



SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Energy Storage

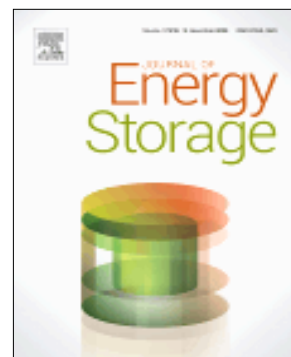
IF: 10.7

Title: Enhanced energy storage performance and superior thermal stability in yttrium-doped bismuth sodium titanate relaxor ferroelectrics through compositional tuning

Author: Das D.; Kerai S.; Majhi S.; Dikshit A.P.; Parashar K.; Parashar S.K.S.

Details: Volume-181, P-B, 15th December, 2026

Abstract: Environmentally friendly ferroelectrics with outstanding energy storage performance (ESP) have gained popularity in recent years due to rising need for environmental protection and pulsed power technologies. This work reports a high W_{rec} (0.27 J/cm³) with an excellent energy efficiency (η) of 65% in (Bi_{0.5}Na_{0.5})_{1-x}Y_xTiO₃ ($x = 0.03$) ceramics at an electric field of 75 kV/cm and shows excellent thermal stability in the temperature range of 30 to 100 °C with η more than 65%, synthesized by conventional solid-state reaction route. The ESP was optimized by creating polar nano regions (PNRs) and reducing grain size to submicron scale using a composition design technique by A-site modification of BNT ceramics. Due to PNRs formation and grain size modification, (Bi_{0.5}Na_{0.5})_{0.97}Y_{0.03}TiO₃ shows improved efficiency, $\eta = 65\%$ (~13.5 fold) as compare to pure BNT ceramics ($W_{rec}[J/cm^3] = 0.11$ J/cm³, $\eta = 4.8\%$, and $E_b[kV/cm] = 75$ kV/cm) and exhibits high E_b value of 105 kV/cm at ambient temperature. The synergistic combination of these features implies promising use in next-generation capacitor devices, particularly in energy storage applications requiring reliable performance in extreme operational environments.



URL: <https://www.sciencedirect.com/science/article/pii/S2352152X26041344?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Hydrology

IF: 7.3

Title: Hydrology-driven transport-storage dynamics, metals interaction, and ecological risk of downstream riverine microplastics

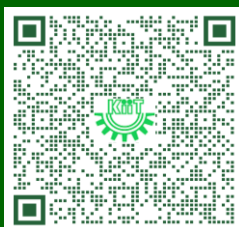
Author: Mahapatra S.; Maity J.P.; Dey G.; Mishra T.; Singha S.; Samal A.C.; Chattopadhyay S.; Mangal S.; Bhattacharya P.

Details: Volume-678, October 2026

Abstract: The occurrence of microplastics (MPs) in monsoon-dominated rivers is influenced not only by the source inputs but also by seasonal hydrological shifts that regulate their transport to storage in downstream regions of the riverine system. The present study investigated MPs in surface water and bed sediments of the downstream riverine system during the pre-monsoon, monsoon, and post-monsoon periods to determine how discharge influences abundance, sediment–water partitioning, polymer-density sorting, metal association, and screening-level ecological risk. The results showed that MPs in surface water followed the order: monsoon (1169.8 ± 68.81 items/m³) > pre-monsoon (951.9 ± 45.42 items/m³) > post-monsoon (598.4 ± 69.42 items/m³), indicating enhanced runoff-driven mobilization and downstream transport under high-discharge conditions. In contrast, sediment MPs showed the trend: post-monsoon (1251.5 ± 32.04 items/kg) > pre-monsoon (976.1 ± 30.67 items/kg) > monsoon (971.9 ± 36.09 items/kg), reflecting a transition from monsoon-driven export to post-monsoon depositional storage. This pattern was further supported by the sediment–water enrichment index, which increased from 0.83 in the monsoon to 2.09 in the post-monsoon, confirming greater sedimentary retention under reduced hydrodynamic forcing. White/transparent particles, fragments, and fibres dominated both matrices, indicating mainly secondary and weathered MPs. Raman analysis identified polymers in the order PP > PE > PET > PS > PVC, and showed density-driven sorting between water and sediment. FESEM–EDX revealed weathered surfaces and associated potentially toxic elements, suggesting that MPs may act as carriers of co-contaminants. This findings highlight that monsoon hydrology strongly regulates MPs transport, storage, and ecological risk in tropical river systems.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0022169426011881?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Industrial and Engineering Chemistry

IF: 7.1

Title: Methanol sensing using UiO-66 MOF coating on laser-induced graphene electrodes

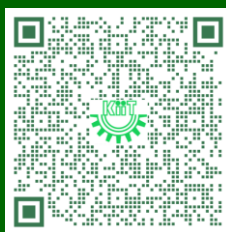
Author: Dhal B.C.; Belal M.A.; Hajra S.; Samal D.; Ghoshal S.; Dutta B.; Panigrahi B.K.; Vivekananthan V.; Kim H.J.; Sahu R.

Details: 11th September, 2026

Abstract: This paper presents the development of a versatile, highly sensitive room-temperature (RT) UiO-66-based gas sensor for methanol (MeOH) detection. Material characterization confirmed the successful synthesis of highly crystalline UiO-66 and the precise patterning of laser-induced graphene interdigitated electrodes (LIG-IDE). Using a spray-coating method, 500 μL of UiO-66 ink was deposited over a highly conductive LIG-IDE pattern on a flexible polyimide substrate. The gas-sensing tests indicated that the UiO-66/LIG-IDE sensor exhibits an n-type response to MeOH at RT, with high selectivity and adequate cyclability. The interaction of UiO-66 with 100 ppm MeOH at RT yields a gas response (R_a/R_g) of 2.75, along with response and recovery times of 68 s and 35 s, respectively. Further, DFT analysis reveals that MeOH sensing arises from reversible interactions, with linker-induced modulation of the electronic structure. This study introduces a promising, economical, and versatile sensing technology with potential applications in non-invasive breath analysis and environmental monitoring.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S1226086X26004971?via%3Dihub>





