SCHOLARLY PUBLICATIONS
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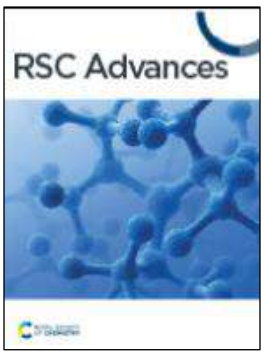
Journal Name: RSC Advances **IF: 6.1**

Title: Phytotoxic effects of methylene blue dye on mustard (Brassica juncea L.): insights from germination bioassays and multivariate analysis

Author: Subudhi L.; Panda A.K.; Mohapatra S.

Details: Volume 16, Issue 30, May 2026

Abstract: Methylene blue (MB), a commonly employed cationic dye, contaminates aquatic and terrestrial ecosystems. Although its presence in polluted environments has been documented, little is known about its phytotoxicity to terrestrial agricultural crops. This study was conducted to assess the effect of MB on the germination and seedling development of a major oil crop, mustard (Brassica juncea L.), in a controlled hydroponic system. MB was found to significantly affect germination and seedling development. This effect was concentration-dependent. Germination was reduced by 50% compared to the control at higher concentrations. Similarly, root growth, shoot growth, seedling vigour index, and biomass were significantly reduced. Principal component analysis, hierarchical cluster analysis, and heatmap correlation analysis revealed a strong negative correlation between MB concentration and growth. Toxicity increased significantly with increasing MB concentration. This study revealed that MB significantly affects germination and seedling development and poses a potential risk to agricultural ecosystems, particularly during the early stages of crop establishment. Furthermore, by statistically identifying radicle elongation and seedling vigour as the most sensitive parameters, this study establishes them as reliable, early-warning biomarkers for agricultural risk assessment. Further field studies are needed to better understand its long-term impact on plant growth and productivity.



URL: https://pubs.rsc.org/ra/article/16/30/27518/1249688/Phytotoxic-effects-of-methylene-blue-dye-on

Journal Name: Inorganic Chemistry Communications **IF: 5.9**

Title: Stir-controlled differential binding of folic acid in hollow silver nanocubes and the PERS enhancement in pre- and post-saturation regimes

Author: Gupta P.; Dadhich B.K.; Patra S.K.; Bhushan B.; Priyam A.

Details: Volume 191, Issue P1, September 2026

Abstract: The chemical identity of the biomolecules on nanostructured substrates is not only defined by plasmon-enhanced Raman spectroscopy (PERS) but also by the nature of the plasmon resonance that is facilitated by the substrate. In this case, we show that the rate of the stirring in the course of the synthesis regulates the sharpness of the corners of hollow silver nanocubes (HAgNCs) that determines the excitation of either the dipolar or both the dipolar and quadrupolar surface plasmon resonances with direct and molecularly specific implications on the PERS of the adsorbed folic acid (FA) capping agent of the hollow silver nanocube.. The transmission electron microscopy proves that both samples produce hollow cubic nanoparticles with similar edge lengths (around 78–79 nm) and void diameters, and the edge of critical morphological distinction is the much sharper corners in HAgNCs-Zero. Second-derivative analysis of UV–Vis extinction spectroscopy shows that HAgNCs-Zero only supports dipolar plasmon modes. Meanwhile, HAgNCs-150, alone, has an extra quadrupolar resonance at 430 nm, the higher-order plasmon mode, which has not been reported in hollow silver nanocubes. Correlatively, PERS measurements reveal that the symmetric and asymmetric NH folic acid vibrations of folic acid at 3200 and 3400 cm−1 are present only in the spectrum of HAgNCs-Zero, the first-ever NH folic acid modes to be observed in any SERS or PERS of folic acid on any substrate. These results provide a direct mechanistic pathway between the synthesis environment to corner geometry, plasmon mode hierarchy, molecular binding orientation, and selective vibrational enhancement to provide new understanding on the rational design of morphology-controlled PERS substrate for bioanalytical applications.

URL: https://www.sciencedirect.com/science/article/pii/S1387700326008580?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Materials Advances **IF: 5.8**

Title: Bridging energy conversion and storage: precursor-engineered Co@CoO–Y2O3 heterostructures for oxygen reduction reaction and battery-type supercapacitor applications

Author: Samanta S.B.; Roy S.; Palit S.; Bharatbhai J.A.; Barik N.; Mo H.; Lee J.; Giri S.; Das S.

