SCHOLARLY PUBLICATIONS
School of Applied Sciences
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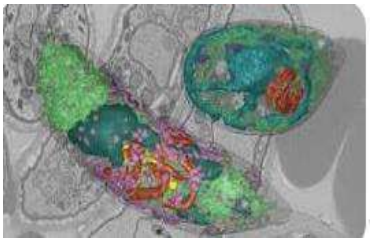
Journal Name: Nature Communications **IF: 14.7**

Title: Evidence of isospin-symmetry violation in high-energy collisions of atomic nuclei

Author: Zwaska R.; Zviagina A.; Zimmerman E.D.; Zherebtsova E.; Zaitsev A.; WyszyÅ„ski O.; WÃ³jcik K.; Witek K.; Wickremasinghe A.; Volkov V.; Vitiuk O.; Vechernin V.V.; VeberiÄ D.; Valiev F.F.; Urbaniak M.; Unger M.; Tveter I.C.; Andronov E.V.; Amin N.; Allison K.K.; Adrich P.; Adhikary H.; Giacosa F.; Gorenstein M.; Poberezhniuk R.; Samanta S.

Details: Volume 16, Issue 1, December 2025

Abstract: Strong interactions preserve an approximate isospin symmetry between up (u) and down (d) quarks, part of the more general flavor symmetry. In the case of K meson production, if this isospin symmetry were exact, it would result in equal numbers of charged (K^+ and K^-) and neutral (K^0 and K^-0) mesons produced in collisions of isospin-symmetric atomic nuclei. Here, we report results on the relative abundance of charged over neutral K meson production in argon and scandium nuclei collisions at a center-of-mass energy of 11.9 GeV per nucleon pair. We find that the production of K^+ and K^- mesons at mid-rapidity is (18.4 ± 6.1)% higher than that of the neutral K mesons. Although with large uncertainties, earlier data on nucleus-nucleus collisions in the collision center-of-mass energy range 2.6<sNN<200 GeV are consistent with the present result. Using well-established models for hadron production, we demonstrate that known isospin-symmetry breaking effects and the initial nuclei containing more neutrons than protons lead only to a small (few percent) deviation of the charged-to-neutral kaon ratio from unity at high energies. Thus, they cannot explain the measurements. The significance of the flavor-symmetry violation beyond the known effects is 4.7σ when the compilation of world data with uncertainties quoted by the experiments is used. New systematic, high-precision measurements and theoretical efforts are needed to establish the origin of the observed large isospin-symmetry breaking.



URL: https://www.nature.com/articles/s41467-025-57234-6

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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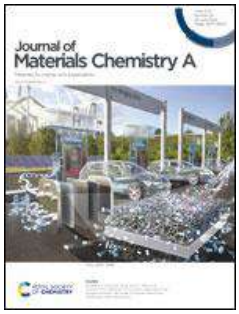
Journal Name: Journal of Materials Chemistry A **IF: 9.5**

Title: Metal-organic frameworks: classifications, synthesis, structure-property-performance relationship, and techno-economic analysis of redox flow batteries

Author: Giri S.; Roy M.; Bandyopadhyay S.; Das S.; Mangal S.; Samanta S.

Details: 03 May 2025

Abstract: Metal-Organic Frameworks (MOFs), which are highly porous materials, offer significant potential across multiple energy storage domains, notably within redox flow batteries (RFBs). Over the past decade, MOFs have garnered increasing attention as advanced electrode and separator materials in RFBs, driven by their intrinsic porosity, tunable architecture, and multifunctional design potential. Prior to discussing MOFs in RFBs, it is important to examine their classification, nomenclature and key properties including their synthesis methodologies across diverse MOF types, as these factors play a vital role in developing efficient RFBs. To date, various metal ions and linkers have been utilized in MOF synthesis, and their selection influences the resulting framework. Correspondingly, a structure-property-performance relationship has been established to correlate the material's properties with its electrochemical performances. We further examined their utilization in RFBs' membranes in a separate section. Additionally, we discuss the challenges and opportunities associated with MOF-based electrodes and membranes. Moreover, special focus is also given to techno-economic analysis for the practical implementation of RFBs. This discussion reveals the potential pathways for advancing MOFs in energy storage applications.



URL: https://pubs.rsc.org/en/content/articlelanding/2025/ta/d5ta01469g

SCHOLARLY PUBLICATIONS
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Journal Name: Results in Engineering **IF: 7.9**

Title: Dielectric characteristics and energy storage capabilities of PVDF-based composite incorporating 2D GnP nanofiller.

Author: Hota S.S.; Panda D.; Panda R.; Mishra S.; Choudhury S.; Biswal L.; Choudhary R.N.P.; Satapathy A.

Details: Volume 26, June 2025, Article number 105593

Abstract: Hybrid nanofiller engineered for polymer nanocomposite are anticipated to achieve superior energy storage performance due to their diverse morphologies and electrical properties. In this study, 2D graphite nanoparticle (GnP) heterostructures were synthesized on surfaces and incorporated into poly(vinylidene fluoride) (PVDF) to develop PVDF-based composite (PVDF-GnP) using the solution casting route. At room temperature and an electric field of 60 kV/cm, the composite exhibits a maximum polarization of 0.079 μC/cm², while the discharged energy density reaches 2.22 J/cm³. The dielectric constant of 0.2 wt% GnP/PVDF at room temperature and at a frequency of 10^3 Hz is ∼52, with a low dielectric loss of 0.25, approximately five times higher than that of pure PVDF (∼10 at 25 °C). Notably, the incorporation of GnP into the PVDF matrix significantly reduces AC conductivity, emphasizing its suitability for energy storage applications. Additionally, the study reveals that adding GnP does not modify the β phase of PVDF, ensuring the stability and compatibility of composite. Impedance analysis further highlights the dominance of grain boundary resistance, providing deeper insights into the electrical properties of the composite. This study contributes to a deeper understanding of GnP nanostructure and highlights their prospective use in cutting-edge nanotechnologies, especially in energy storage systems and high-density magnetic data recording. Current research is anticipated to further optimize the material for wider technological application.

URL: https://www.sciencedirect.com/science/article/pii/S2590123025016639?via%3Dihub

Journal Name: International Journal of Biological Macromolecules **IF: 7.7**

Title: Understanding the structural and functional implications of lysine succinylation in Mycobacterium tuberculosis heat shock protein 16.3

Author: Barik S.; Aldar K.S.; Chakraborty A.; Panda A.K.; Kar R.K.; Biswas A.

