



**SCHOLARLY PUBLICATIONS**  
**School of Applied Sciences**  
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**Journal Name:** Nano Letters

**IF:** 9.6

**Title:** Electrically Controlled Excitons, Charge Transfer Induced Trions, and Narrowband Emitters in MoSe<sub>2</sub>-WSe<sub>2</sub> Lateral Heterostructure

**Author:** Kundu, B; Mondal, P; Tebbe, D; Hasan, MN; Chakraborty, SK; Metzelaars, M; Kögerler, P; Karmakar, D; Pradhan, GK; Stampfer, C; Beschoten, B; Waldecker, L; Sahoo, PK

**Details:** Volume 42, Issue 46, November 2024

**Abstract:** Controlling excitons and their transport in two-dimensional (2D) transition metal dichalcogenide heterostructures is central to advancing photonics and electronics on-chip integration. We investigate the controlled generation and manipulation of excitons and their complexes in monolayer MoSe<sub>2</sub>-WSe<sub>2</sub> lateral heterostructures (LHSs). Incorporating graphene as a back gate and edge contact in a field-effect transistor geometry, we achieve the precise electrical tuning of exciton complexes and their transfer across interfaces. Photoluminescence and photocurrent maps at 4 K reveal the synergistic effect of the local electric field and interface phenomena in the modulation of excitons, trions, and free carriers. We observe spatial variations in the exciton and trion densities driven by exciton-trion conversion under electrical manipulation. Additionally, we demonstrate controlled narrow-band emissions within the LHS through carrier injection and electrical biasing. Density functional theory calculation reveals significant band modification at the lateral interfaces. This work advances exciton manipulation in LHS and shows promise for next-generation 2D quantum devices.



**URL:** <https://pubs.acs.org/doi/10.1021/acs.nanolett.4c03464>





## SCHOLARLY PUBLICATIONS School of Applied Science KIIT Deemed to be University

**Journal Name:** Science of the Total Environment

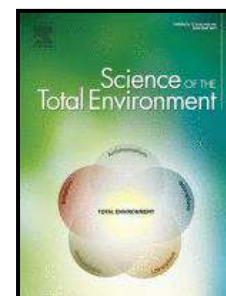
**IF:** 8.2

**Title:** HONO chemistry and its impact on the atmospheric oxidizing capacity over the Indo-Gangetic Plain

**Author:** Pawar, PV; Mahajan, AS; Ghude, SD

**Details:** Volume 947, Article number 174604, October 2024.

**Abstract:** Chemical processes involving nitrous acid (HONO) play a pivotal role as it is a notable source of hydroxyl ( $\cdot\text{OH}$ ) radicals, influencing the oxidation capacity of the atmosphere. We conduct a comprehensive investigation into the temporal dynamics of HONO, other gases (nitrogen oxides ( $\text{NO}_x$ ), ozone ( $\text{O}_3$ ), ammonia ( $\text{NH}_3$ ), sulphur dioxide ( $\text{SO}_2$ ), and nitric acid ( $\text{HNO}_3$ )), particulate matter ( $\text{PM}_{2.5}$ ), and meteorological parameters using measurements that took place during the Winter Fog Experiment (WiFEx) campaign in Delhi, India, during the winter of 2017–2018. Remarkable day-to-day variations in HONO concentrations are observed, with the peak value reaching  $54.5 \mu\text{g m}^{-3}$  during a fog event. This coincides with elevated levels of sulfate and nitrate in aerosols, underscoring the significant role of heterogeneous fog chemistry in HONO production. We investigated HONO sources and sinks during fog periods by using a photochemical box model. The model shows that the gas-phased chemistry of HONO predicts concentrations lower by an order of magnitude compared to observations (peaking at  $0.60 \mu\text{g m}^{-3}$  compared to the average observed value of  $7.00 \mu\text{g m}^{-3}$ ). The calculated production rates of HONO from observations for daytime to nighttime peaks are  $3.10 \mu\text{g m}^{-3} \text{h}^{-1}$  ( $1.1 \times 10^7 \text{ molecules cm}^{-3} \text{ s}^{-1}$ ) and  $2.00 \mu\text{g m}^{-3} \text{h}^{-1}$  ( $7.1 \times 10^6 \text{ molecules cm}^{-3} \text{ s}^{-1}$ ), respectively. This shows the existence of an undefined heterogeneous reaction pathway for HONO production. At the peak of HONO concentration, we estimated an  $\cdot\text{OH}$  formation rate of  $9.4 \times 10^7 \text{ molecules cm}^{-3} \text{ s}^{-1}$  due to the photolysis of HONO, which is much higher than the production of HONO from the reaction of  $\text{O}_1\text{D}$  with  $\text{H}_2\text{O}$ . This underscores the predominant role of HONO photolysis as the primary source of  $\cdot\text{OH}$  radicals compared to other pathways and highlights the significant role of HONO chemistry in influencing atmospheric oxidation capacity.