Details: Volume 7, Issue 12, June 2026

Abstract: The escalating consumption of fossil fuels and the intermittency of renewable power have intensified the need for multifunctional electrochemical materials that can couple efficient energy conversion and durable energy storage while avoiding device-level complexity and reliance on Pt. Herein, we report a non-noble metal-based Co@CoO–Y_2O_3 (CCY) heterostructured composite synthesized via the pyrolysis of a well-defined cobalt–yttrium single-crystal precursor complex. In alkaline media (1 M KOH), CCY demonstrates competitive oxygen reduction reaction (ORR) activity, delivering a half-wave potential of 0.603 V (vs. RHE), an onset potential of 0.79 V, and stable operation for over 24 h. Koutecky–Levich analysis indicates a predominantly two-electron ORR pathway with high peroxide selectivity, highlighting its suitability for non-Pt catalytic systems. Simultaneously, when employed as a battery-type supercapacitor electrode, CCY exhibited electrolyte-dependent faradaic charge storage, achieving specific capacitances of 22, 18.74, and 10.12 F g^{-1} at 0.1 A g^{-1} in KOH, NaOH, and LiOH electrolytes, respectively, along with a low charge-transfer resistance and ∼64.14% capacitance retention over 10 000 cycles. This study establishes a scalable, precursor-driven strategy for designing rare-earth-modified bifunctional materials for integrated energy conversion and storage applications.

URL: https://pubs.rsc.org/ma/article/7/12/6193/1225273/Bridging-energy-conversion-and-storage-precursor

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Journal of Physics and Chemistry of Solids **IF: 4.9**

Title: An ab-initio investigation of Cd-based defect chalcopyrite-type semiconductors: Promising candidates for sustainable energy goals

Author: Nayak, A.; Jena, S.; Parida, P.

Details: Volume 212 May 2026

Abstract: This work focuses on the thermoelectric behavior of CdGaX (X = S, Se, and Te) defect chalcopyrite compounds, carried out using density functional theory (DFT) within the generalized gradient approximation (GGA). The ab-initio structural analysis of these body-centered tetragonal compounds reveals a systematic increase in lattice parameters from CdGaS to CdGaTe, along with the deviation from the ideal chalcopyrite structure. CdGaS exhibits the highest thermodynamic stability, having the lowest cohesive energy. The value of lowest defect formation energy of all the compounds confirmed that the formation of the defects can be done easily. The electronic properties show that all three systems are direct band gap semiconductors. The ductile nature of these compounds is obtained from the elastic behaviors, with CdGaS having the maximum stiffness. All the compounds are found to be thermally stable at elevated temperature (at 800K) through AIMD calculations. The electronic thermoelectric properties are calculated using the semi-classical Boltzmann transport theory. The thermoelectric parameters are calculated w.r.t. temperature, carrier concentration, and chemical potential, revealing enhanced performance under p-type doping. CdGaS and CdGaSe show peak ZT values at high temperatures with a carrier concentration of 10^{18} cm^{-3}, while CdGaTe peaks at 10^{20} cm^{-3}. Using the deformation potential theory and Slack method, the carrier relaxation time and the lattice thermal conductivity are determined, respectively. This study highlights the potential of CdGaX compounds as promising thermoelectric materials, especially at elevated temperatures.

URL: https://www.sciencedirect.com/science/article/pii/S0022369726000235?

SCHOLARLY PUBLICATIONS
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Journal Name: Scientific Reports **IF: 4.9**

Title: Design of a MWCNT integrated advanced ternary composite with dual functionality in energy storage and photo catalytic dye detoxification

Author: Pradhan D.; Biswal S.K.; Nayak N.; Singhal R.; Salim A.; Dash S.K.

Details: Volume 16, Issue 1, December 2026

Abstract: Polluted water harms human health and the planet's wellbeing alike. Tackling the global energy crisis driven by rapid economic expansion and our reliance on power hungry gadgets demands innovative clean energy storage solutions. This study developed a ternary heterojunction photocatalyst based on g-C_3N_4/TiO_2/MWCNTs studied their structural, optical, and morphological properties, the produced materials were thoroughly evaluated via XRD, FTIR, BET, UV-Vis DRS, PL, SEM, TEM, Raman, and XPS studies. The photocatalytic activity of the g-C_3N_4/TiO_2/MWCNTs nanocomposite was evaluated via the degradation of rhodamine B dye under solar light with various parameters, and the results revealed that the g-C_3N_4/TiO_2/MWCNTs nanocomposite had 99% degradation efficiency with Z scheme mechanism and outperformed the pristine g-C_3N_4 sheet and TiO_2, with approximately 1.3 and 1.4 folds higher degradation rates, respectively. The photodegradation process was followed by pseudo first-order kinetics with a rate constant of 0.0922 min^{-1}, resulting in a 2.36 and 3.16 fold increase compared to pristine catalysts. Electrochemical impedance spectroscopy revealed improved electrical conductivity, and cyclic voltammetry investigations revealed an outstanding specific capacitance of 1860 F/g at 30 mV/s nearly six times greater than that of pristine g-C_3N_4 (348 F/g).The remarkable photocatalytic performance and good electrochemical properties of the g-C_3N_4/TiO_2/MWCNTs heterojunction highlight its promise as a multifunctional material for environmental purification and energy storage applications.