Details: Volume 307, May 2025

Abstract: Heat shock protein 16.3 (Hsp16.3), a major immunodominant antigen of Mycobacterium tuberculosis, exhibits molecular chaperone function that is essential for pathogen's survival and slow growth inside hosts, as well as for enhancing the efficacy of Bacillus Calmette-Guérin (BCG) vaccine. Proteomic studies revealed that Hsp16.3 undergoes lysine succinylation in vivo at all lysine residues (K47, K64, K78, K85, K114, K119 and K132) except K136. However, the effects of succinylation on its structure and function remain unexplored. This study investigated the impact of succinylation, induced by physiological (succinyl-CoA) and/or non-physiological (succinic anhydride) donors, on the structure, stability and chaperone function of Hsp16.3. Succinylation of all eight lysine residues, affirmed via fluorescamine assay and mass spectrometry, led to structural (secondary and tertiary) alterations, as indicated by circular dichroism (CD), fluorescence and in-silico analyses. Succinylation induced oligomeric dissociation (dodecamer to dimer) and enhanced surface hydrophobicity of Hsp16.3. Moreover, succinylation reduced protein stability, making it more conformationally flexible and less compact, as revealed by urea-denaturation, chymotrypsin-digestion and computational studies. Despite this reduced stability, succinylated Hsp16.3 exhibited enhanced chaperone activity, offering improved protection to stressed-prone client proteins. These findings provide useful insights into this modification, offering potential therapeutic avenues for targeting Hsp16.3 in M. tuberculosis infection.

URL: https://www.sciencedirect.com/science/article/pii/S014181302502598X?via%3Dihub

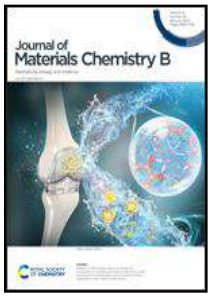
Journal Name: Journal of Materials Chemistry **IF: 5.7**

Title: Ultrasensitive detection of arsenic in water using laser-scribed graphene-based electrodes

Author: Mohanty A.; Upadhye S.; Pradhan G.K.; Nayak P.

Details: 14 May 2025, Article

Abstract: Arsenic contamination in water poses a serious health risk due to its high toxicity, even at ppb levels. In this work, we report a cost-effective graphene-based sensor with ultralow detection capabilities for arsenic. This is achieved by enhancing the catalytic efficiency of graphene electrodes through sunlight-assisted photothermal oxidation of a metal salt into metal oxide nanoparticles. The sensor demonstrated high sensitivity (34.81 ± 1.74 μA cm^{-2} ppb^{-1}) and an ultralow detection limit (LOD 0.0636 ppb). Field tests on water samples from arsenic-contaminated zones in West Bengal, India, showed results consistent with the state-of-the-art ICP-OES analysis, highlighting the sensor's potential for practical, on-site arsenic monitoring.



URL: https://pubs.rsc.org/en/content/articlelanding/2025/tb/d5tb00041f

SCHOLARLY PUBLICATIONS
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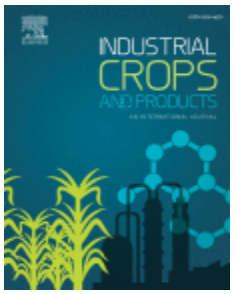
Journal Name: Industrial Crops and Products **IF: 5.6**

Title: Bio-inspired nitrogen-doped carbon quantum dots: A green route for bioimaging and nano-biosensing

Author: Kumar M.; Shrestha B.B.; Chinnathambi S.; Dutta B.; Sivaniah E.; Pandian G.N.

Details: Volume 227, May 2025

Abstract: Carbon quantum dots (CQDs) have emerged as promising nanomaterials due to their tunable fluorescence, high biocompatibility, and diverse applications in bioimaging, diagnostics, and theranostics. Sustainable synthesis approaches utilizing plant biomass-derived carbon sources, such as cellulose, citric acid, and terephthalic acid derivatives, offer an eco-friendly alternative to conventional methods. Here, we report a facile one-pot solvothermal synthesis of novel nitrogen-doped CQDs (ATA100) using 2-aminoterephthalic acid (ATA) as an alternative to biomass-based carbon and nitrogen precursor, with 1,2-ethylenediamine (EDA) as a surface passivation agent. Nitrogen doping enhances fluorescence quantum yield to 38 %, outperforming citric acid-derived CQDs (CA100). Structural characterization via Fourier-transform infrared spectroscopy (FTIR), proton nuclear magnetic resonance (^{1}H NMR), high-resolution transmission electron microscopy (HR-TEM), dynamic light scattering (DLS) confirms the formation of uniform nanoparticles (<5 nm) with enriched amine functionalities. Biocompatibility assessments reveal low cytotoxicity and enhanced cellular uptake, with 2.6-fold higher fluorescence in A549 cancer cells compared to normal chondrocytes, demonstrating its potential as an efficient bioimaging agent. Moreover, ATA100 exhibits fluorescence quenching upon catalase interaction, while its fluorescence intensity increases in response to hydrogen peroxide, highlighting its application for reactive oxygen species (ROS) detection in oxidative stress-related diseases. This study underscores the industrial feasibility of nitrogen-doped CQDs for large-scale bioimaging, biosensing, and therapeutic monitoring. By leveraging renewable resources, ATA100 presents a sustainable, eco-friendly and scalable alternative to traditional semiconductor-based fluorescent probes, advancing bio-inspired nanomaterials for precision medicine and industrial diagnostics.



URL: https://www.sciencedirect.com/science/article/pii/S0926669025003632?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Materials Research Bulletin **IF: 5.3**

Title: In situ Raman and electric modulus study of NBT-ST-KNN ceramics: An insight into temperature evolution of relaxor dynamics

Author: Singha A.; Praharaj S.; Rout D.

Details: Volume 190, October 2025, 113534

Abstract: Polar nanoregions (PNRs) are often argued to be the key factor in enhancing the functional properties of relaxor-based ferroelectrics. The creation and relaxation of these polar entities are believed to be strongly temperature-dependent, but the explanation is still unclear. In this investigation we have chosen a well-established relaxor system $(0.8\text{-}x)(Na_{0.5}Bi_{0.5})TiO_3\text{-}0.2SrTiO_3\text{-}x(K_{0.5}Na_{0.5})NbO_3$; (x = 0.005, 0.01, 0.04 and 0.1) to probe into the thermal dynamics of PNRs using in-situ Raman and electric modulus formalism. The Raman spectra segregate into different temperature zones corresponding to ferroelectric-relaxor transition ($T_{F\text{-}R}$), maximum dielectric constant (T_m) and Burn's temperature (T_B). A closer introspection of width and position of peak peaks around these temperatures depicts the existence of local structural heterogeneities. Further, the frequency-dependent electric modulus, M"(f) study demarcates high-frequency shoulder (related to PNR relaxation) from intermediate frequency peak corresponding to bulk response. Analysis of Z"(f) and M"(f) predict temperature evolution of long-range ordered regions to localized relaxations.