SCHOLARLY PUBLICATIONS
School of Applied Sciences
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Journal Name: Chemistry of Materials

IF: 7.1

Title: Hydrogels for Soft Robotics and Bio-Integrated Devices: Review on Self-Healing to Intelligent Actuation

Author: Bishoyi, KC; Pradhan, AK; Sahoo, SD

Details: 2026

Abstract: Self-healing and shape memory hydrogels have emerged as a transformative class of materials poised to reform next-generation bioelectronics, soft robotics, and actuation systems. By combining biocompatibility, mechanical tunability, and autonomous repair properties, these materials offer unique advantages for designing resilient and multifunctional devices that mimic the adaptability and responsiveness of biological tissues. This review provides a comprehensive analysis of the recent progress in the molecular design, network architectures, fabrication strategies, and functional integration of self-healing hydrogels into smart devices. Emphasis is placed on understanding the dynamic bonding mechanisms involving reversible covalent and supra-molecular interactions that impart self-repair capabilities while balancing mechanical robustness, conductivity, and biocompatibility. Special attention is given to highlighting how self-healing and shape memory functionalities enhance device durability, responsiveness, and long-term performance. We further explore the role of stimuli-responsive mechanisms, such as pH, temperature, and electrical signals, in enabling adaptive actuation and signal transduction. Additionally, the key challenges such as healing speed, operational stability in physiological environments, and seamless multifunctionality have been discussed and outline future directions toward programmable, autonomous, and multifunctional hydrogel systems.

URL: <https://pubs.acs.org/cmaterx/article-abstract/doi/10.1021/acs.chemmater.6c01296/5430479/Hydrogels-for-Soft-Robotics-and-Bio-Integrated?redirectedFrom=fulltext>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Alloys and Compounds

IF: 6.7

Title: Y₂FeMnO₆: A promising lead-free double perovskite for dielectric applications

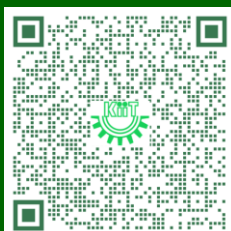
Author: Parida A.K.; Biswal L.; Mangal S.; Roy N.; Hota S.S.

Details: Volume-1080, 25th September, 2026

Abstract: In the present work, Y₂FeMnO₆, a novel second-generation multiferroic rare-earth-based double perovskite, has been synthesised using the conventional solid-state reaction route. XRD confirms the formation of a single-phase orthorhombic phase (Pbnm/Pnma, $a = 5.7209 \text{ \AA}$; $b = 7.5680 \text{ \AA}$, $c = 5.3114 \text{ \AA}$), further supported by the characteristic vibrational modes of Raman spectroscopy. The average crystallite size was 38.68 nm. FESEM analysis reveals a well-defined grain with dense microstructure, and EDS confirms the presence of the expected constituent elements in near-stoichiometric proportions. The average grain size was calculated to be 0.805 μm . The present material is used in optoelectronic and photovoltaic applications, as evidenced by UV-Visible spectroscopy, which shows a direct band gap of 3.4197 eV. Using complex impedance spectroscopy data, the electric polarisation and relaxation phenomena of the material as a function of frequency and temperature are extensively studied. Dielectric studies revealed a strong frequency and temperature dependence, with pronounced low-frequency dispersion associated with space-charge polarisation. Impedance spectroscopy shows a bulk-dominated electrical response, negative temperature coefficient of resistance (NTCR) behaviour, and non-Debye-type relaxation. The frequency-dependent AC conductivity follows Jonscher's universal power law and is consistent with the overlapping large polaron tunnelling (OLPT) model. Overall, the study establishes Y₂FeMnO₆ as a promising multifunctional double perovskite for future applications in electronic, dielectric, and energy-related devices.



URL: <https://www.sciencedirect.com/science/article/pii/S0925838826047067?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Nanoscale Advances

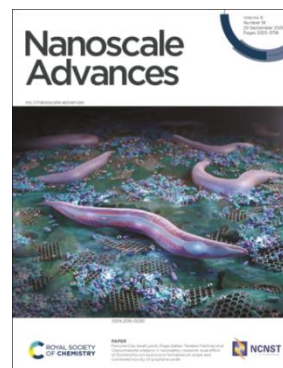
IF: 6.3

Title: MXene-integrated quantum dots: an innovative tool for next-generation healthcare applications

Author: Chakroborty S.; Nath N.; Pati D.K.; Singh S.; Priyadarshini Biswal R.; Mantry S.P.; Kumar M.; Padhee R.; Tiwari K.; Chakraborty C.

Details: Volume-8, Issue-19, 29th September, 2026

Abstract: Due to their superior physical and chemical characteristics, MXene quantum dots (MXQDs) are regarded as outstanding zero-dimensional nanomaterials. The excitation-dependent emission properties, photostability, biocompatibility and dispersion stability of these QDs make them potential candidates for solving biomedical and environmental problems. Owing to their remarkable properties and biocompatibility, MXQDs represent a new generation of smart nanosystems used for cancer diagnostics and treatment, imaging, sensing, tissue engineering, and drug delivery. However, there are many problems related to their biodegradability, photoluminescence, long-term toxicity, and biodistribution properties, which need to be carefully considered. This review focuses on the current developments of MXQDs in healthcare applications and also on the current trends and future perspectives.



URL: <https://pubs.rsc.org/na/article/8/19/5495/1355801/MXene-integrated-quantum-dots-an-innovative-tool>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: RSC Advances

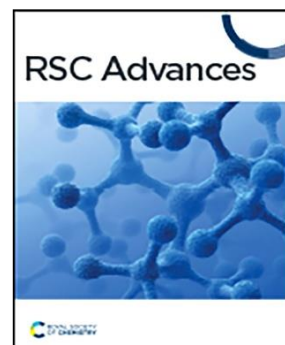
IF: 6.1

Title: Tuning visible-light-driven photocatalytic activity of PrMnO₃ perovskites for tetracycline degradation: mechanistic insights and performance analysis

Author: Nayak L.; Hati T.K.; Panda A.; Patra S.; Das N.; Banerjee S.; Parhi P.