URL: https://www.nature.com/articles/s41598-026-47268-1

SCHOLARLY PUBLICATIONS
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Journal Name: Physics and Chemistry of the Earth **IF: 4.6**

Title: Hidden particles: Abundance, chemical characteristics, metal binding properties, and environmental risk of microplastics in the downstream of riverine sediment-water ecosystems

Author: Mahapatra S.; Maity J.P.; Singha S.; Mishra T.; Mangal S.; Dey G.; Sharma R.K.; Banerjee P.; Bhattacharya P.

Details: Volume 144, October 2026

Abstract: Microplastics (MPs) pollution is a global problem in the current decade due to its contamination, persistence, and risks to ecosystems. The present study aims to investigate the 'occurrence and distribution', physiochemical characteristics, metal binding with MPs, and their environmental risk in the downstream of the riverine ecosystem (water and sediment/soil). The MPs were observed in the range of 50-5000 µm, with a higher abundance in sediment (1356 ± 13 particles/kg) compared to water (582 ± 12 particles/m^3), where the sediments have the potential to act as long-term sinks for MPs. The 'transparent/white color' and 'fragments/fibers' MPs were dominant in both water and sediment. Chemically, the polypropylene (PP) had the highest abundance (Water: 55.56 ± 2%, Sediment: 57.45 ± 3%) compared to polyethylene (PE) polyethylene terephthalate (PET), and polystyrene (PS) in the riverine ecosystem. All MPs are partially weathered (surface roughness/cracks and degradation), and several elements (e.g., As, Cd, Al, etc.) are attached to the MPs surface, suggesting anthropogenic activities as significant contributors. The overall study provides a comprehensive baseline of MPs pollution and risk in the river system, as well as MPs-metal interactions in the aquatic ecosystem, which can help to take proper monitoring strategies and mitigation of plastic-related ecological threats at both regional and global scales, particularly in riverine ecosystems as per SDG-3, 6, 12, and 14.

URL: https://www.sciencedirect.com/science/article/abs/pii/S1474706526002627?via%3Dihub

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

Title: Elemental, morphological and radiation-protective nature of selected low-cost construction materials: Experimental, theoretical and PHITS simulation

Author: Upadhyay D.R.; Khatiwada L.N.; Sunar R.; Praharaj S.; Rout D.; Khanal R.

Details: Volume 244, July 2026

Abstract: The ionizing radiation protective nature at different ranges of energy becomes important in materials. The prime objectives of this work are to investigate density, porosity, elemental, minerological, morphological and radiation shielding properties of low cost construction materials (CM). For this seven varieties of CM are experimentally analyzed using Archimedes principle, energy dispersive X-ray fluorescence, FESEM-EDS, powder X-ray diffraction, theoretical and simulation methods. Comprehensive elemental analysis and mapping demonstrated that Si, Ca, Al, O, and Fe constitute the predominant elemental components of the samples. FESEM analysis revealed well-defined crystalline morphologies and the development of microstructural porosity in selected specimens, while XRD patterns confirmed their crystalline nature. Phase assemblage analysis identified quartz (SiO_2), calcite ($CaCO_3$), alumina (Al_2O_3), and hematite (Fe_2O_3) as the dominant mineralogical constituents. Furthermore, the Particle and Heavy Ion Transport code system (PHITS) was used to determine and evaluate the protective nature, such as attenuation coefficients, radiation protection efficiency, transfer factors, and lead equivalent thickness. Moreover, shielding properties are compared with Phy-X/PSD database. Using Phy-X/PSD, the parameters such as linear, mass attenuation, half and tenth value layers, mean free path, effective conductivities, atomic number, and electron densities were estimated. Furthermore, the neutron shielding is also evaluated using both techniques. indicating significant radiation shielding potential. These findings support their suitability as low-cost, environmentally sustainable materials for radiation shielding applications.