**URL:** <https://www.sciencedirect.com/science/article/abs/pii/S0048969724047533?via%3Dihub>





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**Journal Name:** Inorganica Chimica Acta

**IF:** 6.9

**Title:** Redox transmetallation reaction mediated synthesis of Ni-Pd bimetallic nanocatalyst for pesticide degradation to value added product.

**Author:** Sarkar, S; Pal, T; Maji, PK; Dutta, S; Pal, A

**Details:** Volume 571, Article number 122180, October 2024.

**Abstract:** In this work a wet-chemical recipe has been accounted for the synthesis of bimetallic Ni-Pd nanostructures at ambient condition involving pre-synthesized nickel nanoparticles and aqueous tetrachloropalladate,  $[PdCl_4]^{2-}$  solution. The Galvanic replacement reaction (GRR) starts instantaneously between less noble NiO nanoparticle i.e., zero valent nickel (ZVN) and more noble  $[PdCl_4]^{2-}$ . Thus ZVN is oxidatively etched out as soluble  $Ni^{2+}$  by more noble  $[PdCl_4]^{2-}$  depositing PdO onto the residual ZVN. Concurrently the  $Ni^{2+}$  ions move outwardly into the bulk solution and the PdO enters into the inwardly fashion owing to their different diffusivities and results in the formation of hollow bimetallic nanostructures following diffusion limited nanoscale Kirkendall effect. Finally, the bimetallic nanomaterial was shown to be a competent heterogeneous catalyst for facile hydrolytic degradation of an organothiophosphate pesticide, methyl parathion (MP). After the completion of the degradation, the degraded product, 4-nitrophenolate (4-NP) was subsequently reduced to 4-aminophenolate (4-AP) in the same reaction pot in presence of the same catalyst using borohydride. 4-AP is the principal ingredient for the production of the medicine paracetamol. Hence the bimetallic Ni-Pd nanoparticles turn out to be a promising heterogeneous catalyst for water pollution abatement through pesticide degradation vis-à-vis generation of value added product out of the degraded product of the pesticide.



**URL:** <https://www.sciencedirect.com/science/article/pii/S0020169324002718?via%3Dihub>





## SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

**Journal Name:** Journal of Alloys and Compounds

**IF:** 5.8

**Title:** Effect of milling time on structural and electrical properties of thermomechanically synthesized of Ba<sub>0.1</sub>(Bi<sub>0.45</sub>Na<sub>0.45</sub>)TiO<sub>3</sub> nanoceramics for ferroelectric random-access memory device

**Author:** Hota S.S., Panda D., Biswal L., Joshi S., Shukla A., Choudhary R.N.P.

**Details:** January, 2025

**Abstract:** Lead-free Ba<sub>0.1</sub>(Bi<sub>0.45</sub>Na<sub>0.45</sub>)TiO<sub>3</sub> (BBNTO) nanoceramics were synthesized using high-energy ball milling, followed by a solid-state reaction method. XRD analysis of the microstructure indicated the formation of tetragonal symmetry. The crystallite size of the nanoceramic powder decreased from ~ 28 nm to 10 nm after milling for 0, 30, 60, and 90 hours. The dielectric properties of the nanoceramics showed significant improvement, with a diffuse phase transition occurring around 80 °C). The dielectric constant increased with temperature across various frequencies, reached a maximum value at approximately at temperature ~ 380 °C. At lower temperatures and higher frequencies, the relative permittivity and tangent loss depend on the crystallite size and milling duration. Impedance spectroscopy data analysis revealed size-dependent impedance characteristics and dielectric relaxation. The ac conductivity plot adhered to the Arrhenius relation, and the calculated activation energy confirmed the negative temperature coefficient of resistance (NTCR) behavior. P-E loops confirmed ferroelectric properties, indicating potential for use in future ferroelectric-based storage devices.