Details: August 2026

Abstract: A praseodymium-based perovskite (PrMnO₃) was synthesised via a simple sol–gel route and investigated as a visible-light-active photocatalyst for the degradation of tetracycline. Compared to La, Ce, and Nd based systems, Pr-based materials have received relatively less attention in antibiotic removal, which forms the basis of this study. The structural and physicochemical properties were comprehensively analysed using XRD, FTIR, Raman, FESEM-EDX, XPS, BET, zeta potential, UV-vis DRS, Mott–Schottky, EIS and PL techniques. XRD confirmed the formation of an orthorhombic perovskite phase (Pnma) with an average crystallite size of ~19.8 nm, while spectroscopic analyses verified the presence of MnO₆ octahedra. The material exhibited a porous and agglomerated morphology with a relatively high surface area (70.375 m² g⁻¹). Optical characterisation indicated a band gap of ~2.23 eV, while Mott–Schottky analysis confirmed the n-type semiconducting nature of the material with a flat-band potential of 0.83 V vs. NHE. XPS results revealed mixed-valence states (Pr³⁺/Pr⁴⁺ and Mn³⁺/Mn⁴⁺) and oxygen vacancies, which are beneficial for charge separation. The photocatalytic performance of PrMnO₃ under visible light showed a maximum tetracycline degradation efficiency of 91.04% ($k = 0.016 \text{ min}^{-1}$) within 120 min at near-neutral pH (6.92) in deionised water, with slightly lower efficiency observed in real water matrices (river and tap water). Also, the catalyst maintained excellent stability and reusability, with negligible structural changes after repeated cycles, as evidenced by XRD and FTIR analyses.



URL: <https://pubs.rsc.org/ra/article/doi/10.1039/d6ra06709c/1289989/Tuning-visible-light-driven-photocatalytic>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Inorganic Chemistry Communications

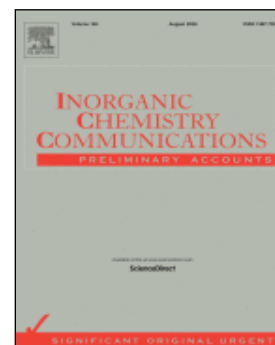
IF: 5.9

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

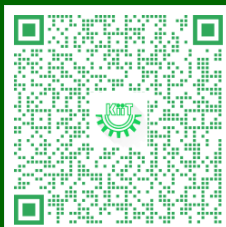
Author: Gupta P.; Dadhich B.K.; Patra S.K.; Bhushan B.; Priyam A.

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 School of Applied Sciences KIIT Deemed to be University

Journal Name: Materials Advances

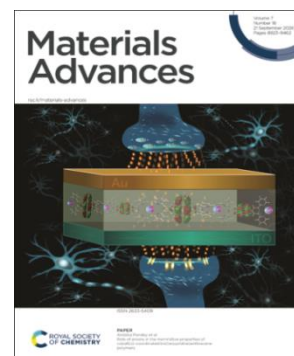
IF: 5.8

Title: Piezo-phototronic effect modulated enhanced photodetection in self-powered P(VDF-HFP)-MoS₂ nanofiber mats

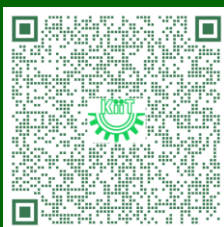
Author: S. P.; Kumar S.; S. S.; Jacob S.K.; Nanda J.; Pradhan G.K.; Mandal P.

Details: 15th September, 2026

Abstract: Multifunctional materials that convert mechanical and optical energy simultaneously into electrical signals can become crucial for the advancement of next-generation self-powered electronic devices. Devices such as piezoelectric nanogenerators and photodetectors harvest one kind of energy thereby limiting their versatility, adaptability, and overall efficiency for real-world applications. A material, integrated through the piezo-phototronic effect, can show enhanced response to both mechanical and optical stimuli through modulation of the interfacial band structure. Here, we demonstrate a dual-functional device based on electrospun ferroelectric P(VDF-HFP)-semiconductor MoS₂ composite nanofibers that simultaneously enables piezoelectric energy harvesting and self-powered photodetection. MoS₂ nanosheets, uniformly embedded in the ferroelectric P(VDF-HFP) matrix, enhance the polar β -phase of P(VDF-HFP) up to 93% and facilitate efficient charge-transfer processes aiding photodetection. The P(VDF-HFP)-MoS₂ piezoelectric nanogenerator delivers a peak-to-peak open-circuit voltage, short-circuit current and power density of 200 V, 14 μ A and 115 μ W cm⁻² respectively under a sinusoidal stress of 20 N. Concurrently, a self-powered photodetector based on the composite exhibits a responsivity, specific detectivity, an on/off current ratio, rapid photo response with a rise/decay time of $\sim 1.08 \mu$ A W⁻¹, $\sim 3.81 \times 10^7$ Jones, $\sim 1.79 \times 10^2$, and 0.30/0.19 s, respectively under white light (300–800 nm) illumination. The photodetector exhibits a large piezo-phototronic effect with about 63% increase in the photocurrent under a longitudinal mechanical tensile strain of 0.11%. The results highlight a design strategy for the development of multi-stimuli responsive devices that integrate ambient light sensing with efficient energy harvesting.



URL: <https://pubs.rsc.org/ma/article/doi/10.1039/d6ma00805d/1356416/Piezo-phototronic-effect-modulated-enhanced>





SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: International Journal of Molecular Sciences

IF: 5.6

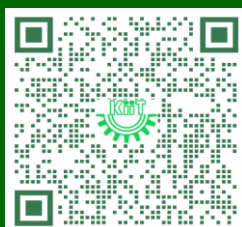
Title: Molecular Insights into Caffeine Stacking, Partitioning, and Organization in DPPC Lipid Bilayers from Microseconds-Long Molecular Dynamics Simulations

Author: Das S.; Karayiannis N.C.; Roy S.