URL: https://www.sciencedirect.com/science/article/pii/S0025540825002429?via%3Dihub

SCHOLARLY PUBLICATIONS
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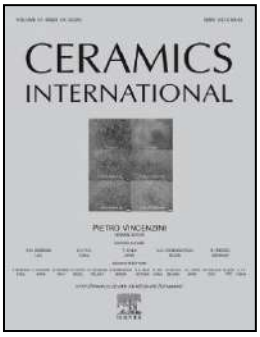
Journal Name: Ceramics International **IF: 5.1**

Title: Unraveling electrical transport and dielectric relaxation in P2-Type NaMg0.25Mn0.75O2: A promising layered oxide for high-temperature electronics

Author: Karmakar S.; Sahoo S.; Mohanty H.S.; Boddhula R.; Reddy G.N.; Mohapatra S.R.; Mahato K.K.; Anirban S.; Nayak P.; Kumar G.R.; Deka N.

Details: 6 May 2025

Abstract: This present work introduces a strategically engineered P2- type $NaMg_{0.25}Mn_{0.75}O_2$ (NNMO) cathode material by sol-gel auto-combustion techniques with optimized cation substitution (Mg^{2+} for Mn^{4+}), which enhances structural stability and high-temperature electrical performance. The X-ray diffraction (XRD) pattern and Raman spectra reveal the P2- type hexagonal crystal structure (space group $P6_3/mmc$) and three sharp Raman active phonon modes A_{1g}, E_{2g}, and E_{1g} at 595, 480, and 390 cm^{-1}, respectively. The ac electrical transport properties i.e., impedance, conductivity, dielectric, and modulus spectra of $NaMg_{0.25}Mn_{0.75}O_2$ investigated at different temperatures from 298 to 523 K (ΔT = 50 K) and frequency range between 100 Hz and 1 MHz. It has been discovered from impedance and conductivity that the NMMO pellet sample contains short-range (AC) and long-range (DC) charge carrier movements, with the former predominating at low temperatures and the latter at high temperatures. The variation of frequency exponent (n) decreases with temperatures which reveals the correlated barrier hopping (CBH) conduction process where the charge carriers (electrons or holes) hop between localized states over a potential energy barrier. The dc activation energy (E_a) was calculated at ~0.48 eV using Arrhenius plots. High dielectric constant (ε_r)~5.4×10^6 and low loss (δ)~23 were obtained at high temperature (523 K) and low frequency (50 Hz) region which recommends its high energy storage capacity at room and high temperatures. The thermal robustness, stable dielectric response, and favorable ac electrical conduction of NMMO demonstrated its possible technological application as a capacitor in high-temperature power electronics and next generation energy storages applications.



URL: https://www.sciencedirect.com/science/article/pii/S0272884225021480?via%3Dihub

SCHOLARLY PUBLICATIONS
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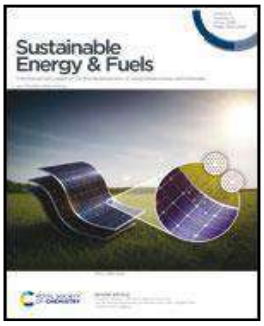
Journal Name: Sustainable Energy & Fuels **IF: 5.0**

Title: Multifaceted DFT analysis of defect chalcopyrite-type semiconductor ZnGa2S4: dynamic stability and thermoelectric efficiency

Author: Jena, S; Priyambada, A; Behera, SS; Parida, P

Details: Article**,** 15 May 2025

Abstract: The drive to transform heat into electricity with peak efficiency is an essential impulse in the quest for next-generation renewable energy technologies. Defect chalcopyrite semiconductors are spearheading this research due to their exceptional heat conduction properties and promising potential as thermoelectric materials for energy conversion applications. This study offers an in-depth analysis of the structural, electronic, mechanical, and thermoelectric properties of the defect chalcopyrite-type semiconductor ZnGa2S4, utilizing first principles density functional theory coupled with semi-classical Boltzmann transport theory. With a direct bandgap of 2.34 eV, the band structure analysis of the optimized structure confirms that the compound exhibits intrinsic semiconducting behavior. A detailed mechanical analysis, including the elastic stiffness constants, suggests that ZnGa2S4 is mechanically stable, but brittle. Phonon dispersion calculations confirm the dynamic stability of the compound. The melting temperature is calculated to be 953.663 K. Additionally, the electronic thermoelectric properties are analyzed using the constant relaxation time approximation (CRTA) within the framework of Boltzmann transport theory. The analysis indicates significantly high Seebeck coefficients at increased temperatures. The lowest lattice thermal conductivity is determined to be 2.529 W m-1 K-1 at 900 K. The figure of merit (ZT) is found to have a peak value of 0.97 at 900 K for a hole concentration of 1018 cm-3. These results highlights ZnGa2S4 as a potential thermoelectric material, particularly suited for high-temperature applications, offering a balance between structural stability and favorable thermoelectric performance.



URL: https://pubs.rsc.org/en/content/articlelanding/2025/se/d4se01740d

SCHOLARLY PUBLICATIONS
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Journal Name: Journal of Inorganic and Organometallic Polymers and Materials **IF: 4.9**

Title: DFT-Guided SCAPS-1D Simulation of Single vs. Double Absorber Layer CsGeI3/CsGeI2Br Perovskite Solar Cells

Author: Mishra H.S.; Mohanty I.; Biswal L.; Mangal S.; Sk M.; Das Pattanayak M.

Details: 11 June 2025, Article

Abstract: In this study, three perovskite halide solar cell device models are proposed and simulated using SCAPS-1D software to explore their performance and potential for practical application. Device 1 features a double-absorber-layer hetero-junction structure combining $CsGeI_3$ and $CsGeI_2Br$, while Devices 2 and 3 utilize single absorber layers of $CsGeI_2Br$ and $CsGeI_3$, respectively. Spiro-OMeTAD and ZnO were employed as the hole and electron transport layer, respectively, in all three structures. Density functional theory (DFT) was used to study the suitability of $CsGeI_2Br$ and $CsGeI_3$ as absorber layers in the proposed device models. Then comprehensive optimization of critical device parameters including absorber layer thickness, defect density, interface defect density and operating temperature were performed to enhance device performance. After optimization, Device 1 demonstrated a significant power conversion efficiency of 21.51%, outperforming Devices 2 and 3 which achieved efficiencies of 16.66% and 15.95% respectively. The superior performance of Device 1 highlights the potential advantages of a double-absorber-layer configuration in improving light absorption and charge carrier dynamics. These results provide a solid foundation for further experimental investigations and feasibility of $CsGeI_3$ and $CsGeI_2Br$-based perovskite structures in the development of high-efficiency solar cells.