**URL:** <https://www.sciencedirect.com/science/article/pii/S0925838824036284?via%3Dihub>





## SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

**Journal Name:** Colloids and Surfaces B-Biointerfaces

**IF:** 5.4

**Title:** Intrinsic physiochemical insights to green synthesized Ag-decorated GO nanosheet for photoluminescence and in vivo cellular biocompatibility with embryonic zebrafish

**Author:** SinghDeo S.; Naser S.S.; Nandi A.; Sinha A.; Shaikh S.A.; Mohapatra S.K.; Suar M.; Verma S.K.; Tripathy J.

**Details:** Volume 245, January 2025

**Abstract:** The advancement of nanotechnology and their application has intrigued a significant interest in green synthesis and application of organic and inorganic nanomaterials like graphene oxide (GO) and silver nanoparticles (AgNP). This study explores the intrinsic physiochemical properties of silver (Ag)-decorated graphene oxide (GO) nanosheets synthesized via a green approach, focusing on their photoluminescence behaviour and in vivo cellular biocompatibility with embryonic zebrafish. The nanocomposites were characterized using various spectroscopic and microscopic techniques to elucidate their structural and optical properties. Results reveal that the Ag-decorated GO nanosheets exhibit enhanced photoluminescence compared to pristine GO with an SPR at 405 nm and emission at 676 nm, attributed to the synergistic effects of Ag nanoparticles and GO. In addition, in vivo biocompatibility assessments using embryonic zebrafish demonstrate minimal cytotoxicity and high cellular viability upon exposure to the nanocomposites with an LC50 of 38 µg/ml, indicating their potential for biomedical applications. Further investigations into the interactions between the nanomaterials and biological systems provide valuable insights into their safety profile and suggest their suitability for various biomedical and therapeutic applications. Overall, this study offers a comprehensive understanding of the physiochemical characteristics and biological compatibility of Ag-decorated GO nanosheets, contributing to the advancement of nanotechnology in biomedicine and related fields.



**URL:** <https://www.sciencedirect.com/science/article/pii/S0927776524004715?via%3Dihub>





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**Journal Name:** Marine Pollution Bulletin

**IF:** 5.3

**Title:** Evaluation and mitigation of potentially toxic elements contamination in mangrove ecosystem: Insights into phytoremediation and microbial perspective

**Author:** Dey G.; Maity J.P.; Banerjee P.; Sharma R.K.; Das K.; Gnanachandrasamy G.; Wang C.-W.; Lin P.-Y.; Wang S.-L.; Chen C.-Y.

**Details:** Volume 209, December 2024

**Abstract:** Mangroves, essential coastal ecosystems, are threatened by human-induced Potentially-toxic-elements (PTEs) pollution. This study analyzed PTEs distribution, phytoremediation potential, and rhizosphere microbial communities in Taiwan's Xinfeng mangrove forest. Significant variations in physicochemical and PTEs concentrations were observed across adjacent water bodies, with moderate contamination in the river, estuary, and overlying water of mangroves sediment. The partition-coefficient showed the mobility of Bi, Pb, Co, and Sr at the water-sediment interface. The geochemical-indices revealed high Bi and Pb contamination and moderate Zn, Sr, Cu, and Cd contamination in sediment. The overall pollution indices indicated the significant contamination, while moderate ecological risk was found for Cd ( $40 \leq E_r^i < 80$ ). Mangroves *Kandelia obovata* and *Avicennia marina* exhibited promising PTEs phytoremediation potential (Bi, Cd, Mn, Sr, and Co). Metagenomics indicated a diverse microbial community with N-fixation, P-solubilization, IAA synthesis, and PTEs-resistance genes. These findings underscore the need for targeted conservation to protect these critical habitats.



**URL:** <https://www.sciencedirect.com/science/article/abs/pii/S0025326X24010129?via%3Dihub>







## SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

**Journal Name:** Ceramics International

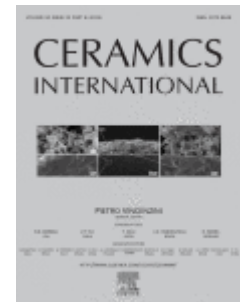
**IF:** 5.1

**Title:** Design and electromagnetic shielding of  $\text{Bi}_0.5\text{Na}_0.5\text{TiO}_3$  ceramics as meta-surface absorber for high-frequency microwave application

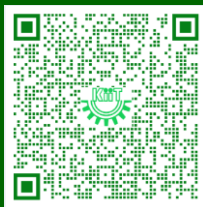
**Author:** Das D.; Samal R.R.; Dikshit A.P.; Parashar K.; Parashar S.K.S.

