.113334.

[2] Maeda K, Wakayama H, Washio Y, Ishikawa A, Okazaki M, Nakata H, et al. Visible-Light-Induced Photocatalytic Activity of Stacked MXene Sheets of Y2CF2. The Journal of Physical Chemistry C 2020;124:14640–5. https://doi.org/10.1021/ACS.JPCC.0C03072.

Rare-Earth (Nd) Substitution Induced Structural and Functional Modulation in Green Synthesized M-Type Ba–Sr Hexaferrites

Astha R. Patel [a], Dharti Tank [a], Rajshree B. Jotania [b], Niranjan M. Devashrayee [c], Chetna C. Chauhan [c], Abhishek A. Gor*[a]

[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar, 382426, Gujarat, India.

[b] Department of Physics, Electronics, and Space Science, University School of Sciences, Gujarat University, Navrangpura, Ahmedabad, 380009, Gujarat, India.

[c] Electronics and Communication Engineering Department, Nirma University, Institute of Technology, Sarkhej-Gandhinagar Highway, Ahmedabad, 382481, Gujarat, India.

*Corresponding author: abhishekgor5@gmail.com

ABSTRACT

Nd-substituted M-type hexaferrites, $Ba_{0.75}Sr_{0.25}Fe_{12-x}Nd_xO_{19}$ with Nd content x varied from 0.0 to 0.5, were synthesized using green synthesis approach employing Moringa oleifera leaf extract, followed by calcination at 1100 °C. The influence of Nd substitution was examined through a systematic study of the structural, microstructural, vibrational, thermal, magnetic, and dielectric properties. A well-developed hexagonal platelet morphology with grain size variation upon Nd incorporation was observed in the FESEM images. X-ray diffraction analysis confirmed single-phase hexagonal M-type structures for all compositions, with lattice distortions consistent with Nd^{3+} substitution at Fe^{3+} sites. Raman spectroscopic analysis showed composition-dependent shifts in characteristic vibrational modes associated with cation substitution. Magnetic studies confirmed hard magnetic behavior accompanied by multi-domain structures in all samples. Cole–Cole plots of frequency-dependent dielectric and impedance data indicate non-Debye relaxation governed by grain and grain-boundary effects. Nd substitution enabled tunable magnetic and dielectric properties, and the biogenically synthesized hexaferrites demonstrate potential for multifunctional applications in magnetic, microwave, and electronic devices.

Keywords: Hexaferrites; Rare-Earth Substitution; Functional Ferrites

References:

[1] Abhishek A. Gor, N.M. Devashrayee, Tanuj Gupta, Chetna C. Chauhan, Rajshree B. Jotania, A study of the effect of the Cu and Cr co-doping on structural, magnetic and dielectric properties of barium hexaferrites synthesized in presence of mentha leaves extract, Materials Today Communications, Volume 37,2023,107214,ISSN 2352-4928.

[2] Devang Anadkat, Chandrababu Badampudi, Abhishek Gor, Anup V. Sanchela, Investigation of frequency dependent dielectric properties of La-doped BaSnO3-ZnSnO3 solid-solutions, Journal of Alloys and Compounds, Volume 958,2023,170350,ISSN 0925-8388.

Credibility and Future Potential of Laser-Induced Breakdown Spectroscopy as a Next-Generation Analytical Technique

Jumisree Sarmah Pathak[*a], Arvind Kumar Saxena [b]
[a] Department of Physics, Indian Institute of Teacher Education, Gandhinagar, Gujarat.
[b] School of Forensic Sciences, National Forensic Sciences University, Gandhinagar, Gujarat.
[*]Corresponding author: [*a] jumishreep@iite.ac.in

ABSTRACT

Laser-Induced Breakdown Spectroscopy (LIBS) has evolved into a versatile atomic emission based analytical technique capable of rapid, multi-element detection with minimal or no sample preparation. Driven by advances in laser sources, spectrometers, detectors, and data analytics, LIBS has transitioned from a primarily qualitative laboratory method to a semi-quantitative and increasingly standardized analytical platform. This paper critically evaluates the analytical credibility of LIBS in terms of accuracy, precision, sensitivity, reproducibility, and robustness, with particular emphasis on its comparison to established techniques such as inductively coupled plasma mass spectrometry and optical emission spectrometry (ICP-MS, ICP-OES), and X-ray fluorescence (XRF). Recent technological developments like double-pulse excitation, femtosecond LIBS and machine-learning-assisted spectral interpretation, are also discussed with special attention to forensic science applications, where LIBS has demonstrated strong potential for rapid screening and discrimination of trace evidence. Current challenges related to matrix effects, standardization, and quantitative reliability are analyzed, and future research directions toward hybrid systems, artificial intelligence integration, and international standardization are outlined. Overall, the paper positions LIBS as a credible next-generation analytical technique with expanding scientific, industrial, and forensic relevance.

Keywords: Laser-Induced Breakdown Spectroscopy (LIBS); analytical credibility; next-generation analytical techniques; forensic analysis; elemental analysis

References:

[1] Zhang, Y., Zhang, T. & Li, H. Application of laser-induced breakdown spectroscopy (LIBS) in environmental monitoring, Spectrochimica Acta Part B: Atomic Spectroscopy, 181, (2021) 106218

[2] Królicka A, Maj A, Łój G. Application of Laser-Induced Breakdown Spectroscopy for Depth Profiling of Multilayer and Graded Materials. Materials. 2023; 16(20), 6641.

Fabrication and Characterization of Dye Sensitized Solar Cells

Bhavesh Motwani[1], Neha Patni[1*], Chetna Chauhan[1]
[1]Institute of Technology, Nirma University, S. G. Highway, Ahmedabad, Gujarat 382 481, India
*Corresponding author: neha.patni@nirmauni.ac.in

ABSTARCT

Dye-sensitized solar cells (DSSCs) are viewed as an affordable and eco-friendly option to traditional solar technologies, yet their broader adoption is constrained by effectiveness and material durability. This research involved the fabrication of a DSSC utilizing naturally sourced dyes and affordable electrode materials. A photoanode made of nanostructured metal oxide was used to improve dye absorption and facilitate efficient charge transfer, whereas the counter electrode allowed for stable redox reactions in the electrolyte. The device's performance was assessed under standard lighting conditions, and the physical, structural, and chemical characteristics of the active layers were analyzed to confirm high film quality and adequate dye interaction. The constructed DSSC exhibited distinct photovoltaic characteristics, reaching a maximum power conversion efficiency of 9.67%. The findings indicate that precise management of material structure and interfacial interactions is crucial for enhancing device performance. This study emphasizes the capability of natural dyes for effective and eco-friendly DSSCs and offers a pragmatic direction for additional optimization.

Keywords: Dye Sensitized Solar Cells, Natural Dyes, IV Characteristics, Conversion Efficiency

References:

[1] N. Patni, S. G. Pillai, and P. Sharma, “Effect of using betalain, anthocyanin and chlorophyll dyes together as a sensitizer on enhancing the efficiency of dye-sensitized solar cell,” Int. J. Energy Res., vol. 44, no. 14, pp. 1–14, 2020.

[2] N. Patni, P. Sharma, and S. G. Pillai, “Newer approach of using alternatives to (Indium doped) metal electrodes, dyes and electrolytes in dye sensitized solar cell,” Mater. Res. Express, vol. 5, no. 3, pp. 1–15, 2018

Ab Initio Study of the Structural Stability and Electronic Behavior of the $MnCo_2Si$ Heusler Alloy

Dipika B Patel*[a], Jaysukh Markna [b], Dev Karelia [C], Bhargavkumar Patel [d]
[a] Center of Education, Indian Institute of Teacher Education, Gandhinagar-382016, India.
[b] Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot-360005.
[c] Center of Education, Indian Institute of Teacher Education, Gandhinagar-382016, India.
[d] Beckman Coulter, Miami, Florida 33196 USA
*Corresponding author: [a] deeps2210@gmail.com

ABSTRACT

This study presents a comprehensive first-principles investigation of the structural and electronic properties of the $MnCo_2Si$ Heusler alloy using spin-polarized density functional theory (DFT). The calculations are carried out using the generalized gradient approximation (GGA) for the exchange–correlation functional. Structural optimization is achieved through total energy minimization, yielding equilibrium lattice. The optimized tetragonal structure was confirmed through total energy minimization and self-consistent field convergence. The thermodynamic stability of $MnCo_2Si$ is evaluated via formation energy calculations. The electronic properties are examined by analyzing the spin-resolved band structure and density of states. The results indicate that the electronic characteristics are predominantly governed by the hybridization of Mn and Co 3d states, while Si contributes mainly to band dispersion at lower energies. The electronic band structure and spin-resolved density of states revealed a half-metallic nature, characterized by a bandgap in the spin-up channel and metallic behavior in the spin-down channel, resulting in 100% spin polarization at the Fermi level. The obtained first-principles insights of $MnCo_2Si$, suggesting its potential applicability in spin-dependent electronic (spintronic) and magneto optical devices.

Keywords: DFT, Spintronic, Heusler alloys, Density of states, Spin-polarized band structure

References:

[1] Al-Douri Y and Ameri M Physical studies of spintronics-based Heusler alloys Critical Reviews in Solid State and Materials Sciences 50 (2025) 189–238.

[2] Lakhani P, Sidhdhapura P, Vala M, Dudhrejiya T, Udani N, Dodia S, Jadav G, Solanki P, Dhruv D and Sharko S A. Investigations on Electronic Structure and Transport Property Modifications of La0. 7Ca0. 3-xKxMnO3 ceramics. Physica B: Condensed Matter 417279 (2025).