URL: https://link.springer.com/article/10.1007/s10904-025-03896-0

SCHOLARLY PUBLICATIONS
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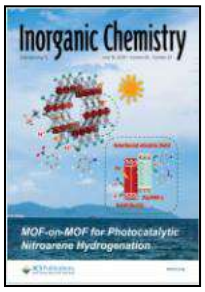
Journal Name: Inorganic Chemistry **IF: 4.7**

Title: Structure-Nanomechanical Property Correlation in Photosalient Isostructural Metal-Organic Crystals

Author: Dutta B.; Mondal A.; Medishetty R.; Choudhury A.; Roy S.; Reddy C.M.; Mir M.H.

Details: Volume 64, Issue 23, Pages 11580 – 11585, 16 June 2025

Abstract: Dynamic photoactuating crystals are making waves for their ability to transform industries, offering groundbreaking possibilities in fields such as medical technology, robotics, and flexible electronics. These crystals respond to light, enabling innovations such as smart devices, artificial muscles, molecular machines, sensors, and microrobots, heralding a new era of highly adaptive and efficient technologies. Herein, we report two iso-structural metal-organic crystals $[Cd(quin)_2(4\text{-nvp})_2]$ and $[Zn(quin)_2(4\text{-nvp})_2]$ [Hquin = quinoline-2-carboxylic acid and 4-nvp = 4-(1-naphthylvinyl)pyridine] based on Cd(II) and Zn(II) ions respectively, that undergo solid-state photochemical [2 + 2] cycloaddition reaction accompanied by photosalient (PS) effect, wherein both the crystals show popping, swelling, and splitting upon UV irradiation, explicitly probed by nanoindentation studies. Thus, these findings may pave the way for the fabrication of photoactuating smart materials.



URL: https://pubs.acs.org/doi/10.1021/acs.inorgchem.5c00943

SCHOLARLY PUBLICATIONS
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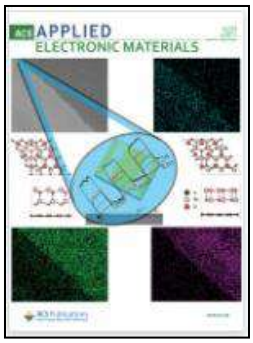
Journal Name: ACS Applied Electronic Materials **IF: 4.7**

Title: Graphene-ZnO Thin-Film Heterostructure-Based Efficient UV Photosensors

Author: Biroju R.K.; Paltasingh S.N.; Sahoo M.R.; Dhara S.; Maity D.; VretenÃ¡r V.; Giri P.K.; Narayanan T.N.;

Details: Volume 7, Issue 11, Pages 4888 – 4897, 10 June 2025

Abstract: Graphene-based ZnO thin-film hybrids (GR-ZnO) have shown interesting properties for electronic and optoelectronic applications, such as enhanced UV photodetection and photocatalysis. The interaction and explicit role of large-area single-layer chemical vapor deposition (CVD)-grown graphene in the improved photophysical properties in such a kind of GR-ZnO hybrids have not been well-understood in recent reports. In the present work, we fabricated a photosensor made with large-area monolayer CVD GR-ZnO thin-film hybrids, which showed improved UV photodetection with high values of UV sensitivity and responsivity compared to bare ZnO films. The GR-ZnO thin-film hybrid photosensors demonstrated about a 20 time improvement in photoresponsivity (9.87×10^3 A/W) compared to the bare ZnO thin film (4.93×10^2 A/W). We investigated the origin of the high photosensitivity of GR-ZnO, and it is explained based on a comparatively large absorption coefficient, enhancement of the number of photogenerated carriers, and a reduction of the recombination rates of these carriers based on density functional theory (DFT) calculations. The high mobility of the graphene layer provides an efficient and faster charge transfer pathway for photogenerated carriers at the interface between ZnO and the graphene layers.



URL: https://pubs.acs.org/doi/10.1021/acsaelm.5c00348

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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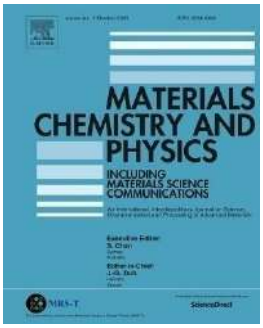
Journal Name: Materials Chemistry and Physics **IF: 4.7**

Title: Insights into the structural and functional properties of potassium based complex perovskite ceramic: dielectric, optical, morphological and electrical perspectives for potential applications.

Author: Rout S.; Moharana K.; Priyadarshini L.; Parida A.K.; Choudhary R.N.P.; Biswal L.

Details: Volume 3431, October 2025, Article number 131050

Abstract: An alkali metal-based compound featuring a disordered complex perovskite structure was successfully synthesized through the conventional solid state reaction technique. Structural characterization using X-ray diffraction (XRD) at room temperature confirmed the formation of a cubic phase with Fm-3m space group symmetry. Rietveld refinement of the XRD data validated the proposed crystal structure. Raman spectroscopy at room temperature further corroborated the XRD findings, supporting the proposed symmetry and structure. Surface morphology and microstructure of the synthesized compound were examined using field emission scanning electron microscopy (FE-SEM) providing insights into the surface features and the overall grain structure of the compound. Energy dispersive X-ray (EDX) analysis was employed to get semi-quantitative information on the distribution of elements and their respective weight percentages indicating successful synthesis of the target material. Optical characterization via UV–visible absorption spectroscopy revealed a direct band gap of 3.20 eV, indicating potential applications in optoelectronic and photovoltaic devices due to its suitability for light absorption and energy conversion. The electrical properties were systematically investigated using complex impedance spectroscopy (CIS), which evaluated dielectric and relaxation behavior across varying temperatures and frequencies. The material demonstrated a stable dielectric response under high-frequency and high-temperature conditions, making it promising for advanced electronic applications. Impedance analysis indicated a negative temperature coefficient of resistance (NTCR), with the bulk effect being the primary contributor to the overall electrical behavior.



URL: https://www.sciencedirect.com/science/article/pii/S0254058425006960?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Materials Today Communications **IF: 4.5**

Title: Synthesis of ferroelectric Bi0.5Na0.5TiO3 ink towards fabrication of a flexible piezoelectric nanogenerator for bio-mechanical energy harvesting.

Author: Das B.; Mohanty S.; Das D.; Parashar S.K.S.