URL: https://www.sciencedirect.com/science/article/abs/pii/S0969806X26002112?via%3Dihub

SCHOLARLY PUBLICATIONS
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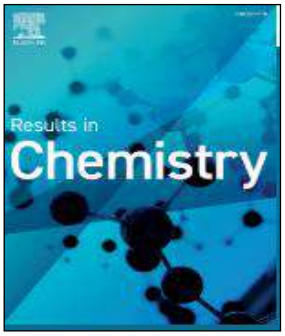
Journal Name: Results in Chemistry **IF: 4.2**

Title: Eco-sustainability of periphyton-inhabited polyvinyl chloride (PVC) and fibre-reinforced plastic (FRP) inferred by in vivo zebrafish embryo oxidative and steatosis responses

Author: Sahoo M.; Naser S.S.; Jena S.; Gupta A.; Barik D.; Sinha A.; Ghosh A.; Vinod C.; Verma S.K.

Details: Vol. 23, May 2026

Abstract: The growing use of synthetic materials in aquaculture, such as polyvinyl chloride (PVC) and fibre reinforced plastic (FRP), has prompted concerns regarding their environmental and biological safety. Despite their durability and cost-effectiveness, the ecological impact of these materials, especially when colonized by periphyton, remains underexplored. This study investigates the developmental and physiological responses of zebrafish embryos (Danio rerio) exposed to water containing periphyton-covered PVC and FRP sheets. Survivability, morphological development, hatching success, heart rate, and cellular responses were evaluated to understand potential toxic effects. While periphyton biofilms were expected to promote ecological compatibility, findings revealed that both periphyton-inhabited PVC and FRP adversely affected embryonic development. Notable effects included delayed hatching, elevated mortality, and increased oxidative stress. However, PVC exhibited relatively higher biocompatibility, causing fewer disruptions to embryo viability and cellular function compared to FRP. At the molecular level, FRP induced stronger toxic responses, likely due to its chemical composition and more aggressive interaction with developing embryos. In contrast, PVC's material characteristics and associated biofilm interactions were less harmful. The study highlights the importance of assessing both material type and biofilm dynamics in aquaculture systems and supports the shift toward eco-compatible infrastructure for sustainable aquatic practices.



URL: https://www.sciencedirect.com/science/article/pii/S221171562600158X?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: ChemCatChem **IF: 4.1**

Title: Stable UiO-66/BaTiO3 Heterostructure for Efficient Solar-Light Ciprofloxacin Degradation and Energy Harvesting Applications

Author: Dhal B.C.; Bhosale P.S.; Hajra S.; Panda S.P.; Das A.; Dutta B.; Kim H.J.; Sahu R.

Details: Volume 18, Issue 11, June 2026

Abstract: The fabrication of robust metal–organic frameworks (MOFs) continues to be difficult in materials science studies. In order to overcome such an obstacle, the design of hybrid framework materials could be an effective solution. Herein, we successfully synthesized UiO-66/$BaTiO_3$ hybrids with different percentages of $BaTiO_3$ mass (10%–50%), which are intended to improve the photocatalytic activity. Considering the widespread pollution of water resources with ciprofloxacin (CIP), leading to the emergence of antibiotic resistance, urgent treatment measures are needed. The optimized U/BTO-25 hybrid showed remarkable photocatalytic activity, with CIP removal reaching 98.37% in 30 min. Such excellent catalytic behavior is due to the complementary nature of both components, where the large specific surface area of UiO-66 helps with the adsorption of CIP, while ferroelectric polarization of $BaTiO_3$ leads to charge separation. In particular, the radical trapping experiments $\bullet O_2^-$ and h^+ to be the dominant radicals. The hybrid showed excellent stability in four successive cycles with a slight decline in efficiency. In addition, the hybrid has significant prospects for use in triboelectric nanogenerators. The output of the nanogenerator was 73 V and 180 nA, respectively, and the output can be harvested in a capacitor to power off-the-shelf electronic devices, demonstrating the potential of MOF-ferroelectric hybrid materials.