Details: Volume-27, Issue-17, September 2026

Abstract: Caffeine (1,3,7-trimethylxanthine) is a widely consumed psychoactive drug and neurostimulant, yet its molecular organization and permeation behavior in lipid membranes are not fully understood. We employ microseconds-long, united-atom molecular dynamics simulations to investigate caffeine interactions with a solvated DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine) bilayer at its fluid phase. Caffeine molecules initially aggregate in the aqueous phase to form ordered stackings, which successively permeate into the membrane. The stacked assemblies gradually dissolve, reaching a stable dispersed state where caffeine molecules preferentially reside near the headgroup–acyl chain interface and orient parallel to the lipid acyl chains, consistent with previous experimental and simulation studies. Simulations initiated with caffeine in the membrane hydrophobic phase converge to the same equilibrium state, indicating a preferred localization at the interface region. Present simulation findings are further supported by free-energy calculations that demonstrate caffeine’s high affinity at the headgroup–acyl chain interface. Caffeine partitioning transiently and slightly reduces bilayer thickness and increases the membrane surface area while enhancing acyl chain stiffness near the hydrophilic part of the membrane. These observed trends are reproducible over different system sizes and independent simulations. Overall, this study provides atomic-level insights into the caffeine permeation process, including its effect on the lipid bilayer structure.

URL: <https://www.mdpi.com/1422-0067/27/17/7704>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: ACS Applied Energy Materials

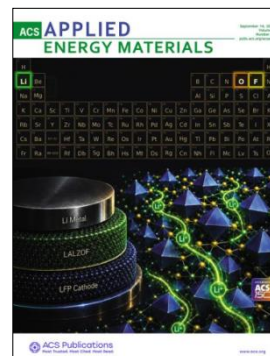
IF: 5.5

Title: Fe₂(MoO₄)₃@Polyindole Nanocomposites for High-Performance All-Solid-State Symmetric Supercapacitors

Author: Pati B.; Rout S.K.; Praharaj S.; Rout D.

Details: Volume-9, Issue-17, 14th September, 2026

Abstract: Synergistic architectures based on binary oxides and conducting polymers address the inherent limitations of individual components, thereby providing enhanced redox kinetics and structural stability for high-performance electrodes. Here, we explore the energy storage performance of Fe₂(MoO₄)₃@polyindole (FMO@PIN) nanocomposites synthesized via in situ oxidative polymerization. The PFM2 (indole:FMO = 2:1 weight ratio) nanocomposite features a unique 3D criss-cross FMO framework with uniformly dispersed PIN globules. This optimized structure, along with multiple oxidation states of FMO, provides efficient conducting pathways and rich redox kinetics, enhancing the overall electrochemical performance. It achieves a high specific capacitance (*C_s*) of 567.6 F/g (at 5 mV/s) and outstanding stability, with 93.3% retention over 15,000 cycles at 5 A/g—performance metrics that significantly surpass those of its pristine constituents. Further, a symmetric device is assembled using PFM2 as both the counter and working electrodes with a PVA/H₂SO₄ gel electrolyte. The resulting symmetric device exhibits a *C_s* value of 288 F/g and a discharge time of 1296 s at 0.1 A/g. It delivers an impressive energy density of 32.23 Wh/kg at 90 W/kg. Three identical devices connected in series successfully powered a red light-emitting diode (LED) for up to 7 min, validating their potential as a compact, efficient energy storage solution.



URL: <https://pubs.acs.org/aaemcq/article-abstract/9/17/11379/5351093/Fe2-MoO4-3-Polyindole-Nanocomposites-for-High?redirectedFrom=fulltext>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Materials Science in Semiconductor Processing

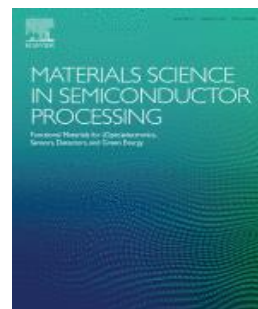
IF: 5.2

Title: Ku-band microwave absorption and EMI shielding of Ni doped ZnO nanoceramics

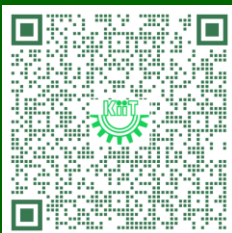
Author: Das B.K.; Das T.; Tudu H.; Das D.; Parashar S.K.S.

Details: Volume-217, January 2027

Abstract: In this study, $\text{Zn}_{1-x}\text{Ni}_x\text{O}$ ($x = 0, 0.01, 0.02$) nanoceramics samples were prepared using the high energy ball milling (HEBM) technique. The phase analysis of the synthesized samples was carried out using X-ray diffraction (XRD). The synthesized sample shows single phase hexagonal wurtzite structure indicating successful doping of Ni in ZnO lattice. The Field Emission Scanning Electron Microscopy (FESEM) micrograph shows a decrease in particle size with Ni^{2+} doping. AFM analysis shows a heterogeneous and rough surface of the synthesized sample. A decrease in the band gap energy was observed for the Ni doped ZnO sample. Raman spectroscopy was used to investigate the various structural vibrational modes of the synthesized samples. The electromagnetic shielding behaviour was investigated using a Vector Network Analyzer (VNA) in the Ku-band frequency range. The composition $x = 0.01$ shows maximum SET value of 29.35 dB at 18 GHz shows the effective EMI shielding behaviour in the Ku-band.



URL: <https://www.sciencedirect.com/science/article/pii/S1369800126007584?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Materials Chemistry and Physics

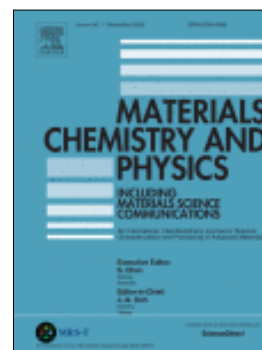
IF: 5.2

Title: Electrical transport and dielectric relaxation mechanisms of NaLaSnO₄: Implications for NTCR thermistor applications

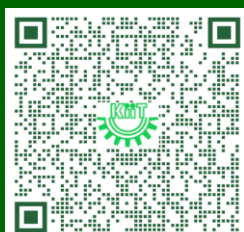
Author: Hota O.P.; Biswal L.; Mangal S.; Hota S.S.