Details: Volume 47, July 2025, Article number 113040

Abstract: Bismuth sodium titanate (BNT) is a widely studied multiferroic material known for its strong ferroelectric and piezoelectric properties, making it a promising candidate for piezoelectric nanogenerators (PENGs). In this study, BNT nanoparticles (BNT NPs) were synthesized using a simple hydrothermal method. The phase purity of the synthesized BNT NPs was verified using X-ray diffraction (XRD) analysis. The inks were prepared by combining BNT NPs with ethanol, glycerol, and ethylene glycol, where the BNT NPs served as the active component imparting piezoelectric properties to the ink. Among the ink formulations, INK: III, containing 30 wt% BNT NPs, exhibited superior piezoelectric and rheological characteristics. For PENG fabrication, the BNT ink was spin-coated onto a polydimethylsiloxane (PDMS) substrate, followed by encapsulation with PDMS and subsequent corona poling. The poled PENG device demonstrated enhanced piezoelectric performance, generating a peak output voltage value of 18.3 V under a human finger-tapping force.

URL: https://www.sciencedirect.com/science/article/pii/S2352492825015521?via%3Dihub

Journal Name: Materials Today Communications **IF: 4.5**

Title: The structural and electrical properties of BiFeO3 â€“ Bi0.5K0.5TiO3 â€“ BaTiO3 based solid solutions at the morphotropic phase boundary

Author: Katragadda N.; Kumar S.; Tulasirao P.; Zhang W.; Halasyamani P.S.; Nanda J.; Pradhan G.K.; ManjÃ³n-Sanz A.M.; Mandal P.

Details: Volume 47, July 2025, Article number 113030

Abstract: Piezoelectric ceramics such as $PbZr_{1-x}Ti_xO_3$ (PZT) show enhanced electro-mechanical properties at morphotropic phase boundary (MPB) separating two ferroelectric polar phases in the compositional phase diagram. Designing MPB in Pb-free perovskite oxide is challenging due to the lack of suitable polar tetragonal oxide with high Curie temperature. In this study, we explored the $BiFeO_3$ – $Bi_{0.5}K_{0.5}TiO_3$ – $BaTiO_3$ ternary phase diagram and searched for Bi-rich perovskite oxides as candidates for piezoceramics near MPB. The phase diagram offers a Bi-rich polar tetragonal ($T_{[001]}$) phase [$0.75BaTiO_3$–$0.25(K_{0.5}Bi_{0.5})TiO_3$] and a well-known rhombohedral ($R_{[111]}$) phase $BiFeO_3$. A solid solution is observed in the entire range between the $T_{[001]}$ phase and the $R_{[111]}$ phase. Structural investigation through powder diffraction and Raman spectroscopy studies suggests the existence of a complex region (MPB), well separated by the rhombohedral and tetragonal phases. The composition $(Bi_{0.670}K_{0.050}Ba_{0.280})(Fe_{0.62}Ti_{0.38})O_3$ at the MPB shows a large signal piezoelectric coefficient of $d_{33}^* = 41.5$ pm/V at room temperature.

URL: https://www.sciencedirect.com/science/article/pii/S2352492825015429?via%3Dihub

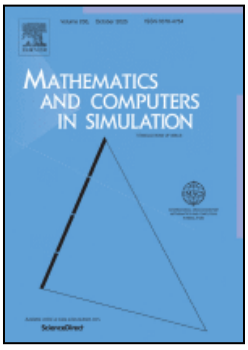
Journal Name: Mathematics and Computers in Simulation **IF: 4.4**

Title: Optimization of a price break policy and advertisement effort based non-instantaneous deteriorating inventory problem with partial backlogged via metaheuristic algorithms

Author: Mondal R.; Manna A.K.; Akhtar M.; Bhunia A.K.

Details: Volume 236, October 2025, Pages 221-247

Abstract: Repeated advertisements of an item in different media, displayed stock in a decorated showroom, and also price break policies play a vital role in an inventory control system. Also, the relationship between products' selling price and market demand is conflicting when all other factors are fixed. Thus, the incorporation of advertisement policy and price break facility in a business is more realistic. This work investigates an inventory problem for non-instantaneous deteriorating items with advertisement and displayed inventory level dependent demand under price break facility. Moreover, partially backlogged shortages and transportation cost for replenishing items are considered in the proposed inventory model. Based on the customer's demand and storage space of the shop, several cases and sub-cases are considered. In this study, different metaheuristic algorithms are considered for maximizing the average profit in each scenario. Then, considering one numerical example, the proposed model is justified. Finally, the sensitivity analysis is carried out to investigate the impact of model parameters on the policy of optimality and a fruitful conclusion is drawn.



URL: https://www.sciencedirect.com/science/article/pii/S0378475425001375?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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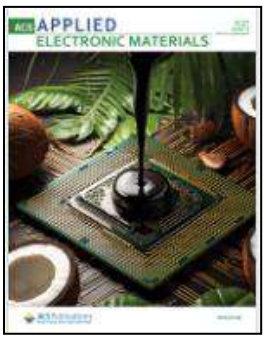
Journal Name: ACS Applied Electronic Materials **IF: 4.4**

Title: Absorption-Dominant Electromagnetic Interference Shielding of Polymer Nanocomposite PVDF/LiNbO3 for High-Frequency Microwave Application

Author: Hota S.S.; Panda D.; Bhoobash S.B.; Mishra S.; Biswal L.; Joshi S.; Shukla A.; Das D.; Choudhary R.N.P.; Parashar S.K.S.

Details: Article, May 7, 2025

Abstract: The swift advancement of wireless communication technology and the miniaturization of electronic devices have significantly increased the need for lightweight, waterproof, and flexible high-performance electromagnetic interference (EMI) shielding materials. This study explores the creation of a multifunctional polymer nanocomposite film utilizing a polyvinylidene fluoride (PVDF) matrix incorporated with lithium niobate, $LiNbO_3$ (LNO) filler, which enhances the attenuation of incoming electromagnetic (EM) radiation. The structural and morphological characteristics of the composite were analyzed through the β-phase fraction of PVDF and field emission scanning electron microscopy (FESEM), respectively. This distinctive magnetodielectric coupling yielded a remarkably high total electromagnetic shielding effectiveness (SE_T) of −62.56 at 8 GHz and −53.62 at 18 GHz, primarily driven by absorption-based shielding. Such high shielding effectiveness underscores the capability of the material to attenuate incoming EM radiation, and the improvement in structural attributes further confirms its suitability for cost-effective and tunable applications. The PVDF-LNO composite exhibits excellent dielectric absorption properties along with dielectric and magnetic loss, making it ideal for EMI shielding. These results position the nanocomposite as a promising specimen to use in the wide frequency range, especially in satellite communication systems.