URL: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cctc.70859

SCHOLARLY PUBLICATIONS
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Journal Name: Frontiers in Antibiotics **IF: 3.9**

Title: Antimycobacterial peptides as natural therapeutics for tuberculosis: mechanisms and structural features

Author: Pritam, P; Das, S; Behera, SK; Sahoo, M; Subudhi, L; Mohapatra, S; Panda, AK

Details: Volume 5, May 2026

Abstract: The disease tuberculosis, caused by *Mycobacterium tuberculosis*, is one of the leading causes of global human mortality. The rise of multidrug and extensively drug-resistant strains of the pathogen and the limited efficacy of the BCG vaccine is one of the major concerns worldwide. Conventional chemotherapy for tuberculosis is often very long and has several side effects. These factors lead to an urgent need for alternative, non-toxic therapeutic strategies with minimal side effects. Antimycobacterial peptides (AMPs), are a class of natural compounds that have shown a broad spectrum of anti-mycobacterial activity with a low propensity for the development of anti-mycobacterial resistance. This review summarizes the current antimycobacterial peptides, highlighting their structural features, physicochemical determinants, and their mechanism of action. Some of the key peptides have been critically discussed with respect to their membrane targeting mechanism. The role of structural modifications, such as disulfide bonding, cyclization, hydrophobicity tuning, and post-translational modifications, in enhancing antimycobacterial efficacy and stability is also examined. Consequently, the broad mechanism of action of these peptides and their role in the development of anti-tuberculosis drugs have been emphasized. This article combines mechanistic and structural insights to show how antimycobacterial peptides could become new anti-TB drugs. It also provides a guide for developing and improving peptide therapies for tuberculosis.

URL: https://www.frontiersin.org/journals/antibiotics/articles/10.3389/frabi.2026.1769369/full

SCHOLARLY PUBLICATIONS
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Journal Name: Industrial & Engineering Chemistry Research **IF: 3.9**

Title: A Chlorophyll-Appended MIL-125-Ti Nanocomposite for Photodriven H2 Generation, Dye Degradation, and CWA Detoxification

Author: Dhal, BC; Swain, J; Acharya, D; Swain, S; Biswas, M; Ghosh, S; Dixit, A; Garg, P; Tyagi, AK; Sahu, R

Details: Volume 65, Issue 25, June 2026

Abstract: The growing environmental crises posed by synthetic dye pollution, chemical warfare agents (CWAs), and energy scarcity necessitate innovative, multifunctional solutions. In this regard, we present a hybrid MIL-125-Ti/Chlorophyll (MTC) nanocomposite that simultaneously addresses these challenges under visible-light irradiation. By integrating natural chlorophyll (0.2 wt %) into the MIL-125-Ti framework, we significantly enhance visible-light absorption and charge-separation efficiency through natural photosensitizers. The composite demonstrates exceptional triple functionality: (a) photocatalytic dye degradation, achieving 100% degradation of Rhodamine B (20 ppm) within 180 min (vs 76.2% for pristine MIL-125) via pseudo-first-order kinetics having rate constant: 0.02037 min-1; (b) hydrogen generation, with a 10-fold increase in photocurrent density (1.7 mu A cm-2) and a 1.5 times higher H2 production rate (265 mu mol h-1) compared to MIL-125; and (c) CWA detoxification, completely degrading Sarin (GB) within 15 min (vs 92.5% by MIL-125 in 30 min) following first-order kinetics. Therefore, the effective generation of the composite acted as a suitable and sustainable catalyst for light-driven environmental applications. Interestingly, the composite's stability remains intact even after four dye-degradation cycles. This work has exhibited a multifunctional platform for environmental remediation and clean energy production.

URL: https://pubs.acs.org/doi/10.1021/acs.iecr.5c04489

Journal Name: Journal of Supercomputing **IF: 3.5**

Title: Efficient hybrid approach for time-fractional (1 + 1)-dimensional Chafee–Infante equation using the Shehu–Adomian decomposition method in the Caputo environment

Author: Nayak S.K.; Jena S.R.

Details: Volume 82, Issue 8, June 2026

Abstract: In this study, we investigate the one-dimensional Chafee–Infante model, where heat diffusion serves as the primary mechanism of energy transfer. The Shehu transform is employed to derive solutions for three distinct forms of the Chafee–Infante equation, incorporating the time derivative in the Caputo fractional sense, and the resulting transformed systems are solved with the nonlinear terms using the Adomian decomposition method. The Chafee–Infante equation is widely used to model nonlinear phenomena in population dynamics, chemical reactions, heat transfer and neural activity. This study provides a new contribution by applying the Shehu decomposition method (SDM) to the time-fractional CI equation. The key advantage of the Shehu decomposition method (SDM) over transform-based hybrid methods such as Laplace–ADM, Sumudu–ADM and Elzaki–ADM lies in its direct handling of nonlinear problems without requiring inverse transforms, which significantly simplifies both analysis and computation. The present method also demonstrates accurate and convergent solutions, supported by error norms and rate of convergence analysis. For each case, the L2 and L∞ norms error norms are evaluated to assess accuracy. Numerical simulations, convergence investigations and comprehensive error and stability analyses consistently confirm excellent agreement between the analytical approximations and the exact solutions. The behavior of the solutions is further illustrated through three-dimensional surface plots and two-dimensional line graphs. Additionally, the numerical results obtained in this work are compared with existing findings in the literature, showing strong consistency and improved performance in terms of computational efficiency cost (CPU time).