Characteristics of Cos Gaussian beams in presence of a Photonic Double-Defect Super-Lattice in photorefractive crystals with both linear and quadratic electro optic effect

Gaurang Potdar [a], Ritesh K Chourasia[b], Aavishkar Katti*[a,]

[a]Affiliation Department of Physics, Dr Vishwanath Karad MIT World Peace University, Kothrud, Pune 411038,

[b] Post-Graduate Department of Physics, Samastipur College (A Constituent Unit of L.N.M.U., Darbhanga-846004, Bihar, India

*Corresponding author: [a] aavishkar.katti@mitwpu.edu.in, [b]riteshphyzics@gmail.com

ABSTRACT

Cos-Gaussian beam (CG beam) is a structured beam from the family of exotic beams and is a preferred choice for studies and application of self-trapping, self-focusing and soliton formations [1],[2]. The Cosine Control Parameter changes the Cosine envelope structure, leading to petal formations for higher order beams. While self-trapping and soliton formation effects for Cos Gaussian beams are studied and well documented, the effect on the spatial propagation of the structured beam after introduction of a photonic lattice remains largely undocumented. For the current study, a novel Photonic Super-Lattice with double defect (PSDD) is considered to be embedded in a PMN-0.33PT photorefractive crystal, and we investigate the propagation characteristics of the cos Gaussian beam through this system. The linear and quadratic nonlinear coefficients are a direct function of the applied electric field and display an interesting interplay while leading to self-trapping effect. The introduction of the PSDD itself induces strong self-trapping effects, which are not directly formed in their absence, but are formed by the scaling of the electric field thus the nonlinear coefficients. The research also focuses on asymmetrical PSDD where one defect is a positive defect while other is a negative defect. The work finds applications in optical communication, and interconnects.

Keywords: Cos Gaussian beam, Photonic lattices, Structured beams, Defect Superlattice, Optical Soliton

References:

[1] Potdar, G. and Katti, A., 2025. Temporal evolution, propagation and mutual interaction of cos-gaussian beams in photorefractive crystals exhibiting both the linear and quadratic electro-optic effect. Physica Scripta, 100(2), p.025525.

[2] Ethuin, C., Bouldja, N. and Wolfersberger, D., 2025. Nonlinear Airy beam propagation in defected photonic lattices. Optics Letters, 50(3), pp.800-803.

Vanadium-Doped Barium Hexaferrite as a Tunable Magnetic-Dielectric Platform for Wideband MIMO Antenna Applications

Dharti Tank [a], Anil Pandya [a], Anmol Jaiswal [a], Niranjana C.S [a], Vidit Patel [a], Vijayalakshmi Iyer [a], Yatharth Thakar [a], Arpan Desai [b], Abhishek A. Gor *[a]

[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India.

[b] Department of ICT, School of Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India.

*Corresponding author: [a] abhishekgor5@gmail.com

ABSTRACT

Vanadium-doped M-type Barium Hexaferrite ($BaFe_{12-x}V_xO_{19}$, (V substitution levels of 0,0.1and 1 at %)) was synthesized via solid-state reaction and investigated for structural, magnetic, and dielectric properties. XRD confirms the hexagonal BaM phase ($P6_3/mmc$), with minor secondary phases at higher doping. FTIR and Raman spectra revealed shifts and broadening of Fe-O vibrations, confirming lattice distortion induced by V doping. FESEM revealed hexagonal platelet morphologies, shifting from smooth edges in pure BaM to wedge-shaped features in V-doped samples, due to lattice strain. Magnetization remained stable at low doping but decreased significantly at higher substitution. Dielectric analysis (20Hz - 20GHz) shows reduced permittivity (ε') and losses at high frequencies, enhancing stability, while AC conductivity increased with frequency due to electron hopping between Fe^{2+}/Fe^{3+} ions at octahedral sites. Electromagnetic characterization using VNA-extracted dielectric parameters was employed to design and simulate a four-element dielectric resonator antenna (DRA) enabling wideband MIMO operation across C-K bands with efficiency >85%, isolation <-30dB, diversity gain >9.5dB, and envelope correlation coefficient <0.005. These results demonstrate the potential of V-doped BaM as a tunable magnetic-dielectric platform for compact, multiband, high-efficiency antennas in next - generation wireless communication.

Keywords: V-doped BaM, Hexaferrite, VNA, MIMO Antennas.

References:

[1] Pullar, Robert C. Progress in Materials Science 57.7 (2012): 1191-1334.

[2] Desai, Arpan, et al. " IEEE Access 10 (2022): 57641-57654.

Study of Physical and Dielectric Properties of Sabarmati River Water in Ahmedabad City

Jeet R. Makkampara, Kushal P. Mehta, Jesalkumar R. Soni, Deepak Gadani*
Department of Physics, University School of Sciences, Gujarat University, Ahmedabad, Gujarat, India
*Corresponding author: *dhgadani@gujaratuniversity.ac.in

ABSTRACT

This study examines the physical and dielectric properties of Sabarmati River water across eight locations in Ahmedabad, using distilled water as a reference. Variation of pH, TDS, conductivity, density, viscosity, and refractive index for the water samples was measured. Acoustic properties, including adiabatic compressibility and impedance, were determined via an ultrasonic interferometer. Results show an increase in Total Dissolved Solids (TDS) from 105 ppm (Chiloda bridge) to 826 ppm (Kamod Bridge), correlating with an increase in electrical conductivity from 217 to 1762 µs/cm. Acoustic analysis using an ultrasonic interferometer revealed that ultrasonic velocity increased from 1511.66 to 1523.33 m/s, while adiabatic compressibility decreased from 4.553×10^{-10} to 4.452×10^{-10} m^2/N, with increase in TDS of water samples. Electrical characterization was performed using a precision LCR meter (Agilent E4980A) (20Hz–2MHz), analysing dielectric constant, losses, tan(δ), and complex impedance. Notably, the dielectric losses at 2 MHz increased from 276.5 from Nana Chiloda bridge water to 2411.49 in downstream samples due to increase in TDS content of water samples. Nyquist plots confirmed distinct relaxation mechanisms related to pollution levels. The integration of acoustic and dielectric measurements provides a sensitive, non-destructive method for monitoring urban river health.

Keywords: Sabarmati River, Dielectric Constant, Water Quality, Dielectric Spectroscopy, Acoustic properties.

Effect of Variation of Moisture and Fertilizer Solution on Complex Permittivity of Soil at Microwave Frequencies

Prahlad Chaudhary*[a], Jayesh Shir[b], Deepak Gadani[c]
[a] M. N. College, Visnagar, Gujarat, India.
[b] Government Arts and Science College, Bavla, Ahmedabad, Gujarat, India.
[c] Department of Physics, Gujarat University, Ahmedabad, Gujarat, India.
*Corresponding author: [a] pdchaudhary009@gmail.com

ABSTRACT

In this study, the complex permittivity ($\varepsilon^* = \varepsilon' - j\varepsilon''$) of the moist and fertilized moist soil was measured across different volumetric moisture contents (MC) within the frequency range from 0.5 to 10 GHz using a Vector Network Analyzer (VNA). The experiment was conducted to measure the complex permittivity of soil samples with varying moisture content (MC) of distilled water (DW), and fertilizer solutions. It is observed that dielectric constant ε' and dielectric loss ε'' for the soil increases with the increase in MC in the soil. As compared to ε', the dependency of ε'' on types of fertilizers present in the soil is clearly observed. The measured values of complex permittivity for the soil samples were compared with the calculated values using the DHG-ADV (Gadani-Vyas) model. A good agreement at 5.35 GHz (C-band) and 9.5 GHz (X-band) frequencies have been observed between the measured values and calculated values using the model, and the results are reported.

Keywords: Dielectric constant, Dielectric loss, Fertilizer, Soil moisture, Microwave.

A DFT Study of Strain-Controlled Chiral Magnon Splitting in Tetragonal β-MnO_2 Altermagnet

Apeksha Gauswami [a] and Prafulla K. Jha[*a]
Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India.
[*a] Corresponding author: prafullaj@yahoo.com

ABSTRACT

In this work, we present a comprehensive first-principles density functional theory (DFT) study of chiral magnons in tetragonal β-MnO_2, a collinear compensated altermagnet. Phonon and AIMD calculations confirm the dynamical and thermal stability of the tetragonal lattice and establish an antiferromagnetic ground state exhibiting momentum-dependent spin splitting, a hallmark of altermagnetic order. Using a DFT+Wannier approach, we extract Heisenberg exchange parameters and find that the magnetic interactions are dominated by nearest-neighbour antiferromagnetic coupling, leading to non-degenerate magnon modes. The spin-wave spectra, calculated within linear spin-wave theory, clearly reveal chiral magnon behaviour in the form of non-reciprocal dispersion and chirality-dependent magnon band splitting. This splitting originates from exchange anisotropy interactions allowed by the crystal symmetry, even in the absence of net magnetization. We further investigate the role of lattice strain on magnon excitations and demonstrate that compressive strain significantly enhances the magnon spin splitting, whereas tensile strain suppresses it. These results establish strain as an effective external knob to control chiral magnon properties. Overall, our findings identify β-MnO_2 as a promising altermagnetic material for spintronic and magnonic applications, offering field-free unidirectional spin transport and strain-tunable chiral excitations.

Keywords: Altermagnetism, Spin-splitting, Exchange interaction, Spin-wave theory and Chiral Magnons.

References:

[1] Y. Noda, K. Ohno, and S. Nakamura, Momentum-Dependent Band Spin Splitting in Semiconducting MnO2: A Density Functional Calculation, Phys. Chem. Chem. Phys. **18**, 13294 (2016).
[2] L. Šmejkal et al., Chiral Magnons in Altermagnetic RuO_2, Phys. Rev. Lett. **131**, 1 (2023).