Details: Volume-367, November 2026

Abstract: In the current study, we developed a cubic crystalline material, NaLaSnO₄ (NLSO), via a high-temperature solid-state method. The crystallite size of the sample was determined by the W–H graph to be 5.3 nm. FESEM micrographs show that the obtained solid has a fine microstructure with an average grain size of approximately 1.6 μm . FTIR and Raman studies confirmed the presence of related vibrational bonds. The temperature and frequency-dependent dielectric analysis indicates the presence of Maxwell–Wagner interfacial polarisation, with the material exhibiting a high dielectric constant ($\epsilon_r \approx 592.47$ at 25 °C) and a low dielectric loss (≈ 0.4) at 100 Hz. Nyquist plots provided information on the separation between resistive and capacitive properties of the ceramic material, as well as the contributions from both the grain and grain boundary. The decrease of activation energy for the conduction process of the compound, corresponding to the frequency range, suggests the involvement of oxygen vacancies in the conduction mechanism. The conductivity behaviour of the compound was modelled according to Jonscher's Power Law, indicating a negative temperature coefficient of resistance (NTCR) behaviour, making it suitable for thermistor use, with a sensitivity of 19744.64 and a temperature coefficient of $-2.9\%/K$. This multifunctional material provides a comprehensive platform for developing high-performance systems and presents promising prospects for next-generation technologies, including non-volatile memory and spintronic devices.



URL: <https://www.sciencedirect.com/science/article/pii/S0254058426009880?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

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

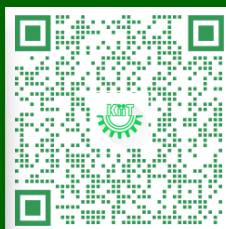
Author: Pradhan D.; Biswal S.K.; Nayak N.; Singhal R.; Salim A.; Dash S.K.

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 $g\text{-C}_3\text{N}_4/\text{TiO}_2/\text{MWCNTs}$ 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 $g\text{-C}_3\text{N}_4/\text{TiO}_2/\text{MWCNTs}$ nanocomposite was evaluated via the degradation of rhodamine B dye under solar light with various parameters, and the results revealed that the $g\text{-C}_3\text{N}_4/\text{TiO}_2/\text{MWCNTs}$ nanocomposite had 99% degradation efficiency with Z scheme mechanism and outperformed the pristine $g\text{-C}_3\text{N}_4$ 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 $g\text{-C}_3\text{N}_4$ (348 F/g). The remarkable photocatalytic performance and good electrochemical properties of the $g\text{-C}_3\text{N}_4/\text{TiO}_2/\text{MWCNTs}$ 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
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Journal of Molecular Structure

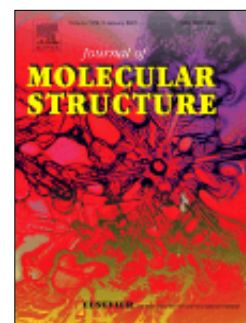
IF: 4.9

Title: Fabrication of Schottky device using 9-anthracenecarboxylate based binuclear Cd(II) compound

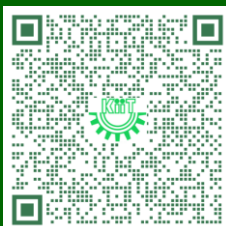
Author: Sk R.; Hossain E.; Sil S.; Pramanik S.; Dutta B.; Ray P.P.; Mir M.H.; Mukhopadhyay S.

Details: Volume-1381, P1, 5th February, 2027

Abstract: Here, we report the synthesis of a binuclear Cd(II) coordination compound, [Cd₂(9-aca)₄(pyz)(MeOH)₃] (1), constructed from the π -conjugated ligand 9-anthracenecarboxylic acid (H-9-aca) and the N-heterocyclic ligand pyrazine (pyz). The compound assembles into a one-dimensional (1D) supramolecular chain through strong $\pi\cdots\pi$ stacking interactions. Electrical measurements of 1 reveal semiconducting behavior with Schottky diode characteristics, where the enhanced conductivity is attributed to through-space charge transport facilitated by the $\pi\cdots\pi$ interactions. The experimental results are further corroborated by density functional theory (DFT) calculations with HOMO–LUMO band gap and density of states (DOS) analyses.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0022286026021228?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Next Materials

IF: 4.7

Title: Theoretical advances in $\text{CH}_3\text{NH}_3\text{SnI}_3$ -based perovskite solar cells: A comprehensive review

Author: Mohanty I.; Muduli S.; Singh U.P.; Mangal S.

Details: Volume-13, October 2026

Abstract: Methylammonium tin iodide (MASnI_3) has emerged as one of the most promising lead-free perovskite absorbers for next-generation photovoltaic devices owing to its suitable direct band gap, high absorption coefficient, excellent charge-carrier mobility, and environmentally benign composition. Over the past decade, extensive theoretical investigations have been conducted to understand and optimize the performance of MASnI_3 based perovskite solar cells (PSCs) using computational approaches such as density functional theory (DFT), SCAPS-1D, SILVACO-TCAD, COMSOL, SETFOS, MATLAB-based simulations, and machine learning techniques. This review provides a comprehensive overview of these theoretical advancements, focusing on the intrinsic properties of MASnI_3 , simulation methodologies, device optimization strategies, and the evolution of predicted power conversion efficiencies (PCEs). Analysis of the reported studies reveals that improvements in absorber thickness, defect density, interface quality, energy-level alignment, and charge-transport layer selection are the primary factors driving enhanced device performance, with several optimized device architectures theoretically achieving PCEs exceeding 30%. However, the review also identifies important limitations in current modeling frameworks, including simplified defect assumptions, inadequate representation of Sn^{2+} oxidation and self-doping effects, limited consideration of degradation pathways, and insufficient validation against experimental observations. Based on these findings, future research should prioritize the development of realistic multiscale models that incorporate defect evolution, stability-related phenomena, and stronger simulation–experiment correlations. By synthesizing the current theoretical landscape, this review highlights both the opportunities and challenges associated with MASnI_3 and provides guidance for the design of efficient, stable, and environmentally sustainable lead-free PSCs.