URL: https://pubs.acs.org/doi/10.1021/acsaelm.5c00316

SCHOLARLY PUBLICATIONS
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Journal Name: Journal of Physics and Chemistry of Solids **IF: 4.3**

Title: Solvothermally synthesized nanocrystalline CoSb3: Insights into lattice dynamics, thermal stability, and thermal conductivity

Author: Mohanty A.; Deheri P.K.; Khatei J.; Mallick S.; Rout D.; Pradhan G.K.

Details: Volume 200, May 2025

Abstract: Binary skutterudite $CoSb_3$ is considered as one of the most promising thermoelectric (TE) materials for power generation. However, relatively high thermal conductivity limits its application. The nanocrystalline phase addresses this issue by introducing numerous grain boundaries that scatter phonons and hinder their movement. This phonon scattering diminishes the material's heat conduction capability, effectively lowering its thermal conductivity while possibly preserving or improving its electrical properties. Hence, in search for lower thermal conductivity, we have successfully synthesized nanocrystalline $CoSb_3$ with an average grain size of ~60 nm using solvothermal method. The nanocrystalline nature of the $CoSb_3$ powder is confirmed through various characterization techniques, including X-ray diffraction, high resolution transmission electron microscopy, and Raman spectroscopy. Our study focuses on understanding the temperature-dependent phase stability and lattice dynamics of nanocrystalline $CoSb_3$ skutterudites using Raman scattering. Raman spectroscopy reveals that the skutterudite phase in the nanocrystalline form remains stable up to 653 K, after which secondary phases start to develop due to oxidation in the air. Additionally, we discuss the temperature dependent Raman frequency shift for individual optical phonon modes that emphasizes the necessity of using mode-dependent parameters for the modelling of lattice thermal conductivity.

URL: https://www.sciencedirect.com/science/article/pii/S0022369725000381?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Journal of Physics and Chemistry of Solids **IF: 4.3**

Title: Correlation-driven interface magnetism and conductivity in CaNbO3/Ca2VMoO6 perovskite oxide heterostructure: An ab initio approach

Author: Priyambada A.; Parida

Details: Volume 203, August 2025

Abstract: In this work, we investigate the effect of strong electron correlation on the structural, magnetic, and electronic properties at the interface of the $CaNbO_3/Ca_2VMoO_6$ heterostructure using the density functional approach. The heterostructure is designed along the (010) direction. The relaxed heterostructure is also found to be stable in the orthorhombic phase as the bulk individuals. The transition metal–oxygen bond lengths vary more along the y-axis, than the other two perpendicular axes. This makes the octahedra in this heterostructure more distorted than that of bulk constituents. The individual compounds, i.e., $CaNbO_3$ and Ca_2VMoO_6, exhibit G-type antiferromagnetic and ferromagnetic behavior, respectively, at their ground state. Conversely, in the heterostructure, $CaNbO_3$ experiences a spin-flip, converting the compound to a ferromagnetic material, whereas, the spin alignment of Ca_2VMoO_6 remains unchanged. The spins of $CaNbO_3$ and Ca_2VMoO_6 are aligned in the opposite direction, making the interface of the heterostructure antiferromagnetic. The electronic behavior of the heterostructure is obtained to be metallic. The reason behind the metallicity is found to be the partially occupied t_{2g} orbital of Mo atoms, which is clear from the spin-orbital projected density of states, and orbital-projected electronic band structure diagrams with U = 7 eV.

URL: https://www.sciencedirect.com/science/article/pii/S0022369725001829?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Materials Chemistry and Physics **IF: 4.3**

Title: Exploring the role of strong electron correlation on the structural, magnetic, and electronic properties of CaNbO3/La2MnVO6 perovskite oxide heterostructure: An ab initio study

Author: Priyambada A.; Parida P.

Details: Volume 342, 15 September 2025, 130912

Abstract: In this work, we have investigated the structural, magnetic, and electronic properties at the interface of $CaNbO_3/La_2MnVO_6$ oxide heterostructure using density functional theory considering the strong correlation effect. The heterostructure is found to be stable in orthorhombic symmetry same as the bulk individuals. The heterostructure is designed along the (010) direction, hence it is associated with longitudinal strain along y-axis. Therefore, the variation in transition metal and oxygen bond lengths is more along (010) compared to other directions. As a result, the heterostructure possesses more distorted octahedra than the bulk compounds. The spin of the Nb atom present at the Nb–Mn interface is flipped due to strong ferromagnetic coupling, whereas, that in the V–Nb interface remain unchanged. The electronic behavior of the heterostructure is found to conducting, whereas, $CaNbO_3$ and La_2MnVO_6 are found to be insulator and conductor, respectively. The reason for the conducting nature of this heterostructure is partially filled Mn e_g orbital at the Fermi level.

URL: https://www.scopus.com/pages/publications/105004416836

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Environment Development and Sustainability **IF: 4.2**

Title: Green level and expiry time dependent demand based production inventory model with interval uncertainty via tournament differential evolution

Author: Akhtar M.; Ali H.; Manna A.K.; Shaikh A.A.; Bhunia A.K.

Details: 04 June 2025, Article

Abstract: The parameter(s) of practically all real-world optimization problems involving decision-making are complicated due to uncertainty. For that reason, it is essential for solving optimization problem when dealing with unknown optimization problems. In this study, a production inventory model with interval uncertainty is proposed for manufacturing green products.Once more, the demand from customers is regarded as interval-valued and is dependent on the green level. The objective of this work is to address an interval optimization problem, focusing on an interval-valued objective function (average profit) associated with a production inventory model that determines the optimal green level and business period. To achieve this, a simple yet powerful differential evolution algorithm is hybridized with a tournamenting process, aided by interval ranking, to solve the inventory problems within an interval environment. This hybrid approach is termed as tournament differential evolution (TDE) algorithm. The first two variants of TDE technique are employed to obtain the best-found solutions for optimizing the interval-valued average profit. The results from these two TDE variants are then compared with those from several other well-known metaheuristic algorithms. Following this, statistical comparisons and a statistical test are performed on the centre value of the average profit to assess the effectiveness and performance of the proposed hybrid algorithm. Finally, a sensitivity analysis is conducted on the centre value of the average profit, the product's green level, the production run time and the cycle length by varying one model parameter at a time while keeping the others constant. Also, a managerial implications related to proposed work is discussed along with future direction of research.

URL: https://link.springer.com/article/10.1007/s10668-025-06323-z

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Polymer Bulletin **IF: 4.0**

Title: Polyvinylidene fluorideâ€“barium tungstate nanocomposite for advanced energy storage devices

Author: Hota S.S.; Panda D.; Bhoobash S.B.; Biswal L.; Mishra S.; Choudhary R.N.P.