Analysis of dielectric properties of sweet basil leaves cultivated hydroponically over the 100 Hz to 15 GHz frequency range

Pratipal D. Chauhan[a], Deepak H. Gadani[b]*, Vipin A. Rana[c]
[a,b,c] Department of Physics, University School of Sciences, Gujarat University, Ahmedabad-380009, Gujarat, India.
*Corresponding author: dhgadani@gujaratuniversity.ac.in

ABSTRACT

Sweet Basil was cultivated hydroponically in a laboratory environment, under controlled atmosphere of lighting using LEDs of suitable wavelengths, and a nutrient solution containing NPK fertilizers. The complex permittivity ($\varepsilon^* = \varepsilon' - j\varepsilon''$) of the Basil leaves was measured over 100 Hz to 2 MHz using a precision LCR-Meter in association with a parallel plate capacitive solid test fixture (Agilent 16451-B), and 0.5 GHz to 15 GHz using a semi-rigid coaxial probe connected with a vector network analyzer (Anritsu Shockline Model-MS46322A). The dielectric constant (ε') and dielectric loss (ε'') decrease as moisture content in the Basil leaves decreases. At a given moisture level, both (ε') and (ε'') decrease with increase in frequency from 100 Hz to 2 MHz. In microwave frequency range it has been observed that, the dielectric loss decreases with increase in frequency, but at higher moisture contents in the leaves dielectric loss increases with increase in frequency from 5 GHz towards 14 GHz, which represents the presence of free water. The relative dielectric loss of the leaves with respect to that of drier leaves over the microwave frequency range provides clear distinction of bound water from free water in the leaves at frequency approaching towards 14 GHz.

Keywords: Dielectric properties, Sweet Basil leaves, Moisture content, Bound/Free water, Hydroponics

References:

[1] Gadani D.H, Rana V.A, Vyas A.D, & Bhatnagar S.P, Effect of saline water on emissivity of soil, Indian Journal of Radio & Space Physics, 40 (4) (2011) 218–226.

[2] Ulaby F.T & Jedlicka R.P, Microwave Dielectric Properties of Plant Materials, IEEE Transactions on Geoscience and Remote Sensing, vol. GE-22(4) (1984) 406-415.

Multiphysics Simulation of Electromagnetic-Thermal Coupling in Metal-Ceramic Compacts During Microwave Heating

Dr. Shruti C Bhatt *[a]
[a] Mechanical Engineering Department, Nirma University
*Corresponding author: [a]shruti.mehta@nirmauni.ac.in

ABSTRACT

Microwave heating of materials fundamentally couples electromagnetic field distributions within the resonant cavity to volumetric heat generation and subsequent thermal transfer processes. This numerical investigation develops a 3D multiphysics model using COMSOL Multiphysics 6.2 to simulate the microwave heating behavior of Al/SiC metal matrix composites inside a multimode microwave cavity applicator. Symmetry boundary conditions are strategically applied to develop model geometry, significantly reducing mesh density and computational time. Key analyses examine electric field intensity patterns, sample heating rates , and spatial temperature uniformity, with systematic parametric studies quantifying the influences of variable microwave source power (500–1000 W range) and alternative sample mold materials on both temperature evolution and cavity field parameters. The coupled electromagnetic-thermal solver accurately predicts hotspot formation driven by SiC reinforcement's selective microwave absorption within the aluminum matrix. Experimental validation against infrared pyrometry measurements during controlled heating trials demonstrates excellent model fidelity, achieving temperature prediction errors below 5% across full ramp-up cycles. These findings advance fundamental understanding of complex multimode heating dynamics in Al/SiC composites and provide optimizing power profiles and mold configurations to maximize heating rates while minimizing thermal gradients, ultimately enhancing sintering uniformity.

Keywords: Microwave Heating, Composites, Multiphysics Simulation, Heating Dynamics

References:

[1] Rybakov, Kirill I., Eugene A. Olevsky, and Ekaterina V. Krikun. "Microwave sintering: fundamentals and modeling." Journal of the American Ceramic Society 96.4 (2013): 1003-1020.

[2] Devi, Jutika, and M. Jaleel Akhtar. "Multiphysics modeling of metal ceramic compact for microwave processing." 2012 7th European Microwave Integrated Circuit Conference. IEEE, 2012.

Synthesis and Multifunctional Properties of $Fe_2(MoO_4)_3$ for Magneto-Electronic Applications

Devarshi A. Brahmakshatriya [a], Dharti Tank[a], Dr. Abhishek Gor*,
[a]Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge corridor, Raisan, Gandhinagar, Gujarat, India - 382426
*Corresponding author: abhishekgor5@gmail.com

ABSTRACT

This study investigates the structural, optical, dielectric, magnetic and magneto-transport properties of $Fe_2(MoO_4)_3$ synthesized via a solid-state reaction route. X-ray diffraction confirms a single-phase monoclinic structure with a P*nma* symmetry. UV–Vis analysis yields a direct band gap of approximately 1.47 eV, indicating bandgap with direct transitions. Dielectric and impedance spectroscopy reveal strong Maxwell–Wagner interfacial polarization, non-Debye relaxation and hopping-type AC conduction dominated by resistive grain boundaries. Magnetoresistance measurements constitute a key result of this work, showing a small negative MR (up to ~7%) at room temperature together with a field hysteresis between up- and down-field sweeps. The slow and transient relaxation observed in current-time measurements under stepped magnetic fields signifies non-equilibrium transport beyond the scope of simple R_H scaling. Notably, this behavior mirrors the resistive state switching observed with applied voltage, suggesting that $Fe_2(MoO_4)_3$ may support field-tunable switching driven not only by electric fields but also by magnetic fields. Overall, synthesized sample exhibits complex charge dynamics and magnetic-field-dependent behavior, suggesting potential for magnetic sensing and multifunctional oxide-based electronic applications.

Keywords: $Fe_2(MoO_4)_3$, Magnetoresistance, Field-induced switching, Sensing

References:

[1] J.Wang, H. Liu, H. Xiong, and J. Xiao, “Mixed-potential NH3 sensor with Fe2(MoO4)3 as the sensing electrode: Performance and mechanistic insights,” Solid State Ionics, vol. 422, p. 116814, 2025.

DFT Investigation of Electronic and Thermoelectric Properties of Bulk and Two-Dimensional LiGeN

Dev Yogeshbhai Karelia[a], Dipika B Patel*[b], Pratik M. Gadhavi*[c]
[a,b] Centre of Education, Indian Institute of Teacher Education, Gandhinagar-382016, Gujarat, India
[c]Government Engineering College, Gandhinagar-382028, Gujarat, India
*Corresponding author: [b]deeps2210@gmail.com , [C]pratikphd29@gmail.com

ABSTRACT

We present a comprehensive density functional theory (DFT) investigation of the structural, electronic and thermoelectric properties of bulk LiGeN and its two-dimensional (2D) monolayer forms. Structural optimization confirms the energetic stability of both phases. Bulk LiGeN crystallizes in a hexagonal structure with space group $P6_3mc$, characterized by strong Li–N and Ge–N bonding typical of nitride-based materials [1,2]. The electronic band structure reveals a semiconducting nature, with the valence band maximum and conduction band minimum located at distinct high-symmetry points, indicating an indirect band gap. Upon dimensional reduction to the monolayer limit, significant modifications in the electronic band dispersion are observed compared to the bulk phase. Thermoelectric transport coefficients, including the Seebeck coefficient, electrical conductivity, power factor, and dimensionless figure of merit (ZT), are evaluated using Boltzmann transport theory. The 2D LiGeN monolayer exhibits enhanced thermoelectric performance relative to its bulk counterpart, highlighting its promising potential for future thermoelectric applications.

Keywords: LiGeN; Density functional theory; Electronic structure; Thermoelectric properties; Two-dimensional materials

References:

[1] P. K. Kamlesh, P. Pravesh, S. Kumari, and A. S. Verma, "Effect of hybrid density functionals on half-Heusler LiZnX (X = N, P and As) semiconductors: Potential materials for photovoltaic and thermoelectric applications," Phys. Scr., vol. 95, Art. no. 095806, 2020.
[2] C. H. Hu, Y. Yang, and Z. Z. Zhu, "Structural stability and electronic properties of LiNiN," Solid State Commun., vol. 150, nos. 13–14, pp. 669–674, 2010.

Janus HfSeO monolayers for neurotoxicant gas sensing: A first-principles study

Bharat Avdheshsingh Rajput[a], Pratik Gadhavi*[b], Shardul Vadalkar[c], and Narayan N. Som*[d]
[a] Research Scholar, Gujarat Technological University, Ahmedabad, 382424, Gujarat, India
[b] Government Engineering College, Gandhinagar, Gujarat-382028, India.
[c] Department of Applied Science & Humanities, Sardar Vallabhbhai Patel Institute of Technology, Vasad, Gujarat – 388306, India.
[d] Centre for Advanced Materials and Technologies (CEZAMAT), Warsaw University of Technology, 19 Poleczki St, Warsaw 02-822, Poland
*Corresponding author: [b]pratikphd29@gmail.com,[d]somnarayan4@gmail.com

ABSTRACT

Carbon monoxide (CO) and ammonia (NH_3) are widely encountered neurotoxicant gases, with CO regarded as strong and NH_3 comparatively weaker, posing risks in the environment. In this work, the gas-sensing performance of Janus HfSeO monolayers toward CO and NH_3 is investigated using the density functional theory (DFT) framework, employing the GGA functional with vdW-D2 dispersion correction. Pristine HfSeO exhibits semiconducting behavior with a band gap of 1.6 eV. Adsorption energies are evaluated at five distinct sites: Hf-top, O-top, hollow, bridge, and Se-top, and the most energetically favorable configurations are analyzed. CO exhibits moderate physisorption at the Hf-top site with an adsorption energy of −0.41 eV. In contrast, NH_3 shows strong chemisorption at the Hf-top site (−1.1 eV), accompanied by spontaneous migration from less favorable sites. Löwdin charge transfer is higher for NH_3 (∼0.3 |e|) compared to CO (∼0.1 |e|), leading to noticeable electronic structure modulation. Recovery-time estimates indicate rapid desorption for CO (∼8 microseconds at 298 K) and longer recovery for NH_3 ($\sim 10^6$ s), suggesting enhanced sensitivity toward NH_3. Compared to strained $HfSe_2$[1] and Janus MoSSe[2], Janus HfSeO demonstrates superior NH_3 affinity due to its asymmetric Hf–O polarity, establishing its candidature as a material for toxic gas-sensing.