URL: https://link.springer.com/article/10.1007/s11227-026-08572-9

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Food and Humanity **IF: 3.5**

Title: Biochemical insights of alpha-amylase activity in determining starch digestibility and glycaemic response in rice

Author: Nayak L.; Biswal M.; Das J.; Panda S.; Lal M.K.; Ngangkham U.; Kumar S.; Kumar A.

Details: Volume 7, December 2026

Abstract: Rice's impact on blood sugar is significant, particularly for those with diabetes. This study looks at the function of alpha (α)-amylase, a main starch-hydrolyzing enzyme, and its relationship to glycaemic index (GI), glycaemic load (GL), amylose content (AC), and resistant starch (RS) in the selected rice genotypes. Sixteen genotypes, comprising high-protein, scented, general, and pigmented rice, were tested for α-amylase activity during seed germination, and in mature grain eGI, GL, AC, and RS were also carried out. All four traits showed significant genotypic differences ($p < 0.05$) with the ranges of AC (4.42–25.5%); RS (0.4–1.86%); α-amylase (1.8–7.51U/100seeds) and eGI (54.46–72.15). Amylose content ($r = -0.53$) and RS ($r = –0.90$) were negatively correlated with GI; while α-amylase ($r = 0.94$) and GL ($r = 0.83$) were positively associated with eGI. Regression analysis confirmed a strong relationship of α-amylase with eGI ($R^2=0.88$), while a moderate relationship to GL ($R^2=0.62$). Principal Component Analysis and hierarchical clustering grouped genotypes into distinct clusters, with pigmented rice often exhibiting a desirable combination of high AC, high RS, and low eGI. This study proposes seed α-amylase activity as an exploratory correlation study proposing a potential screening marker for identifying rice genotypes with altered starch digestibility and suggesting its use helps screening in rice breeding programs for developing health-oriented rice cultivars.

URL: https://www.sciencedirect.com/science/article/abs/pii/S2949824426002673?via%3Dihub

SCHOLARLY PUBLICATIONS
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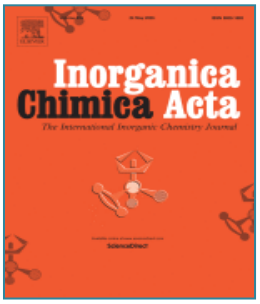
Journal Name: Inorganica Chimica Acta **IF: 3.2**

Title: Crystallographic and quantum chemical methods to elucidate the structural and electronic characteristics of a Zn(II) complex

Author: Patla, A.; Dutta, B.; Paul, A.; Subramanian, R.; Konar, S.

Details: Volume 595 , May 2026

Abstract: A new zinc(II) complex [Zn(L)$(SCN)_2$] (1) of NNN donor Schiff base ligand L (where "L" = N-(4,6-dimethyl-pyrimidin-2-yl)-N'-pyridin-2-ylmethylene-hydrazine) is synthesized and characterized by elemental analysis and single crystal X-ray crystallography (XRD). Using the single-crystal X-ray diffraction technique, the structure of Complex 1 exhibits a distorted trigonal bipyramidal geometry. The crystal packing of 1 exhibits intermolecular S···H, π···π stacking interactions to generate a 1D network. These unique S···H interactions significantly affect the stability, arrangement, and prospective functional uses of the Complex. DFT calculations were used to determine the complex's electronic structure, using the pseudo-potential LANL2DZ for the zinc atom and the 6-31G+(d,p) basis set for the remaining atoms, at the B3LYP level. At this computational level, the optimized structure can accurately replicate the crystal structure. To comprehend the complex's reactivity properties, the molecule's electrostatic potential (MEP) and frontier molecular orbital analysis have been assessed. Natural bond orbital (NBO) analysis was used to illustrate the charge transfer between donor and acceptor sites. Additionally, fingerprint plots and Hirshfeld surface analysis are used to examine the complex's intermolecular interactions. Hirshfeld surface analysis, combined with two-dimensional fingerprint plots, provided a comparative visualization of the non-covalent interaction patterns in the synthesized complex.