Details: 03 June 2025, Article number 217601

Abstract: Composite films of polyvinylidene fluoride–barium tungstate (PVDF-$BaWO_4$) were created through the solution casting method, wherein ceramic powder was integrated into the PVDF polymer matrix. The synthesized films underwent structural, morphological, and electrical characterization. The vibrational spectroscopy illustrates the enhancement of electroactive β phase F(β) of the polymer. In the frequency range of 100 Hz to 1 MHz, the dielectric constant of the composite increases with the rise in filler concentrations. The PVDF film loaded with 0.9 wt% $BaWO_4$ filler exhibits the highest dielectric constant, attributed to the smaller size of the filler and their homogeneous and discrete dispersion in the matrix. In-depth examination of electrical attributes with impedance spectroscopy unveils the respective influences of grains and grain boundaries on the resistive and capacitive properties of the composite. The study of frequency-dependent electrical conductivity at various temperatures suggests the applicability of Jonscher's power law supports the transport properties of the composites. The observed low electrical conductivity, high dielectric constant, and low loss indicate the potential use of PVDF/BWO composites in developing optoelectronics and capacitive energy storage devices.

URL: https://link.springer.com/article/10.1007/s00289-025-05822-3

SCHOLARLY PUBLICATIONS
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Journal Name: Applied Organometallic Chemistry **IF: 3.7**

Title: Structure of Protonated Baclofen [AuCl4]â^', Theoretical Elucidation and Biological Studies

Author: Chowdhury K.; Shit M.; Halder S.; Samanta A.; Dutta B.; Ali M.; Jana K.; Sinha C.

Details: Volume 39, Issue 5, May 2025

Abstract: Baclofen (3-(4-chlorophenyl)butyric acid, HBAC), a useful medicine of CNS depressant, muscle relaxant, and GABA agonist, has been used to isolate Au (III) ionic solid, $[H_2BAC]^+[AuCl_4]^-$ (1). The confirmed structure of 1 is established by the single crystal X-ray diffraction measurements along with various other physicochemical studies. The anticancer activity of 1 is evaluated on MCF-7, HeLa, MDA-MB-231, A549 cancer cells and has been compared with human normal lung fibroblast cell line (WI-38) and kidney epithelial cell line NKE. The results have been compared with Cisplatin as a standard reference. The toxicity of 1 is accounted from the MTT assay. Notably, the complex 1 has exhibited higher efficacy in inhibiting the proliferation of MCF-7 (IC_{50}: 11.36 ± 1.58 µM) compared to other cancer cells, such as HeLa (IC_{50}: 18.23 ± 2.31 µM), A549 (IC_{50}: 32.09 ± 2.17 µM), and MDA-MB-231 (IC_{50}: 27.07 ± 2.42 µM). A thorough examination of Hirshfeld surfaces and fingerprint plots were used for the comparison of intermolecular interactions, which are critical in the formation of various supramolecular designs. Using the crystallographic parameters of complex 1, DFT computation determines the energy gap ($\Delta E = E_{HOMO} - E_{LUMO}$), 2.50 eV, which is within the range of semiconducting materials and may help for anticarcinogenic action.

URL: https://onlinelibrary.wiley.com/doi/10.1002/aoc.70142

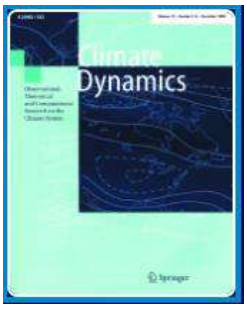
Journal Name: Climate Dynamics **IF: 3.7**

Title: Dynamic and thermodynamic conditions influencing the tropical cyclogenesis in the Bay of Bengal and Arabian sea during warm ENSO-IOD event: a case studyDynamic and thermodynamic conditions influencing the tropical cyclogenesis in the Bay of Bengal

Author: Xalxo K.L.; Mahala B.K.; Routray A.; Mohanty P.K.

Details: Volume 63, Issue 6, June 2025, Article number 258

Abstract: Tropical cyclogenesis in the Bay of Bengal (BoB) and Arabian sea is significantly modulated by dynamic and thermodynamic conditions during warm El Niño-Southern Oscillation (ENSO) and Indian Ocean Dipole (IOD) events. The current study investigates the parameters such as sea surface temperature, vertical wind shear, wind and wind vectors, mid-level relative humidity, low-level relative vorticity, and cloud covers that are conducive to genesis of tropical cyclone and its intensity in the BoB and the Arabian sea during Indian post-monsoon season. This study includes one tropical cyclone named “Titli” in the BoB and another named “Chapala” in the Arabian sea. The role of ocean heat content at 0-700 m depth was also discussed for the seasons April–May-June and October–November-December. Results show that warm ENSO-IOD events enhance low-level convergence, upper-level divergence, and weak wind shear, creating an environment favouring the tropical cyclogenesis. Thermodynamically, warm waters provide a significant source of latent heat through evaporation. Rising moist air cools and condenses, releasing latent heat and fuelling the intense convection. Thermodynamic conditions, particularly under ENSO-IOD events, when coupled with favourable dynamical factors such as low vertical wind shear, positive vorticity significantly contribute to the genesis and intensification of tropical cyclones in the BoB and the Arabian sea. This study highlights the critical role of dynamic and thermodynamic interactions in tropical cyclogenesis during warm ENSO-IOD events, providing insights for improved predictability and mitigation strategies.



URL: https://link.springer.com/article/10.1007/s00382-025-07746-0

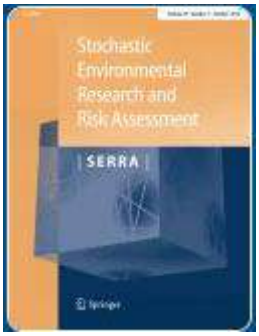
Journal Name: Stochastic Environmental Research and Risk Assessment **IF: 3.6**

Title: Evaluation of NCUM-R 4DVAR assimilation techniqueâ€™s performance on simulation of tropical cyclones over NIO region

Author: Patel S.S.; Routray A.; Singh V.; Dutta D.; Bhatla R.; Mahala B.K.; Opatz J.

Details: 27 May 2025, Article number 100536

Abstract: The present study evaluates the forecasting skill of a regional model (NCUM-R) with the 4DVAR analysis system on the simulation of pre- and post-genesis phases of three tropical cyclones (TCs) over the North Indian Ocean (NIO) region. Specifically, the study aims to determine whether the NCUM-R model can identify pre-genesis of the storm 2–3 days in advance to accurately predict the intensity and track of TCs. The selected storms include the Severe Cyclonic Storm (SCS) 'Asani' (2022), the extremely severe cyclonic storm (ESCS) 'Mocha' (2023), and ESCS 'Biparjoy' (2023). The initial conditions (ICs) are prepared for the NCUM-R forecasting model by assimilating various observations through the 4DVAR data assimilation (DA) technique. Various thermodynamic and dynamic variables, such as genesis potential parameters (GPP), potential vorticity (PV), relative humidity (RH), landfall position and time errors are examined. The study highlights equatorial moisture's role in storm development. Moist winds from the equator release latent heat, greatly intensifying storms. The study shows that the track error forecast significantly improved by the NCUM-R model about 7%, 11.2%, 22.8% and 21.9% on 00, 24, 48 and 72 UTC forecasts. The landfall position and time error are relatively less in the regional model. Further, the NCUM-R model's outputs are validated against India Meteorological Department (IMD) observations and Fifth Generation of ECMWF Atmospheric ReanalysisERA-5, demonstrating a good match in TCs' pattern and intensity.