Keywords: Density Functional Theory; Adsorption; Janus Monolayers; 2D Materials; Toxic Gas Sensing

References:

[1] H. Yang, J. Li, Z. Shao, C. Tan, C. Gao, H. Cui, X. Tang, Y. Liu, H. Ye, G. Zhang, Strain-engineered S-HfSe 2 monolayer as a promising gas sensor for detecting NH 3 : A first-principles study, Surfaces and Interfaces. 34 (2022) 102317.

[2] C. Jin, X. Tang, X. Tan, S.C. Smith, Y. Dai, L. Kou, A Janus MoSSe monolayer: A superior and strain-sensitive gas sensing material, J. Mater. Chem. A. 7 (2019) 1099–1106.

Propagation and Transmission Characteristics of Quasiperiodic Fibonacci Chalcogenide–Polymer Bragg Fibers

Dakshata Mandloi [a], Ritesh K Chourasia[b], Aavishkar Katti*[a,]
[a] Department of Physics, Dr Vishwanath Karad MIT World Peace University, Kothrud, Pune 411038,
[b] Post-Graduate Department of Physics, Samastipur College (A Constituent Unit of L.N.M.U., Darbhanga-846004, Bihar, India), Samastipur 848134 Bihar, India
*Corresponding author: [a] aavishkar.katti@mitwpu.edu.in

ABSTRACT

We numerically analyze light propagation in a chalcogenide–polymer Bragg fiber incorporating a quasiperiodic Fibonacci cladding. The structure consists of a low-index core surrounded by alternating low- and high-index chalcogenide–polymer layers arranged according to fourth, fifth, and sixth-order Fibonacci sequences and periodically repeated to form supercell claddings, enabling systematic investigation of the effects of quasiperiodic order on the transmission response. A cylindrical transfer matrix formulation based on Bessel and Hankel functions is employed to model H-polarized wave propagation. High refractive-index contrast configurations are considered, and the incidence angle is varied to examine its influence on the transmission characteristics. The computed transmission spectra reveal distinct photonic bandgaps and multiple transmission windows arising from the quasiperiodic Fibonacci cladding, with enhanced spectral selectivity compared to periodic Bragg fibers. These findings highlight the potential of Fibonacci-based chalcogenide–polymer Bragg fibers for tailored light guidance and sensing applications.

Keywords: Fibonacci quasiperiodic structures, Supercell claddings, Chalcogenide–polymer materials, Cylindrical transfer matrix method

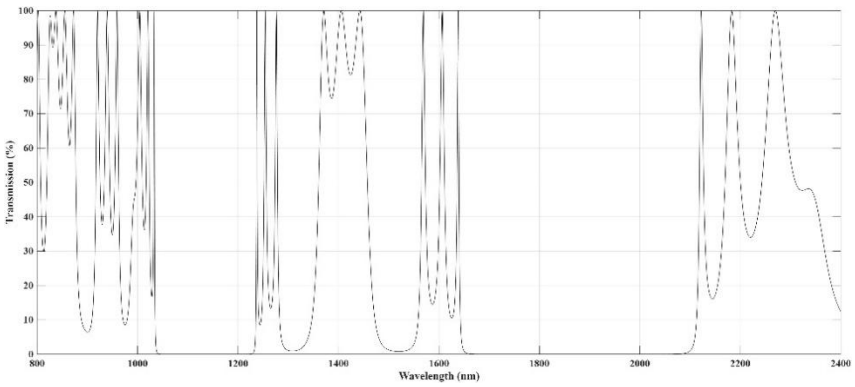


Fig. 1. Transmission spectrum of a sixth-order Fibonacci supercell chalcogenide–polymer Bragg fiber with high refractive-index contrast under H-polarized excitation at a core incidence angle θ = 65°, illustrating quasi periodicity induced photonic bandgaps and transmission windows.

Systematic computational study of external field effect on stability and electronic properties of inorganic nanoring

Riddhi Sainda [a], Prafulla K. Jha*[a]
[a] Department of physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat-390002.
*Corresponding author: [a] prafullaj@yahoo.com

ABSTRACT

The electronic structure of nanorings is highly sensitive to the choice of the basis set and hybrid functionals; however, systematic investigations of these effects remain limited. In the present work, we examine the influence of different basis sets and hybrid exchange–correlation functionals on the electronic and geometric properties of the well-known inorganic Al_9N_9 and B_9N_9 nanorings. Key properties including frontier molecular orbitals, HOMO–LUMO energies, band gaps, density of states, reactivity descriptors, and infrared spectra are computed and analyzed. Our results indicate that the ωB97X-D functional combined with the 6-311G++(d,p) basis set provides the most reliable description of these nanorings, as it incorporates correct long-range exchange and dispersion interactions essential for capturing van der Waals forces. Based on this optimized computational framework, we further investigate the effect of a normal external electric field (0.01–0.05 a.u.) on both nanorings. Field-induced variations in electronic structure, geometry, and aromaticity are systematically examined. The results revels significant changes in ring diameters as well as in reactive parameters. The observed electric-field tunability highlights the potential of these nanorings for applications in nanoelectronic and optoelectronic devices. This study offers critical guidance for accurate theoretical modeling of inorganic nanorings and establishes a robust platform for the rational design of field-tunable nanomaterials.

Keywords: Inorganic nanoring, external field, hybrid functional.

References:

[1] G. V. Baryshnikov, R.R. Valiev, A. V. Kuklin, D. Sundholm, H. Ågren, Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling, J. Phys. Chem. Lett. 10 (2019) 6701–6705.

[2] C. Wang, B. Likozar, M. Huš, J. Wu, Z. Wang, K. Yang, How does an external electric field in the normal-direction affect the cyclo[18]carbon molecule?—a DFT study, Phys. Chem. Chem. Phys. 27 (2025) 19488–19499.

Study of dielectric properties of spices as a function of frequency and density

Renykumari Champavat, Minal Makvana, Pratipal D. Chauhan, Deepak Gadani*

Department of Physics, University School of Sciences, Gujarat University,

Ahmedabad-380009, Gujarat, India.

*Corresponding author: *dhgadani@gujaratuniversity.ac.in

ABSTRACT

The present work investigates the dielectric properties of spices like turmeric powder, coriander powder, and cumin powder over 1 kHz to 2 MHz frequency range for different densities. The complex permittivity ($\varepsilon^* = \varepsilon' - j\,\varepsilon''$) of pure spices was measured using a Precision LCR Meter (Agilent E4980A) with a parallel plate capacitive solid test fixture (Agilent 16451B). The dielectric constant (ε') and dielectric loss (ε'') of pure spices are found to decrease with increase in the frequency. At a fixed frequency of 2 MHz, the dielectric constant and dielectric loss of pure spices is found to increase with the increase in the density of spices. The variations in complex electric conductance (σ), electric impedance (Z), and electric modulus (M), as a function of frequency, were calculated for all the spices at different densities. The results indicate the absence of any relaxation mechanism in all the dry spice samples across the studied frequency range.

Keywords: complex permittivity, precision LCR meter, spices, density.

References:

[1] Hernández-Nava, Ruth & Meza-Arenas, Juan & Sarmiento-Narvaez, Diego & Kaur, Tejinder & Corona, Alonso & Rojas-Laguna, Roberto & Sosa-Morales, María.. Dielectric Properties of Mexican Dried Chili Peppers (Capsicum annuum L.): De Árbol, Guajillo, and Pasilla at Microwave and Radiofrequency Ranges. Journal of Food Process Engineering. 48. (2025)

[2] S. M. Delmade, A. S. Mule, P. G. Gawali. Agreement of experimental and theoretical values of dielectric parameters of powder turmeric at X-band microwave, International e-Conference on Recent Trends in Material Science (ICRTMS) in association with International Journal of Scientific Research in Science and Technology Volume 11 | Issue 9 | Print ISSN: 2395-6011 (2024)

Compressive study of $LaTMO_3$ (TM= Fe, Mn) Electronic, Structural, Mechanical and Thermodynamical properties- using computational investigation (DFT)

R. N. Kharatmol[*], N. Y. Pandya*[a], Dhara Raval[&], Adwait Mevada[+], P. N. Gajjar[#]
[*]Parul University, P.O. Limda, Tq. Waghodiya, Vadodara, 391760, Gujarat, India
[*a]Government Commerce and Science College, Dahej, Gujarat, India
[&]Department of physics, Faculty of science, University of Ostrava, Ostrava-701103, Czech Republic
[+]Jeel Goswami College of Science and Research, Monark University, Vahela-Dahegam, 382433, Gujarat, India
[#]Department of Physics, University School of Sciences Gujarat University, Ahmedabad, 380009, Gujarat, India
[*]Corresponding Author: [a] nypandya85@gmail.com

ABSTRACT

Elastic constants of condensed cubic space group Pm3m of LaTMO3 (TM = Fe, Mn) have been calculated by density functional theory (DFT) under a plane-wave basis set with generalized gradient approximation with Perdew-Burke-Enzerhof functional exchange-correlation methods as implemented in the Quantum ESPRESSO suite. For structure optimization, the experimental lattice constant has been employed. Its pressure derivative, bulk modulus, and lattice constants are determined. The electronic profile shows a metallic nature. Fermi surface analysis, contour plots, and DOS provide a clear explanation for the decline of these physical parameters. Elastic constants, Debye temperature, Young's, bulk & shear modulus, Poisson's ratio, (n) and the anisotropic factor (A), all in Voigt-Reuss-Hill approximations, have been presented at 0 GPa. The thermodynamic properties include the Grüneisen parameter, specific heats, and thermal expansion coefficient have been examined for the entire pressure range of 0 GPa and temperature range of 0 to 1073 K.

Keywords: Perovskites, Electronic properties, Mechanical properties, Thermodynamic properties, DFT.

References:

[1] Imane Koriba, Brahim Lagounb, Abdenacer Guibadja et al, Structural, electronic, magnetic and mechanical properties of three LaMnO3 phases: Theoretical investigations, computational condensed matter (2019) vol. 29Computational Condensed Matter 29 (2021) e00592.