URL: <https://www.sciencedirect.com/science/article/pii/S2949822826017387?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Next Materials

IF: 4.7

Title: Borophene in energy storage technologies: Structural insights, functional performance, and future directions

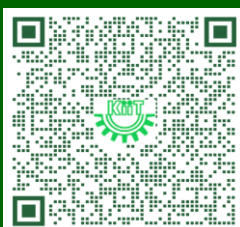
Author: Chakroborty S.; Nath N.; Yadav A.S.; Chakraborty C.; Garai S.; Alam T.; Sharma A.; Mohan M.

Details: Volume-13, October 2026

Abstract: Borophene, a novel two-dimensional (2D) allotrope of boron, has rapidly emerged as a promising material for next-generation energy storage technologies owing to its exceptional physicochemical, mechanical, electronic, and thermal properties. This review provides a comprehensive outline of current advances in the synthesis, structural characteristics, and functional capabilities of borophene and its derivatives. Key synthesis routes, including both top-down and bottom-up approaches, are discussed in the context of material quality, scalability, and substrate interactions. The unique polymorphic nature and anisotropic behavior of borophene are examined through a structural understanding, supported by density functional theory and experimental findings. Particular attention is given to the application of borophene in energy storage systems such as lithium-ion and sodium-ion batteries, supercapacitors, and hydrogen storage devices. Functional enhancements through heterostructure formation, elemental doping, and surface modifications are critically analyzed. The paper concludes with a discussion on the challenges and future directions for leveraging full potential of borophene in sustainable and high-performance energy storage applications.



URL: <https://www.sciencedirect.com/science/article/pii/S294982282601347X?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

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

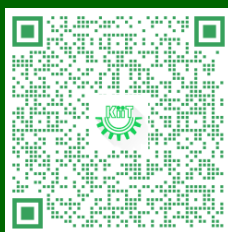
Author: Mahapatra S.; Maity J.P.; Singha S.; Mishra T.; Mangal S.; Dey G.; Sharma R.K.; Banerjee P.; Bhattacharya P.

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: $55.56 \pm 2\%$, Sediment: $57.45 \pm 3\%$) 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 KIIT Deemed to be University

Journal Name: Synthetic Metals

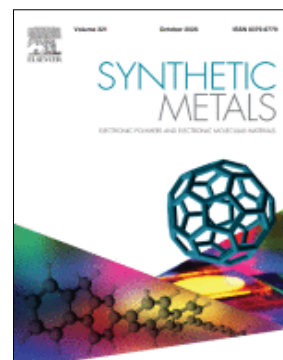
IF: 4.5

Title: Mechanistic and thermodynamic evaluation of H₂O₂-assisted methylene blue degradation with green-synthesized CuO/rGO nanocomposites

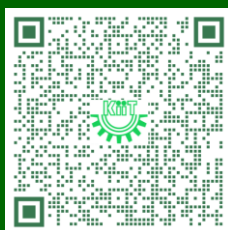
Author: Deo R.; Apta D.; Devi M.

Details: Volume-321, October 2026

Abstract: In the present study, a cost-effective ultrasonication method was employed for the green-synthesized CuO/rGO nanocomposites and used as a photocatalyst for MB dye degradation. The crystal structure, morphology, optical response and stability of the nanocomposites were analyzed using XRD, FESEM, EDS, XPS, FT-IR, UV-Vis, PL and TGA, respectively. The effects of catalyst dosage and reaction temperature on dye degradation were examined. At room temperature, $93.97 \pm 0.27\%$ dye degradation occurred in 35 min of visible light irradiation with an optimum dosage (0.2 g/L) of the catalyst in the presence of H₂O₂ as a synergistic oxidant. The dye degradation efficiency increased with rising reaction temperature. From the thermodynamic analysis, the activation energy (E_a) was determined to be 101.60 kJ/mol. The positive value of activation enthalpy 95.71 kJ/mol indicates the endothermic nature of the reaction. The positive activation entropy confirms the process to be entropy-driven, and Gibbs free energy confirms the spontaneity of the reaction. The role of reactive species involved in dye degradation was validated from scavenger studies. The stability and regeneration of the photocatalyst were analyzed from the zeta potential and recyclability studies, which show 88% dye degradation efficiency even after five cycles, confirming the sustainability of the photocatalyst for MB dye degradation.



URL: <https://www.sciencedirect.com/science/article/pii/S0379677926002079?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Materials Science

IF: 4.4

Title: Machine learning-guided design and electrochemical performance of bamboo-derived activated carbon/SrFeO composite as high-performance supercapacitor electrode

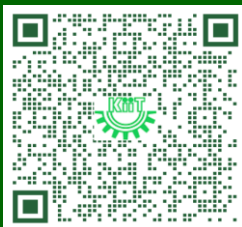
Author: Samantaray S.; Mohanty D.; Manjunatha C.; Hung I.-M.; Hsu X.C.; Bahumanya R.G.; Biswal L.; Satpathy S.K.

Details: August 2026

Abstract: The advancement of supercapacitor technology is contingent upon the creation of robust and effective electrode materials. This study used activated carbon (AC) made from bamboo leaves by high-temperature carbonization at 800 °C to create a novel SrFe₁₂O₁₉-activated carbon (SFO-AC) composite by reflux method. The composite was assessed as cathode material in supercapacitors, which electrochemical performance was significantly improved due to synergistic interaction between AC and SrFe₁₂O₁₉. The conductivity of the composite is 2.78 Ω⁻¹ m⁻¹ with an elevated specific capacitance of 453.3 F g⁻¹. In comparison with bare SFO, the electrochemical properties of composite were greatly affected by addition of AC to the SFO matrix making it appealing supercapacitor electrode material. Machine learning (ML) models were further developed to predict the electrochemical response of SFO-AC supercapacitor electrode as a function of time. Among the evaluated algorithms, random forest model tends to yield the precise agreement between the ML-predicted and measured current responses.