URL: https://link.springer.com/article/10.1007/s00477-025-02999-x

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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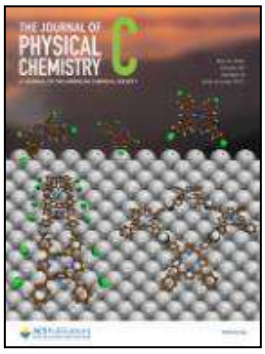
Journal Name: Journal of Physical Chemistry C **IF: 3.3**

Title: Resonance Raman Process and Exciton Engineering in MoS2-WS2 Vertical Heterostructure

Author: Panigrahi A.K.; Sahoo S.; Mallik S.K.; Kumar A.; Pradhan M.; Roy S.; Senapaty S.R.; Sahu P.; Mohanty H.N.; Padhan R.; Pradhan G.K.; Sahoo S.

Details: Vol 129/Issue 19, Article, May 6, 2025

Abstract: Two-dimensional (2D) materials have emerged as a fascinating platform to explore novel optical and electrical properties at the nanoscale. Designing suitable heterostructures has the potential to offer enhanced and tunable physical properties and to broaden their applications in the field of nanoelectronics and optoelectronics, which are not achievable using individual monolayers. In this study, we present the optical characterization of a salt-assisted chemical vapor deposition-grown MoS_2-WS_2 vertical heterostructure, where a continuous monolayer of MoS_2 is transferred over WS_2 layers with different stacking configurations using a PMMA-assisted transfer method. The heterostructures are characterized by micro-Raman and photoluminescence spectroscopy under various conditions, revealing a few interesting results. The resonance Raman effect with different laser excitations leads to a noticeable increase in intensity for both the characteristic and low-frequency vibrational modes in WS_2 compared to MoS_2. Additionally, as the layer number of WS_2 increases, two novel Raman modes have emerged from the subject heterostructure, which show crossed polarization dependency. Low-temperature photoluminescence spectroscopy reveals the evolution of interlayer exciton peaks as a consequence of type-II band alignment in the MoS_2-WS_2 heterostructures. Furthermore, our first-principles density functional theory (DFT) calculations shed light on the observed optical properties of the vertical heterostructure. These findings highlight the potential for tailoring the structural and vibrational properties of 2D heterostructures by engineering a van der Waals heterostructure.



URL: https://pubs.acs.org/doi/10.1021/acs.jpcc.5c01463

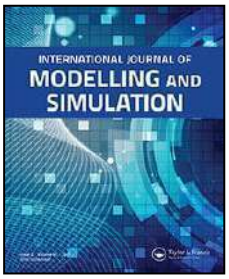
Journal Name: International Journal of Modelling and Simulation **IF: 3.1**

Title: Qualitative analysis of magnetohydrodynamics Powellâ€“Eyring fluid with variable electrical conductivity

Author: Swain S.; Sarkar S.; Sahoo B.; Makinde O.D.

Details: Volume 45, Issue 2, 2025

Abstract: The non-Newtonian fluid model helps to visualize the fluid movements in modern industrial materials for the enhancement of work productivity. Therefore, this numerical investigation examines the flow behaviour of Powell–Eyring fluid over the stretching sheet with variable electric conductivity and thermal radiation. We have used the Lie group analysis method to reduce the governing momentum and energy equations into ordinary differential equations (ODEs). The resultant system is then numerically solved using the shifted Chebyshev collocation method. The accuracy of the numerical method has been verified by comparing the current work to existing literature, and it is found to be in excellent agreement. The effects of rheological parameters like stretching sheet parameter, magnetic field parameter, material parameters, suction/injection parameter, radiation parameter and Prandtl number on fluid velocity and temperature profiles are examined in detail through tables and graphs. The main motivation behind this study is to examine the effects of Lorentz force on fluid velocity and temperature in the presence of thermal radiation, which has several industrial applications. It is observed that the velocity profile decreases when the magnetic field parameter increases. Furthermore, it is noticed that increasing thermal radiation parameter increases the temperature profile.



URL: https://www.tandfonline.com/doi/full/10.1080/02286203.2023.2231613

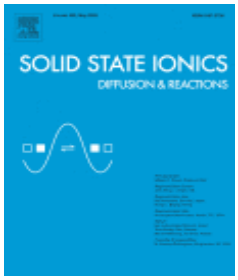
Journal Name: Solid State Ionics **IF: 3.0**

Title: Exploring structural, optical, dielectric and electrical attributes of a La based complex perovskite

Author: Priyadarshini L.; Biswal L.; Rout S.; Moharana K.; Parida A.K.; Choudhary R.N.P.; Satpathy S.K.

Details: Volume 45, Issue 2, 2025

Abstract: A rare-earth based novel compound with a disordered perovskite structure has been synthesised using the conventional solid-state reaction approach. The structural phase of the compound is analysed using room temperature X-ray diffraction (XRD) data. The refinement of XRD data suggested formation of compound in trigonal phase with R-3c symmetry. Position of peaks in Raman spectra obtained at room temperature further support the proposition of above structure and symmetry of formation. Using scanning electron microscope (SEM) images, the microstructure of the compound and the surface morphology is revealed. EDX analysis presented semi-quantitative information on distribution and weight percentage of elements present, from which the synthesis of the expected compound is substantiated. Examination of optical characteristics via UV–Visible absorption spectroscopy revealed a band gap of 3.2 eV suggesting possible potential applications in optoelectronic and photovoltaic devices. The electric polarisation and relaxation phenomena prevailing in the material as a function of frequency and temperature are extensively studied using data acquired via complex impedance spectroscopy (CIS) technique. A temperature and frequency stable dielectric response in high frequency region recommends use of compound for application at high frequency and temperature. Dominating bulk contribution to overall electrical response and negative temperature coefficient of resistance (NTCR) behaviour is observed. The frequency-dependent ac conductivity data adheres to Jonscher's power law. To estimate the activation energy, which facilitates the identification of the specific charges involved in the ac conduction process, the temperature-dependant ac conductivity data is utilised



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