[2] Saad Tariq, A.A. Mubarak, et al, Repercussion of pressure on thermodynamic, optoelectronic, thermoelectric and magneto-elastic rectitude of cubic LaFeO3: Quantum DFT perspective., Journal of Alloys and Compounds 831 (2020) 154600

Valorization of Algal Waste via Conventional Pyrolysis: Production and Characterization of Bio-oil and Bio-char

Lakshmana Rao Jeeru[a], Balasubramanian Ragunathan[a], Kotaiah Naik Dhanavath[*b], Narasimha Reddy Ravuru[c]

[a] Department of Petroleum Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar-382426, India

[b] Department of Chemical Engineering, Jawaharlal Nehru Technological University Hyderabad, Hyderabad-500085, India

[c] Department of Chemical Engineering, Institute of Technology, Nirma University, Ahmedabad-382481, India

[*] Corresponding Author: [b] dhanavath_koti@yahoo.co.in

ABSTRACT

The aim of the present work is to develop processes for the production of bio-oil and bio-char from algae waste using the pyrolysis at controlled conditions. The pyrolysis was carried out at different temperatures 450-575 °C and different heating rates 10-40 °C/min. The algal waste, bio-oil and bio-char were successfully characterized using Elemental analysis, Chemical composition, the samples were analysed by Fourier-transform infrared spectroscopy (FT–IR), X–ray powder diffraction and gas chromatography–mass spectroscopy (GC–MS) for physicochemical properties of algal biomass, bio–char and bio–oil. The FT–IR study represents a reduction in the quantities of O–H (hydroxyl), C–H (alkanes), C=O (esters), –C–H (alkenes), and C–O (primary alcohol) groups, under algal biomass at the expanding pyrolysis temperatures. The GC–MS investigation showed the highest concentrations of 4–Methylpentanamide, n–Heptadecane, 2–Methyl naphthalene and n–Hexadecanoic acids in bio–oil. A maximum yield of 20.1% by weight of bio–oil outcome is reported at 575°C in 45 minutes. Results show that the bio-oil cannot be used as bio-fuel, but can be used as a source of value-added chemicals. On the other hand, the bio-char is a promising candidate for solid fuel applications and for the production of carbon materials.

Keywords: Pyrolysis; Algal waste; Bio-oil; Bio-char; Characterization

References:

[1] Sekar, M., Vinu, R. & Baskar, G. A review on the pyrolysis of algal biomass for bio-oil and biochar production. Journal of Analytical and Applied Pyrolysis 153, 104967 (2021).

Screening and Characterization of Indigenous Microbes for Crude Oil Biodegradation

Lakshmana Rao Jeeru[a], Surendra Sasikumar Jampa[a], Narasimha Reddy Ravuru[b], Balasubramanian Ragunathan*[a]
Department of Petroleum Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar, Gujarat – 382426. India.
Department of Chemical Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar, Gujarat – 382426. India.
Department of Chemical Engineering, Institute of Technology, Nirma University, Ahmedabad-382481, India
*Corresponding author: balaschem@gmail.com

ABSTRACT

Crude oil contamination remains a significant environmental concern, necessitating efficient and sustainable bioremediation approaches. This study investigated the isolation, screening, and characterization of indigenous hydrocarbon-degrading bacteria from oil-contaminated soil to evaluate their crude oil biodegradation potential. Four morphologically distinct bacterial isolates were obtained using enrichment culture techniques with crude oil as the sole carbon source. Primary screening using the 2,6-dichlorophenol indophenol (DCPIP) assay identified two highly efficient degraders, designated PDB-2 and PDB-4, which showed rapid decolorization rates of 95.8% and 91.3%, respectively, within 72 hours. Molecular identification based on 16S rRNA gene sequencing confirmed PDB-2 as *Pseudomonas aeruginosa* and PDB-4 as *Bacillus subtilis*. Both strains were mesophilic (optimal growth at 30–37 °C), neutrophilic (pH 7.0), moderately halotolerant, and exhibited notable tolerance to heavy metals such as Pb^{2+} and Zn^{2+}. Gravimetric analysis over a 21-day incubation period revealed crude oil degradation efficiencies of 65.7% for *P. aeruginosa* and 58.4% for *B. subtilis*. Notably, a defined bacterial consortium demonstrated a significant synergistic effect, achieving a higher degradation efficiency of 78.5% ($p < 0.01$). These findings highlight the strong potential of indigenous bacterial consortia for effective bioaugmentation-based remediation of oil-contaminated environments.

Keywords: Phylogenetic Catabolic Profiling; Metabolic Pathway Complementation; Biosurfactant-Mediated Bioavailability; Heavy Metal Co-Tolerance; Enrichment Culture Selection.

References:

[1] Bisht, A., Bhagat, M.S., Abdul Rasheed, M., & Archana, G. Isolation and characterization of oil degrading bacteria isolated from artificially crude oil-contaminated soil, Biochemical Engineering Journal, 225 (2026) 109928.
[2] Shokranian, S., Yousefzadi, M., Biuki, N.A., Yaghoubi-Avini, M., & TaheriAkerdi, M., Isolation, characterization, and bioremediation potential of oil-degrading bacteria from contaminated soils in Shiraz and Bandar Abbas, Iran. Scientific Reports, 15(2025) 42101.

Influence of Texture Structure and Moisture Content on Complex Permittivity of Soils at Microwave Frequencies

Jayesh Shir[a], Prahlad Chaudhary[b], Virendra Patel [c], Vipinchandra Rana[d], Deepak Gadani[e*]
[a] Government Arts and Science College, Bavla, Ahmedabad, Gujarat, India.
[b] M. N. College, Visnagar, Gujarat, India.
[c, d, e] Department of Physics, Gujarat University, Ahmedabad, Gujarat, India.
[*]Corresponding author: dhgadani@gujaratunivrsity.ac.in

ABSTRACT

The complex permittivity of three soil samples with varying textures and moisture content (MC) was measured using an open-ended coaxial probe with the help of a vector network analyser over the frequency range 0.5 GHz to 8.0 GHz. We studied 3 soil samples for their dielectric behaviour. Soil sample 1 is natural soil with a texture 58.4% sand, 14.7% silt and 26.9% clay. Soil sample 2 and soil sample 3 were prepared by manually adding pure sand to natural soil collected from the farm field of the Kheda district of Gujarat, India. This resulted in sandy loam (68.4% sand, 11.11% silt, and 20.48% clay) and loamy sand (78.4 % sand, 7.52 % silt, and 14.06 % clay), respectively. The results show that the dielectric constant and dielectric loss increased as the MC increased. At a given MC, the dielectric constant and dielectric loss decrease as frequency increases. At higher MC the dielectric loss decreases as frequency increases above 5 GHz, approaching towards relaxation frequency of free water. The measured values of the real and imaginary parts of permittivity were compared with the Wang and Schmugge, Hallikainen et al., and DHG-ADV models and found very good agreement with the models.

Keywords: complex permittivity, soil moisture, Soil Texture, Microwave

References:

[1] Hallikainen, M. T., Ulaby, F. T., Dobson, M. C., El-Rayes, M. A., & Wu, L. K. (1985). Microwave dielectric behavior of wet soil-part 1: Empirical models and experimental observations. IEEE Transactions on geoscience and remote sensing, (1), 25-34.

[2] Gadani, D. H., & Vyas, A. D. (2015). Dielectric mixing model for the estimation of complex permittivity of wet soils at C and X band microwave frequencies. Indian Journal of Pure & Applied Physics (IJPAP), 53(3), 190-198.

Preparation and Characterization of Karanja Cake Powder Filled Jute Fibre Reinforced Epoxy Composites

Venkata Saikumar Reddy Ravipati [a], Balasubramanian Ragunathan [b], Lakshmana Rao Jeeru*[b], Mohana Krishnudu Doni [a], Venkateshwar Reddy Pathapalli [c]

[a] Department of Mechanical Engineering, G. Pulla Reddy Engineering College, Kurnool, Andhra Pradesh, India.

[b] Department of Petroleum Engineering, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar, Gujarat, India.

[c] Department of Mechanical Engineering, Vardhaman College of Engineering, Hyderabad, Telangana, India

*Corresponding author: [b] lakshmanarao.jeeru@spt.pdpu.ac.in

ABSTRACT

Lightweight materials with high mechanical strength are increasingly required in modern engineering applications. Fibre-reinforced polymer composites have gained strong attention due to their excellent strength-to-weight ratio, durability, and design flexibility. In this study, an environmentally friendly and cost-effective composite was developed using jute fibres as reinforcement and Karanja cake powder as filler. The fibres were subjected to alkali treatment to improve interfacial bonding with the polymer matrix. Composite specimens were fabricated using the hand-layup technique and evaluated for tensile, flexural, and impact characteristics following standard testing procedures.

The optimum mechanical performance was achieved at a filler content of 6 wt.%, showing a tensile strength of 126 MPa, a flexural strength of 194 MPa, and an impact strength of 138 kJ/m². SEM analysis confirmed improved fibre–matrix adhesion, while FTIR analysis verified the presence of characteristic functional groups. Thermal analysis using TGA demonstrated enhanced thermal stability, with a final residual mass of 9.927% at 810°C, indicating improved resistance to thermal degradation. Overall, the results highlight the potential of the developed composite for both structural and non-structural applications across various industries.

Keywords: Natural Fibre, SEM, TGA, FTIR, Alkali treatment.

References:

[1] Iqbal, R. M., Ahammad, R., Arifuzzaman, M., Islam, M. S., & Islam, M. M. Manufacturing and Properties of Jute Fiber-Reinforced Polymer Composites—A Comprehensive Review. Materials, 18(5), 1016 (2025).