URL: <https://link.springer.com/article/10.1007/s10853-026-13465-6>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Transactions on Electrical and Electronic Materials

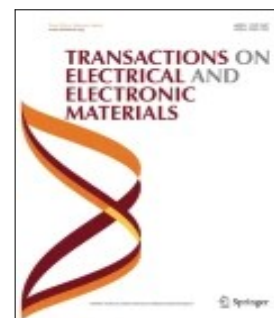
IF: 4.2

Title: High Dielectric Constant Observation in Cerium Site Substitution on $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$

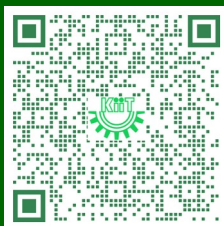
Author: Subudhi D.K.; Biswal B.; Jena S.; Pattanaik P.; Das J.; Mishra D.K.

Details: Volume-27, Issue-4, August 2026

Abstract: $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ (LCMO), $\text{La}_{0.67}\text{Ca}_{0.32}\text{Ce}_{0.01}\text{MnO}_3$ (LCMO@1Ce) and $\text{La}_{0.67}\text{Ca}_{0.23}\text{Ce}_{0.1}\text{MnO}_3$ (LCMO@10Ce) samples were synthesized successfully by solid state reaction technique at a sintering temperature of 1300 °C. A mixed phases of orthorhombic LaMn_2O_5 and $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ with space group pbam and pnma, respectively have been observed in both LCMO and LCMO@10Ce. Only single phasic compound has been observed in LCMO@1Ce which suggest that 1% Ce substitute at Ca site plays role in forming stable single phasic LCMO. High dielectric constant value in the order of 10^{10} is observed in LCMO@10Ce at a frequency of 1 kHz and 40 °C. However, high dielectric loss and low impedance value is observed in LCMO@10Ce because of the presence of defects and impurity phases in the sample. Even LCMO@1Ce shows the dielectric constant value in the order of 10^7 at a frequency of 1 kHz and 40 °C, the low dielectric loss and single phasic nature proves this material appropriate for dielectric applications in the field of data storage. With increase in temperature, the magnitude of impedance gradually decreases which suggests the negative temperature coefficient of resistance (NTCR) behavior in undoped LCMO and Ce substituted samples.



URL: <https://link.springer.com/article/10.1007/s42341-025-00663-3>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Next Nanotechnology

IF: 3.7

Title: Exploring the effect of graphene@Fe₃O₄ hybrid filler with TPU/PPy nanocomposites for microwave absorption in C, X, Ku bands with minimum reflection

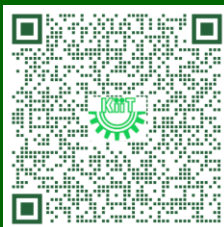
Author: Acharya S.; Rout S.R.; Samal R.R.; Parashar S.K.S.; Sahoo B.P.

Details: Volume-10, December 2026

Abstract: The issue of electromagnetic (EM) radiation pollution is a significant concern in modern society, as it has negative impacts not only on electronic devices but also on the environment. The goal of this research is to fabricate TPU/PPy/gra@Fe nanocomposites via cost-effective solvent casting. The fabricated nanocomposites undergo structural and morphological characterization using FTIR, Raman, XRD, FESEM, HRTEM, and XPS. The dielectric, magnetic, and microwave absorption properties are investigated in the C, X, and Ku bands, i.e., 5–18 GHz. The dielectric and magnetic properties of nanocomposites are significantly enhanced by combining dielectric and magnetic fillers, such as gra@Fe, at appropriate weight ratios, as confirmed by the Cole-Cole plot. The total effectiveness (SETot) of all nanocomposites across the microwave spectrum ranges from 22 to 37 dB. The SETot for TPU/PPy at a 1:3 gra@Fe ratio is 37 dB, accompanied by a SEAbs of 34 dB and a low SRef of less than 3 dB. The 95:5:1(1:3) composite exhibited $SE_{t\ ot} > 30$ dB across 6.0–12.0 GHz (6.0 GHz effective bandwidth) and maintained $SE_{t\ ot} > 25$ dB within the Ku band (12–17 GHz), corresponding to an effective bandwidth of approximately 5 GHz. All microwave nanocomposites exhibit a reflection rate below 20%. Importantly, the reflection rate of TPU/PPy 1:3 gra@Fe nanocomposite is less than 10% in the X and Ku bands. The TPU/PPy/gra@Fe nanocomposite exhibits a low reflection rate and broadband performance, rendering it suitable for microwave and radar-absorption applications, especially in the military field.



URL: <https://www.sciencedirect.com/science/article/pii/S2949829526003074?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Food and Humanity

IF: 3.5

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

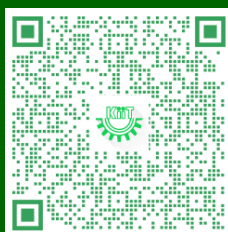
Author: Nayak L.; Biswal M.; Das J.; Panda S.; Lal M.K.; Ngangkham U.; Kumar S.; Kumar A.

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 School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of the Indian Chemical Society

IF: 3.4

Title: Essential oil-based phytochemicals as antibiofilm agents against methicillin-resistant *Staphylococcus aureus*: From in silico screening to in vitro validation

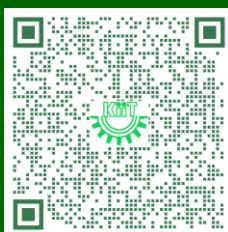
Author: Pattnaik S.; Behera S.K.; Mishra S.; Rath B.P.; Kumar S.; Mohanty C.