URL: https://www.sciencedirect.com/science/article/pii/S002016932600040X?via%3Dihub

SCHOLARLY PUBLICATIONS
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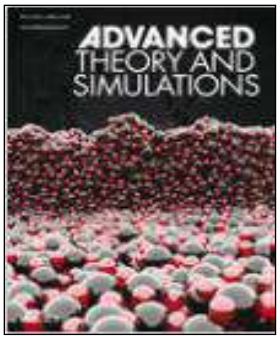
Journal Name: Advanced Theory and Simulations **IF: 3.2**

Title: Hermite Wavelet Simulation of the Time-Fractional Whitham–Broer–Kaup System for Nonlinear Dispersive Wave Dynamics

Author: Nayak S.; Gupta A.K.

Details: Volume 9, Issue 5, May 2026

Abstract: Modeling nonlinear long-wave motion becomes more challenging when the underlying medium exhibits memory effects or delayed temporal responses. Classical integer-order models cannot capture these hereditary behaviors, which are observed in many natural wave processes. To address this limitation, we investigate the time-fractional Whitham–Broer–Kaup (TFWBK) system, where memory is introduced through the Caputo fractional derivative. A numerical scheme based on Hermite wavelet collocation is utilized to solve TFWBK. This method converts the original nonlinear fractional system into a sparse algebraic structure that is efficient to compute and stable over long simulation intervals. Numerical tests show rapid convergence and high spectral accuracy for both classical and fractional cases, with errors remaining consistently small. The performance of the method is examined through comparison with several well established approaches including the B-spline collocation, the variational iteration method (VIM), the Adomian decomposition method (ADM), and two versions of the optimal homotopy asymptotic method (OHAM1 and OHAM2). The results indicate that the present scheme offers improved accuracy while maintaining computational economy. Overall, the wavelet-based framework provides a reliable and memory-aware tool for simulating nonlinear dispersive wave dynamics described by the TFWBK model.



URL: https://advanced.onlinelibrary.wiley.com/doi/10.1002/adts.70423

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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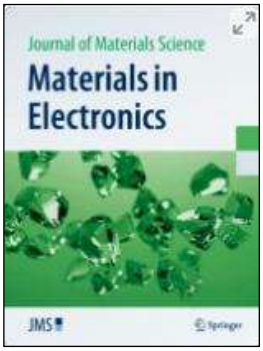
Journal Name: Journal of Materials Science: Materials in Electronics **IF: 3.2**

Title: Influence of precursor molarity on Sb2(S,Se)3 thin films prepared by a solution-based dip-coating method

Author: Bal S.S.; Basak A.; Behera D.; Singh U.P.

Details: Volume 37, Issue 16, June 2026

Abstract: Antimony sulfo-selenide ($Sb_2(S,Se)_3$) has emerged as a promising absorber material for thin-film solar cell applications owing to its suitable band gap, high absorption coefficient, earth-abundant constituents, low toxicity, and excellent stability. The present work focuses on examining the effect of varying precursor molarity on the crystallinity, composition, morphology, and optical behavior of $Sb_2(S,Se)_3$ thin films. In this work, Sb_2S_3 thin films were synthesized using a solution-based deposition method employing antimony (III) chloride ($SbCl_3$) and thiourea (CH_4N_2S) as precursor materials with dimethylformamide (DMF) as the solvent. To examine the impact of concentration on film characteristics, precursor solutions with varying molar concentrations (0.1 M, 0.6 M, and 1.1 M) were made. Selenium was then incorporated into the deposited Sb_2S_3 films by annealing them at 400 °C in a selenium environment to prepare antimony sulfo-selenide ($Sb_2(S,Se)_3$). The structural, morphological, compositional, and optical characteristics were studied. Among the prepared samples, the film deposited using the 0.6 M precursor solution exhibited a dislocation density of 9.50×10^{15} m^{-2} with the highest crystallite size of 10.26 nm with a reduced full width at half maximum (FWHM) value of 0.84°, indicating improved crystallinity and film compactness and a lower band gap of 1.16 eV compared to the 0.1 M and 1.1 M films. These findings Indicate that the 0.6 M precursor concentration is favorable for obtaining high-quality $Sb_2(S,Se)_3$ absorber layers suitable for thin-film solar cell applications