[2] Thimmegowda, D. Y., Hindi, J., Markunti, G. B., & Kakunje, M. Enhancement of Mechanical Properties of Natural Fiber Reinforced Polymer Composites Using Different Approaches—A Review. Journal of Composites Science, 9(5), 220 (2025)

Optoelectronic Properties of Quaternary Chalcogenides: A First-Principles Study toward Photovoltaic Applications

Namrata A. Tukadiya *[a], Prafulla K. Jha [a]
[a] Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002
*Corresponding author: [a] namratatukadiya1884@gmail.com

ABSTRACT

The search for novel chalcogenide materials with favorable optoelectronic characteristics is essential for the development of next-generation photovoltaic and optoelectronic devices. QUTERNARY chalcogenides based on Li have gained attention due to their structural diversity and tunable electronic properties. In this work, we present a first-principles investigation of the structural, electronic, and optical properties of $Li_2BeTMSe_4$ (TM = Fe, Cr) compounds. In order to analyze structural stability, density functional theory calculations are used to determine total energy minimization, band structure, density of states, and key optical parameters, such as absorption coefficients and dielectric functions This study indicates that incorporating transition metal elements significantly influences the bandgap of these materials, which is found to be 1.1-2.6 eV, as well as the electronic states near Fermi levels, which leads to increased near-infrared and visible optical absorption. These features suggest the potential suitability of $Li_2BeTMSe_4$ materials for optoelectronic and photovoltaic-related applications. The work focuses on evaluating their solar-cell-relevant properties and assessing their applicability as absorber materials through further theoretical analysis and provides material-level insights and a screening framework for emerging quaternary chalcogenides with multifunctional characteristics.

Keywords: Density functional theory, Quaternary Chalcogenides, Optoelectronic properties

Electronic Structure Modulation and Adsorption Mechanism of Ciprofloxacin on Graphene Oxide and Reduced Graphene Oxide using DFT approach

[†]Ananya Shandilya[a], [†]Vaishnavi Khalas[b] , Satyam Shinde[b], Abhishek A. Gor*[b]
[a] Smt. NHL Municipal Medical College (NHLMMC), Pritan Rai Cross Road, Ellis Bridge, Paldi, Ahmedabad- 380006, Gujarat, India.
[b] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India.
[†] Equal contributing first author
*Corresponding author: [a] abhishekgor5@gmail.com

ABSTRACT

The development of graphene-based nanocarriers offers a promising pathway to overcome antibiotic resistance, yet the atomic scale interactions governing drug stability on these surfaces remain distinctively complex. In this work, we present a systematic Density Functional Theory (DFT) study of the adsorption mechanism of the fluoroquinolone antibiotic Ciprofloxacin on Graphene Oxide (GO) and Reduced Graphene Oxide (rGO) surfaces. Structural stability, binding energetics, and charge distribution at the drug-material interface are analysed using suitable basis set and functionals to accurately describe long-range non-covalent interactions. Our calculations reveal that Ciprofloxacin exhibits a preferential adsorption on rGO characterized by strong π-π stacking interactions, with a calculated adsorption energy significantly exceeding that of the GO surface. Electronic analysis such as Density of states (DOS) and charge transfer mechanism indicate modification in energy levels of graphene oxide upon drug adsorption suggesting a stable physisorbed complex. These theoretical insights provide a fundamental understanding of the interfacial electronic properties necessary for designing stable, rGO-based drug delivery systems for clinical applications.

Keywords: GO/rGO, Ciprofloxacin, DFT, Non-Covalent Interactions, Density of States (DOS).

References:

[1] Interactions between Antibiotics and Graphene-Based Materials in Water: A Comparative Experimental and Theoretical Investigation; Xuntong Zhang, Jiachun Shen, Ning Zhuo, Ziqi Tian, Peiran Xu, Zhen Yang, and Weiben Yang; ACS Applied Materials & Interfaces 2016 8 (36), 24273-24280; DOI: 10.1021/acsami.6b09377

Influence of Heating Temperature on Structural, Electrical, Magnetic and Optical Properties of Ni_2W Hexaferrites Prepared Using *Musa acuminata* Leaves Extract

Manasi Raval[a,b], Heena H. Rathod[a], Manali N. Shah[c], Devang D. Shah[d], Abhishek Gor[b], Rajshree B. Jotania[e]

[a] Department of Physics, Faculty of Science, Ganpat University, Mehsana- 384012, Gujarat, India
[b] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Gandhinagar- 382426, Gujarat, India
[c] School of Forensic Science, National Forensic Sciences University, Gujarat Campus, Gandhinagar- 382007, Gujarat, India
[d] Department of Physics, Govt. Arts and Science College, Morva Hadaf- 389115, Gujarat, India
[e] Department of Physics, Electronics and Space Science, University School of Sciences, Gujarat University, Ahmedabad- 380 009, Gujarat, India
*Corresponding authors: mansibraval@gmail.com, manalitrvd@yahoo.co.in

ABSTRACT

In present study, we investigated the effect of various heating temperature on the structural, electrical, magnetic, and optical properties of nickel-substituted W-type (Ni_2W) hexaferrites ($SrNi_2Fe_{16}O_{27}$) synthesized in presence of *Musa acuminata* (banana) leaves extract as a chelating and fuel agent via a–sol-gel auto-combustion method. A series of samples were prepared by varying temperature from 900°C to 1300°C and characterized using FTIR, XRD, dielectric, VSM and UV-Vis spectroscopic measurements. FTIR spectra shows two bands. XRD analysis confirms the formation of the pure W-type phase at 1300 °C, whereas W- type phase along with secondary phases (M type, spinel and α- Fe_2O_3) has been found at 900 °C to 1200 °C. Low frequency (20Hz-2MHz) dielectric measurements carried out at room temperature and dielectric constant found to decrease with frequency and explained using a Maxwell-Wagner polarization model and electron hopping mechanisms. Formed ferrites possess a soft magnetic characteristic with a maximum saturation magnetization of 63.22 emu/g. Optical properties shows that band gap varies from 1.52 to 1.54 eV. This study highlights the successful green synthesis of $SrNi_2Fe_{16}O_{27}$ hexaferrite, demonstrating a sustainable alternative to conventional methods. The obtained material is promising candidate for high frequency and microwave applications.

Keywords: Ni_2W hexaferrites, Banana leaves extract; Structural properties, Dielectric properties, Optical properties

DFT and Vibrational Spectroscopy-Based Theoretical and Experimental Investigation of Nobiletin

Vaishnavi A. Khalas [a], Satyam Shinde*[a], Prahlad K. Baruah [a]
[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Raysan, Gandhinagar-382426, India
*Corresponding author: [a]dr.smshinde@gmail.com

ABSTRACT

Nobiletin, a polymethoxylated flavonoid with established antioxidant, anti-inflammatory, and anticancer activity, along with three of its derivatives, was investigated using a combined computational and experimental approach. Density Functional Theory (DFT) calculations were employed to analyze structural, electronic, and vibrational properties, with benchmarking performed using B3LYP, M06-2X, and PBE0 functionals in conjunction with 6-31++G(d,p), def2-TZVP, and cc-PVDZ basis sets. The B3LYP/6-31++G(d,p) level showed the best balance between accuracy and computational efficiency and was therefore selected for detailed analysis. Theoretical vibrational frequencies were correlated with experimental FTIR and Raman spectra, and mode assignments were validated through Potential Energy Distribution (PED) analysis. Solvent effects in water and dimethyl sulfoxide were examined using the IEF-PCM model, highlighting environment-dependent variations in molecular properties. Frontier molecular orbital analysis revealed enhanced electronic characteristics in the demethylated derivatives, including increased electron affinity, ionization potential, and electronegativity. Molecular electrostatic potential mapping identified carbonyl and hydroxyl-rich regions as dominant reactive sites. In addition, the electronic structure and polarizability trends observed for Nobiletin suggest its potential suitability for surface-enhanced Raman scattering (SERS) enhancement when interfaced with plasmonic nanostructures.

Keywords: Nobiletin, Density Functional Theory, Vibrational Analysis, Solvent effects.

References:

[1] Moazamiyanfar R, Rezaei S, AliAshrafzadeh H, Rastegar-Pouyani N, Jafarzadeh E, Mouludi K, et al. Nobiletin in Cancer Therapy; Mechanisms and Therapy Perspectives. Curr Pharm Des;29 (2023).

[2] Mıhçıokur Ö, Özpozan T. Molecular structure, vibrational spectroscopic analysis (IR & Raman), HOMO-LUMO and NBO analysis of anti-cancer drug sunitinib using DFT method. J Mol Struct;1149 (2017)

Nonlinear Optical Response of M-Type Hexaferrite Thin Films: A Thickness-Dependent Study

Abhishek A. Gor*[,a], Dikisha Patel[a], Pinkal Patel[a], Chetna Chauhan[b], Prahlad Kumar Baruah *[a,c]
[a] Department of Physics, School of Energy Technology, Pandit Deendayal Energy University, Knowledge Corridor, Gandhinagar-382426, Gujarat, India.
[b] Department of Electronics and Communication, Institute of Technology, Nirma University, S G Highway, Ahmedabad-382481, Gujarat, India.
[c] Institute Lumière Matière, Université Claude Bernard Lyon 1, Lyon, France.
*Corresponding author: [a] abhishekgor5@gmail.com; prahlad.iitg@gmail.com

ABSTRACT

M-type hexaferrite thin films of barium hexaferrite ($BaFe_{12}O_{19}$) and strontium hexaferrite ($SrFe_{12}O_{19}$) were fabricated on glass substrates using RF and DC magnetron sputtering, respectively, to investigate the influence of deposition time (film thickness) on their structural, linear, and third-order nonlinear optical properties. X-ray diffraction confirmed the formation of the hexagonal M-type phase in both systems, while SEM revealed thickness-dependent grain growth, surface smoothing, and film densification. Raman spectroscopy verified characteristic Ba–O/Fe–O vibrational modes in $BaFe_{12}O_{19}$ films. UV–Vis spectroscopy showed thickness-dependent optical transmittance and absorption, with optical band gaps decreasing from 3.53 to 3.16 eV for $BaFe_{12}O_{19}$ and from ~3.66 to 3.44 eV for $SrFe_{12}O_{19}$, attributed to quantum confinement, internal stress, and improved structural ordering. Third-order nonlinear optical parameters were evaluated using the Z-scan technique under CW Nd:YAG laser excitation (λ = 532 nm). Both ferrite systems exhibited positive nonlinear refraction (self-focusing) and strong reverse saturable absorption, with thinner films showing enhanced nonlinearity. The results demonstrate that M-type hexaferrite thin films combine strong third-order nonlinearity with magnetic functionality, making them promising candidates for photonic, magneto-optical, and optical limiting applications.