Details: Volume-103, Issue-10, October 2026

Abstract: Methicillin-resistant *Staphylococcus aureus* (MRSA) is a significant human pathogen which causes life threatening and recurrent infections. This is largely attributed to its biofilm formation, which promotes bacterial persistence and resistance to antimicrobial therapy. The present study investigated essential oil-based phytochemicals as potential antibiofilm agents against MRSA using combined in silico and in vitro approaches. In silico screening identified two phytochemicals (α -Terpineol and Phthalic Acid) as suitable candidates based on their predicted interactions with the MRSA biofilm regulators SarA and AgrA. Disc diffusion and minimum inhibitory concentration (MIC) assays confirmed measurable antibacterial activity of α -Terpineol and Phthalic Acid against MRSA, with MICs of 900 and 1800 $\mu\text{g/mL}$, respectively. The treatment with α -Terpineol reduced MRSA biofilm formation by 79.02% at MIC/2 (450 $\mu\text{g/mL}$), whereas Phthalic Acid produced a 56.26% reduction at MIC/2 (900 $\mu\text{g/mL}$). Microscopic analysis showed that α -Terpineol disrupted biofilm structure and prevented aggregation at sub-MICs, while Phthalic Acid treated samples resembled the untreated control. The Alamar Blue assay indicated that both the compounds exhibited a non-bactericidal effect on MRSA at the tested concentrations. Furthermore, α -Terpineol significantly reduced slime production compared to Phthalic Acid. Overall, the study identifies α -Terpineol as an effective antibacterial and antibiofilm agent against MRSA, capable of significantly reducing biofilm formation at sub-inhibitory concentrations. These findings support the potential of α -Terpineol for the development of formulation-based strategies against MRSA biofilm-associated infections.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0019452226006540?via%3Dihub>





SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Journal of the Indian Chemical Society

IF: 3.4

Title: Exploration of titanocene(III) chloride in deiodination reaction of benzyl iodide

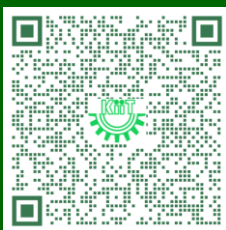
Author: Panigrahi R.K.; Jana S.

Details: Volume-103, Issue-10, October 2026

Abstract: Titanocene (III) chloride mediated deiodination reaction of benzyl iodide has been reported. The reaction proceeds through the formation of benzyl radical. The benzyl radical reacts with another benzyl radical to afford a bibenzyl product. Also, the radical can be trapped using one electron deficient double bond. Titanocene (III) chloride has been generated by reduction of titanocene dichloride using activated zinc dust in deoxygenated THF under argon condition. As Ti(III) is a single electron donor, it can readily reduce the active iodo compound to form the corresponding carbon radical, which further reacts with appropriate functionality to obtain the desired product.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0019452226006084?via%3Dihub>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Materials Science: Materials in Electronics

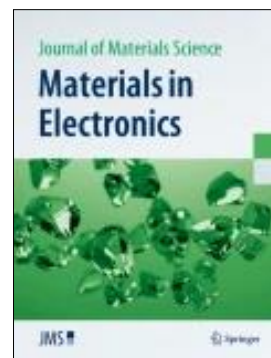
IF: 3.2

Title: Understanding of dynamic scaling behavior, pyroelectric energy storage and electrocaloric performance of MnO-modified BaCaZrTiO ceramics

Author: Nanda S.; Badapanda T.; Joardar H.; Sumit; Arockiarajan A.; Rout S.K.

Details: Volume-37, Issue-22, August 2026

Abstract: This work involved the dynamic scaling hysteresis behavior of MnO₂-doped BCZT (Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O₃) perovskite compounds synthesized by a traditional solid-state reaction technique. The single-phase perovskite symmetry is observed at all dopant concentrations, as authenticated by X-ray diffraction. A small deviation in the transition temperature and electrical permittivity with rising dopant value was indicated by temperature-driven dielectric measurements. The temperature-driven ferroelectric hysteresis measurement was carried out and the correlation of remanent polarization (Pr), coercive field (Ec), and the mean hysteresis loop area (A) with temperature was analyzed. The exponents associated with the temperature-driven hysteresis quantities were obtained using a standard power-law relationship. The storage performance of the compositions was measured using conventional formula. An Olsen electrothermal cycle was utilized to assess the energy harvesting (thermal) capabilities of all compositions. The electrocaloric performance of the doped compositions was estimated using the indirect method. These results indicate that integrating MnO₂ into BCZT ceramics is an effective method for improving energy storage capacity and pyroelectric and electrocaloric properties.



URL: <https://link.springer.com/article/10.1007/s10854-026-18031-z>





SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

Journal Name: Journal of Physical Chemistry A

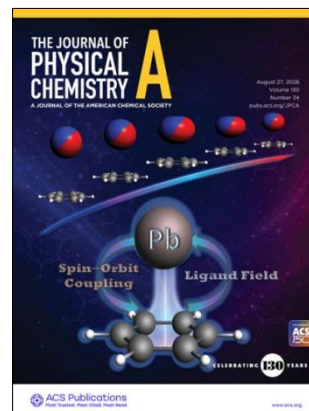
IF: 3.0

Title: Predictive Molecular-Level Recognition of Pesticides by Co(II)-Based Coordination Polymer: A Theoretical Study of Host-Guest Interactions

Author: Hasan, MN; Dutta, B; Bhowmick, R; Mahapatra, M; Halder, S

Details: Volume-130, Issue-34, August 2026

Abstract: The strategic design of advanced sensing materials for pesticides is increasingly challenged by regulatory restrictions and limited experimental accessibility to several hazardous agrochemicals. This work reports a comprehensive theoretical investigation of a well-characterized Co(II)-based coordination polymer (CP), synthesized using a slow diffusion process, as a potential sensing platform for pesticide recognition. The CP has been thoroughly characterized by X-ray single-crystal diffraction analysis, and its interaction with nine representative pesticides has been systematically explored using density functional theory (DFT) and time-dependent DFT. Optimized host-guest geometries reveal favorable binding affinities driven by a combination of hydrogen bonding, electrostatic interactions, pi-interactions, etc., depending on the chemical nature and molecular structure of the pesticide. Optical response, chemical reactivities, charge transfer characteristics, frontier molecular orbital analysis, and noncovalent interaction (NCI) analyses provide molecular-level insights into the recognition mechanism and relative selectivity of the CP toward different pesticides. The results demonstrate that the electronic structure of the Co(II) coordination framework is sensitively modulated upon guest binding, highlighting its potential as a sensing material. This study establishes a predictive computational sensing strategy for environmentally relevant pesticides that are difficult to access experimentally (sometimes banned) and offers valuable guidelines for the future design of CP-based sensors targeting emerging and regulated contaminants.



URL: <https://pubs.acs.org/jpcafh/article-abstract/130/34/6794/5254000/Predictive-Molecular-Level-Recognition-of?redirectedFrom=fulltext>