URL: https://link.springer.com/article/10.1007/s10854-026-17686-y

SCHOLARLY PUBLICATIONS
School of Applied Sciences
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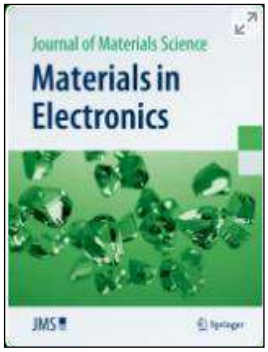
Journal Name: Journal of Materials Science: Materials in Electronics **IF: 3.2**

Title: K0.5La0.5BaTi2O6: an exploration of structural and multifunctional properties

Author: Priyadarshini L.; Rout S.; Moharana K.; Roy N.; Biswal L.

Details: Volume 37, Issue 16, June 2026

Abstract: Substituting cations of different ionic radii and valence states in A-site of perovskite oxides creates ionic size mismatch and mixed valence environment, further resulting in lattice distortions and local strain fields. Thus, introducing controlled disorderness in A-site has become an effective approach for tailoring and optimising the properties of perovskite oxides. This work reports the systematic and comprehensive analysis of structure, optical and dielectric study of a rare earth-based A-site disordered complex perovskite $K_{0.5}La_{0.5}BaTi_2O_6$ synthesized through solid state reaction route. The study presents a comparative analysis of crystallite size, internal stress, lattice strain, and elastic properties derived from X-ray diffraction (XRD) data. The commonly used Scherrer method estimates crystallite size but neglects microstructural effects like lattice strain. To address these limitations, three variations of the Williamson-Hall (W–H) method have been employed. The XRD pattern revealed the tetragonal structure of the synthesised sample which was further confirmed by Raman Spectroscopy. Raman spectroscopy gave an insight of the vibrational modes of compound whilst Fourier Transform Infrared (FTIR) spectroscopy elucidates the vibrational dynamics and bonding characteristics of the material. Photoluminescence (PL) spectroscopy interpreted the charge carrier recombination mechanisms and defect-related emissions within the compound. Comprehensive optical analysis using UV–Visible spectroscopy reveals band gap of 3.08 eV and Urbach energy around 0.114 eV. The AC conductivity spectra at various temperatures are analysed using Jonhscher's power law, indicating that the conduction mechanism aligns with the overlapping large polaron tunnelling (OLPT) model. The thermally activated nature of the conduction is described by the Arrhenius relation, and activation energies across different temperature ranges are calculated to identify the charge carriers involved.



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SCHOLARLY PUBLICATIONS
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Journal Name: Journal of Materials Science: Materials in Electronics **IF: 3.2**

Title: Effect of stoichiometry ratio on the properties of CZTSe thin-film absorber layers for photovoltaic applications

Author: Sahoo S.; Kumar V.; Mangal S.; Singh U.P.

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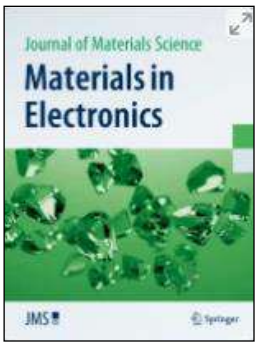
Abstract: Thin-film solar cells (TFSCs) have received much attention as efficient and economical solutions for solar energy conversion. $Cu_2ZnSnSe_4$ (CZTSe) has emerged as a promising absorber material because it is made from earth-abundant and environmentally friendly elements, has a high absorption coefficient, and possesses a suitable bandgap for photovoltaic applications. However, achieving high-quality CZTSe films requires careful control of stoichiometry, as minor compositional deviation can significantly impact their structural and optoelectronic properties. In this work, CZTSe thin films were deposited on soda-lime glass (SLG) and Mo-coated SLG substrates. One sample was kept as-deposited, another sample was annealed at 450 °C for 15 min in a selenium atmosphere, and to ensure correct stoichiometry, an additional Cu was sequentially deposited onto the as-deposited film and subsequently annealed at the same temperature to obtain the optimized film. XRD and Raman analyses indicate improved crystallinity and dominant CZTSe phase formation, with no prominent secondary phase peaks observed within the detection limits of the measurements. The optimized films exhibited larger grain size, enhanced electrical conductivity and mobility, and a reduced bandgap. These results demonstrate that maintaining an appropriate stoichiometric ratio significantly enhances CZTSe thin-film quality, improving its suitability for high-performance solar cell applications. In this work, Cu capping was employed as a post-deposition approach to improve the stoichiometry of CZTSe thin films and investigate its influence on material properties.



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