Keywords: Hexaferrites, M-type, Z-Scan, Nonlinear optics, Ferrite Films.

References:

[1] Pullar, Robert C. Progress in Materials Science 57.7 (2012): 1191-1334.

[2] Gor, Abhishek A. et. al. Journal of Materials Science: Materials in Electronics 35 (2024): 584.

Strain-induced Modulation of Electronic Structure and Van Hove Singularities in Metallic $PdBiS_2$: A First-Principles study

Nikunj Joshi[a], Ankur Pandya[b] and Prafulla K. Jha[c*]
[a] Department of Applied Sciences, Faculty of Engineering and Technology, Parul University, Vadodara
[b] Institute of Technology, Nirma University, Ahmedabad-382481 Gujarat, India
[c] Department of Physics, Faculty of Science, The M. S. University of Baroda, Vadodara-390002 Gujarat, *India*

ABSTRACT

Understanding the tunability of electronic properties under external perturbations is essential for the design of functional materials. $PdBiS_2$ is a layered metallic chalcopyrite that has attracted attention due to its robust metallicity and lattice stability. While its equilibrium electronic and vibrational properties have been previously investigated, the response of its electronic structure to lattice strain remains unexplored. In this work, we employ density functional theory to study the effect of biaxial in-plane strain on the electronic structure of $PdBiS_2$. Controlled compressive and tensile strains up to $\pm 1\%$ are applied in the basal plane to simulate realistic lattice deformation conditions relevant to epitaxial growth and residual stress. Our results reveal that the electronic bands near the Fermi level (E_F) exhibit pronounced sensitivity to strain, with noticeable shifts in band dispersion and bandwidth under both compressive and tensile deformation. In particular, Pd-d and S-p derived states close to the E_F show strain-induced modulation, indicating a tunable metallic response. The absence of structural instability within the considered strain range suggests that $PdBiS_2$ can sustain moderate lattice deformation while maintaining its metallic character. Strain-induced modulation of the electronic band structure reveals a tunable Van Hove singularity (VHS) in close proximity to the E_F. The relative shift of the nearest VHS with respect to E_F under small biaxial strain indicates strong sensitivity of the density of states near the Fermi energy, which is expected to influence charge transport and thermoelectric response. The present study offers a useful framework for exploring strain-driven electronic tuning in layered metallic chalcopyrites.

Keywords- Density of states,Van Hove singularity, Strain engineering, Fermi level tuning, First-principles calculations

Green synthesis of Cobalt doped Ba–Zn X-type hexaferrites using Indian gooseberry extract: Structural, electrical and magnetic property evaluation

Hemal Khatri [a, b], Chetna C. Chauhan*[a, b], Tanuj Gupta[b], Rajshree B. Jotania **[c]
[a] Institute of Science, Nirma University, Ahmedabad-382481, India.
[b] Institute of Technology, Nirma University, Ahmedabad -382481, India
[c] Department of Physics, Electronics and space science, School of Sciences, Gujarat University, Ahmedabad -380 009, India.
*Corresponding author: *chetna.chauhan@nirmauni.ac.in, **rbjotania@gmail.com

ABSTRACT

Cobalt-substituted X-type hexaferrites $Ba_2Zn_{2-x}Co_xFe_{28}O_{46}$ (x = 0.0 – 2.0, step = 0.25) were synthesized via green sol-gel method using Phyllanthus emblica (Indian Gooseberry, amla) extract and calcined at 1300°C for 6 h. Phase purity was confirmed by XRD, revealing major X-phase formation across all compositions. Minor lattice parameter variations arise from localized distortions due to slight ionic radius differences between Zn^{2+} (0.74 Å) and Co^{2+} (0.745 Å). Room-temperature VSM measurements showed soft magnetic behavior with narrow, smooth M-H loops, saturation magnetization increasing from 47.5 to 65.07 Am^2/kg with Co substitution, alongside measured remanence, squareness ratio, and coercivity. Frequency-dependent dielectric studies (20 Hz–2 MHz) revealed real dielectric constant values of 1–11 at low frequencies, becoming nearly frequency-independent above 10 kHz. Cole-Cole plots exhibited complete semicircles, indicating dominant grain boundary contributions to the dielectric response and confirming the single relaxation mechanism in these X-type hexaferrites.

Keywords: Green synthesis, X-type hexaferrites, XRD, VSM, Dielectric measurement

Cr^{3+} Substitution Effects on Multidomain Magnetism in Co_2-X Hexaferrites

Tanuj Gupta[a*], Sahil Menpara[a], Hemal Khatri[a], Chetna C. Chauhan[a*], Rajshree B. Jotania[b**]
[a] Institute of Technology, Nirma University, Ahmedabad, India, 382481
[b] Department of Physics, Electronics and Space Science, University School of Sciences, Gujarat University, Ahmedabad, India, 380009
*Corresponding author: * tanuj.gupta@nirmauni.ac.in ; chetna.chauhan@nirmauni.ac.in ** rbjotania@gmail.com

ABSTRACT

A series of Cr^{3+} substituted X-type hexagonal ferrite with composition $Sr_2Co_2Cr_xFe_{28-x}O_{46}$ (x = 0.0, 0.25, 0.5, 0.75, and 1.0) has been prepared through the heat treatment method. The obtained precursors were heated at 1300 ºC for 6 h and then characterized using various instrumental techniques. FTIR investigation confirms the ferrite phase formation in all the samples. All samples display two absorption peaks in the range between 420 cm^{-1} and 580 cm^{-1}, attributed to the Fe–O stretching bond. The XRD pattern of all the samples depicts the X-phase as a major phase with minor impurities. Magnetic parameters like saturation magnetization (M_S), coercive field (H_C), and remanent magnetization (M_r) were estimated from hysteresis loops of the samples. Magnetic analysis revealed that the prepared ferrite samples possess a multi-domain nature.

Keywords: simple heat treatment; X-type hexaferrite; XRD analysis; magnetic properties

References:

[1] R.C. Pullar, Hexagonal ferrites: A review of the synthesis, properties and applications of hexaferrite ceramics, Prog Mater Sci 57 (2012) 1191–1334. https://doi.org/10.1016/j.pmatsci.2012.04.001.

[2] M.K. Dmour, E.S. Al-Hwaitat, Y. Maswadeh, I. Bsoul, S.H. Mahmood, Preparation and characterization of rare earth-zinc substituted X-type hexaferrites, J Alloys Compd 836 (2020). https://doi.org/10.1016/j.jallcom.2020.155396.

Electronic Band Structure of LuN: Comparative Study Using LDA, GGA, and HSE Approaches

Snehal Paladiya[a], Mina Talati*[a,]
[a] Gujarat Technological University, Chandkheda, Ahmedabad 382424, Gujarat, India
[b] Shri K J Polytechnic, Bharuch 392002, Gujarat, India
*Corresponding author: [a] mina.talati@gmail.com

ABSTRACT

Lutetium Nitride (LuN), a rare-earth nitride, has emerged as a promising candidate for optoelectronic and spintronic applications due to its unique electronic properties. In this work, we investigate the band structure of LuN in its three-dimensional crystalline form using *ab initio* density functional theory (DFT) calculations implemented in Quantum ESPRESSO. The study employs three exchange–correlation functionals: Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), and the hybrid Heyd–Scuseria–Ernzerhof (HSE) functional. Our results demonstrate that LDA and GGA significantly underestimate the band gap, consistent with their known limitations, while the HSE function provides improved accuracy and better agreement with expected experimental trends. The comparative analysis highlights the importance of hybrid functionals in capturing the electronic behavior of LuN, particularly for applications requiring precise band gap engineering. This work contributes to the fundamental understanding of LuN's electronic structure and underscores its potential for integration into advanced semiconductor and optoelectronic devices.

Keywords: Lutetium Nitride, Band Structure, DFT, LDA/GGA, HSE

References:

[1] Holmes-Hewett, W. F., Miller, J. D., Ahmad, H. G., Granville, S., & Ruck, B. J., Rare-Earth Nitrides: Fundamental Advances and Applications in Cryogenic Electronics, arXiv:2505.15238 [cond-mat.mtrl-sci] (2025).

[2] Singh S. K., & Verma U. P. (2015). Investigation of high-pressure phase transition and electronic properties of Lutetium Nitride. Journal of Physics: Conference Series, 640, 012029.

Effect of Annealing on Structural and Morphological and Magnetic Properties of $NiCo_2O_4$ Thin Films

Kapil Kalme[a,b], Tanuj Gupta[c], Ambrish Dwivedi[d], Salil Modak[b] Anil Gome[d,e], Yksh Gupta[f], Keval Gadani[g], Sourav Chowdhury[h] Sanjay Kumar Upadhyay[j], Mohd Rehan Ansari[j] Ratnesh Gupta[f], Sagar Sen [*a]

[a]Department of Physics, Maharaja Bhoj Govt. P.G. College, Dhar, India
[b]School of Physics, Devi Ahilya Vishwavidyalaya, Indore, India
[c]Intitute of Technology, Nirma University, Ahmedabad, Gujrat 382481
[d]UGC DAE CSR, Indore Campus, Indore, India
[e]Department of Physics, Medi-Caps University, Indore, India
[f]School of Instrumentation, Devi Ahilya Vishwavidyalaya, Indore, India
[g]Center of Education, Faculty of Physics, Indian Institute of Teacher Education (IITE), Gandhinagar, India
[h]Deutsches Elektronen-Synchrotron DESY Notkestrasse 85, 22607, Hamburg, Germany.
[i]HNB Garhwal University Srinagar Garhwal, Uttarakhand -246174, India
[j]Department of Electronic Science, University of Delhi South Campus, New Delhi, 110021, Indian.
[*]Corresponding author: sagar.sen@mp.gov.in

ABSTRACT

$NiCo_2O_4$ (NCO) thin films have attracted significant attention due to their cubic spinel structure, high chemical stability, and potential applications in spintronic and energy-storage devices [1]. In this study, NCO thin films were deposited on Si (100) substrates using pulsed laser deposition (PLD). The as-deposited pristine film is referred to as S0**,** while post-deposition vacuum-annealed films at 250 °C (S1)**,** 350 °C (S2)**,** and 450 °C (S3) were prepared to investigate the influence of annealing temperature on structural, morphological, and magnetic properties. Vacuum annealing plays a crucial role in tailoring oxide thin films by reducing defect density, relieving residual strain, and promoting grain growth. X-ray reflectivity analysis shows a gradual decrease in total film thickness from ~512 Å (S0) to ~465 Å (S3), indicating film densification with increasing annealing temperature. Grazing incidence X-ray diffraction confirms the formation of a phase-pure cubic spinel NCO structure with a pronounced (400) preferred orientation. An increase in crystallite size accompanied by a reduction in microstrain from S0 to S3 signifies improved crystallinity due to thermally activated atomic rearrangement. Atomic force microscopy reveals reduced surface roughness upon annealing, demonstrating enhanced surface smoothness. Magneto-optical Kerr effect measurements show a monotonic decrease in coercivity with increasing annealing temperature, indicating reduced magnetic pinning. Overall, vacuum annealing significantly improves the structural quality and magnetic performance of NCO thin films, making them suitable for spintronic and energy-storage applications.

Keywords: $NiCo_2O_4$; thin film; Grazing incident X-ray diffraction, X–Ray Reflectivity

References:

[1] Xiaoshan Xu, Corbyn Mellinger Zhi Gang Cheng, Xuegang Chen, and Xia Hong, Epitaxial NiCo2O4 Film as an Emergent Spintronic Material: Magnetism and Transport Properties, Journal of Applied Physics,132(2) (2002) 020901.

Comparative Study of The Thermal Behavior of PVC/Silicon Nanocomposites Produced by Different Cooling Modes

Afsana Surkhayli[1]

[1]Department of Optics and Molecular physics, Baku State University, Azerbaijan.

[*]Corresponding author: afsana.surxayli@bsu.edu.az

ABSTRACT

Polymer nanocomposites attract significant interest due to enhanced mechanical, thermal, and functional properties at low filler contents. Polyvinyl chloride (PVC) is widely used because of its low cost, chemical resistance, flame retardancy, and processing versatility. Incorporation of silicon-based nanoparticles into PVC matrices influences structural ordering and thermal behavior. This study investigates the effect of cooling rate on PVC reinforced with porous silicon nanoparticles. Si–PVC nanocomposite films were prepared under slow cooling, iced water cooling, and quenching in liquid nitrogen. Structural and thermal properties were analyzed by XRD, SEM, and DSC [1]. XRD results show that slow cooling produces sharper Si-related diffraction peaks, indicating higher ordering and partial crystallinity. Water- and liquid-nitrogen-cooled samples exhibit broader peaks, reflecting increased amorphous content. According to free-volume theory, Si nanoparticles occupy interchain voids, reducing free volume and limiting polymer chain mobility, which suppresses crystallization during rapid cooling. DSC analysis shows that Tg depends strongly on cooling mode: 83 °C for slow cooling, 85 °C for water cooling, and 98 °C for liquid-nitrogen quenching. SEM images reveal that slow-cooled samples have a compact and ordered morphology, water-cooled samples are moderately homogeneous with localized amorphous regions, and liquid-nitrogen-cooled samples are highly disordered with extensive amorphous domains.

Keywords: Polymer nanocomposites, Polyvinyl chloride (PVC), Silicon nanoparticles, Cooling rate effect, Thermal and structural properties

Reference:

[1] Shirinova, H. A., Surkhayli, A. E., & Pashayev, B. G. (2025). Fabrication, characterization and thermal properties of PVC+Si based polymer nanocomposites. Composite Interfaces, 32(9), 1289–1304. https://doi.org/10.1080/09276440.2025.2467563

Synthesis and Characterization of Trimethylbenzylammonium Tetrachloridocuprate Single Crystals Grown by the Slow Evaporation Technique

Kajal B. Chudasama[a], Bharatkumar B. Parekh[a]*
[a] Pandit Deendayal Energy University, Gandhinagar 382007
*Corresponding author: dr.bharatparekh@gmail.com

ABSTRACT

An organic–inorganic hybrid metal halide, trimethylbenzylammonium tetrachloridocuprate, $(C_{10}H_{16}N)_2[CuCl_4]$, was synthesized by the slow evaporation technique from an aqueous 1.0 M HCl medium through the reaction of trimethylbenzylammonium chloride and $CuCl_2$ in a 2:1 molar ratio. Powder X-ray diffraction confirmed the phase purity and good crystallinity of the material, while single-crystal X-ray diffraction revealed a centrosymmetric crystal structure belonging to the monoclinic space group $P2_1/n$. Fourier-transform infrared spectroscopy verified the presence of the expected functional groups, and EDAX analysis corroborated the elemental composition and stoichiometry. Optical transmittance studies in the UV–Vis–NIR region showed high transparency in the ultraviolet region and very low transmittance across the visible window (≈500–750 nm), indicating suitability for optical-limiting applications, along with near-complete opacity in the infrared region. The optical band gap, estimated from a Tauc plot, was found to be approximately 2.2 eV. Thermogravimetric analysis demonstrated that the compound is thermally stable up to about 200 °C. To complement the experimental results, molecular electrostatic potential (MEP) analysis was carried out to examine the charge distribution within the molecule. The calculated MEP reveals significant charge asymmetry despite the centrosymmetric crystal packing, suggesting potential for nonlinear optical (NLO) activity. Open- and closed-aperture Z-scan measurements were performed to investigate the third-order nonlinear optical response. The observed nonlinear transmission behaviour and measurable third-order nonlinearity further support the material's applicability in optical-limiting and NLO device applications. Overall, the combined structural, optical, thermal, theoretical, and nonlinear optical investigations identify $(C_{10}H_{16}N)_2[CuCl_4]$ as a promising candidate for future photonic and optoelectronic applications.

Keywords: Trimethylbenzylammonium tetrachloridocuprate; Nonlinear optics; Z-scan; Optical limiting; Molecular electrostatic potential (MEP).

Investigating Structural, Magnetic and Dielectric Properties of U-Type Hexaferrite

Chirag Patel[1], Abhishek Gor[2], Rajshree Jotania[3], Chetna Chauhan[4*]
[1]Institute of Science, Nirma University, Ahmedabad– 382 481, Gujarat, INDIA
*Email: chetna.chauhan@nirmauni.ac.in

ABSTRACT

U-type hexaferrites with composition ($(Sr_{1-3x}Pr_{2x})_4Co_2Fe_{36}O_{60}$), x = 0.0,0.05,0.10,0.15,0.20,0.25, were successfully synthesized using *Syzygium aromaticum* (clove) extract as a green and eco-friendly fuel. The plant-assisted route enabled phase formation at relatively lower processing conditions while avoiding toxic chemical reagents. Structural analysis confirmed the formation of the U-type hexaferrite phase with good crystallinity, and microstructural features were found to be influenced by Pr substitution. Magnetic measurements revealed systematic variations in saturation magnetization and coercivity with increasing Pr content, attributed to cation redistribution and magnetocrystalline anisotropy. Dielectric studies showed frequency-dependent behaviour consistent with Maxwell–Wagner interfacial polarization and hopping conduction mechanisms. UV–visible spectroscopy indicated modified optical absorption characteristics and band gap variation due to rare-earth substitution. The results demonstrate that clove-assisted green synthesis is an effective approach for tailoring the multifunctional properties of U-type hexaferrites for potential applications in high-frequency, microwave, and electromagnetic devices.

Keywords: ($(Sr_{1-3x}Pr_{2x})_4Co_2Fe_{36}O_{60}$) and clove and holy basil composites, Green synthesis technique, XRD, VSM, dielectric measurement.

Germanene-Graphene Heterostructure For Early Earthquake Sensing

Haard Shah [a] , Karan Mungra [a], Ankur Pandya [*a]
[a] Department of Mechanical Engineering, Nirma University, Ahmedabad- 382481, India
[*]Corresponding author: [a]ankur.pandya@nirmauni.ac.in

ABSTRACT

Heterostructures such as germanene-graphene present us with a promising pathway for the development of ultra sensitive nanoscale sensors because of their numerous properties such as high carrier mobility, complementary mechanical stiffness and other tunable electronic properties. In our present work, a doubly clamped germanene-graphene nanoresonator has been proposed by us as a seismic strain detector for a nextgeneration technology of early warning earthquake detection systems. The prediction of resonant behaviour of the heterostructure is done through the usage of a continuum mechanics framework which is based on Euler-Bernoulli beam theory. This framework incorporates both bending rigidity and built in axial tension. The induced axial strain and its resulting modulation of electrical conductivity through the piezoelectric effect is done in order to analyze the interaction taking place between the seismic acoustic waves and the nanoribbon used by us. Quantification if the conversion efficiency between incoming mechanical vibration energy and the electrical output is done through the development of an electromechanical coupling model. This enables the evaluation of device performance under extremely low amplitude seismic excitation. Our paper indicates high resonant frequency tunability and measurable conductivity shifts even under micro strain levels can be obtained through our germanene graphene bilayer. This study thus reveals the potential of our device as a compact, low cost, and a highly sensitive component in dense early warning sensor networks. Our aim is to lay out a groundwork for future fabrication and experimental validation of 2D materials based seismic NEMS sensors.

Keywords: Heterostructure, nanoresonator, continuum mechanics, piezoelectric effect, NEMS.

Glimpse of Previous RAMAN