**Details:** Volume 50, Issue 22, Pages 46621 - 4663115 November 2024

**Abstract:** EMI shielding reduces ambient electromagnetic (EM) radiation by reflecting and absorbing EM waves. Rapid technological growth has increased electronic gadgets and EM radiations, threatening the environment. Microwave materials with high absorption power and cheap cost are crucial for eliminating electromagnetic difficulties in stealth technologies. This study used a conventional solidstate reaction technique to prepare  $\text{Bi}_0.5\text{Na}_0.5\text{TiO}_3$  (BNT) solid solutions and examined their structural, ferroelectric, dielectric, and shielding characteristics. This research describes an EMI shielding material that efficiently absorbs EM wave-induced radiation. Characterizations have been done to evaluate material behavior to support EMI shielding and confirm its absorbing nature. Field emission scanning electron microscopy (FESEM), Raman spectroscopy, and X-ray diffraction (XRD) were employed to examine the surface morphology, local lattice deformation with ionic configuration, and crystal structure. BNT exhibited a rhombohedral structure with  $R3c$  symmetry space group with crystallize size 81.5 nm and showed eight Raman active modes with an average grain size of 1.67  $\mu\text{m}$ . The high dielectric constant, reduced dielectric tangent loss, and enhanced polarization value make BNT ceramic a good choice for electrical devices and microwave applications. BNT ceramics showed EMI shielding owing to absorption (SET  $\sim -23.65$  dB, SEA  $\sim -18.91$  dB) at 9.2 GHz in the X-band (8.2–12.4 GHz). Meta-surfacebased BNT absorbers were designed and simulated in the CST software. The peak depicted the absorption at 9.2 GHz with absorptivity of 91.56 %, 85.03 %, 84.36 %, and 64.6 % for designs 1, 2, 3, and 4, respectively. BNT ceramics have exceptional dielectric absorption properties, and dielectric and magnetic losses, which make them suitable for EMI shielding and absorption applications in the microwave region.



**URL:** <https://www.sciencedirect.com/science/article/pii/S0272884224039749?via%3Dihub>





## SCHOLARLY PUBLICATIONS School of Applied Science KIIT Deemed to be University

**Journal Name:** Journal of Photochemistry and Photobiology A: Chemistry

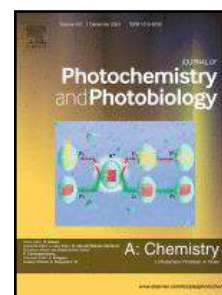
**IF:** 4.7

**Title:** Reduced graphene oxide supported Bismuth-Iron mixed oxide nanocomposite: A potent photocatalyst for crystal violet dye degradation and antimicrobial application.

**Author:** Das, D; Panigrahi, UK; Giri, J; Panda, AK; Satapathy, PK; Mallick, P

**Details:** Volume 457, 1 December 2024, Article No. 115912.

**Abstract:** The nanocomposites of rGO-[BixFe(1-x)]<sub>2</sub>O<sub>3</sub> (x=0.02, 0.05, 0.10 and 0.20) are successfully synthesized with the help of a cost-effective co-precipitation procedure. Influence of Bi on to the magnetic, optical, microstructural and antimicrobial properties of Fe<sub>2</sub>O<sub>3</sub> are investigated. The presence of pure  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> is being witnessed through the characteristic intensity of XRD peak where phase impurity is not noticed up to 10 % of Bi loading. Presence of various defects have been realized in the sample from PL spectra. The direct band gap of the adsorbent nanocomposite with Bi loading up to 10 % with that of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> is found to be 2.51 eV and it may be taken as a suitable photocatalyst of choice towards the photodegradation of Crystal Violet with 97.69 % by maintaining the pH-10 and time-60 min as optimum condition. Adsorption capacity (qm) and rate constant (kapp) are found to be 28.50 mg/g and 0.0473 min<sup>-1</sup> respectively. The antimicrobial analysis of the synthesized material signifies its antibacterial activity against Staphylococcus aureus (Gram +Ve) and Klebsiella pneumonia (Gram -Ve). On the basis of our finding, the synthesized nano composite may be the materials of choice for the optical device application, memory storage device as well as in the biomedical application.



**URL:** <https://www.sciencedirect.com/science/article/abs/pii/S1010603024004568?via%3Dihub>







**SCHOLARLY PUBLICATIONS**  
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**Journal Name:** Inorganic Chemistry Communications

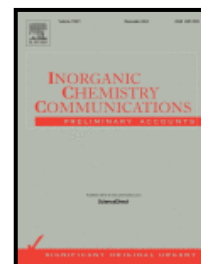
**IF:** 4.4

**Title:** Investigation of structural, dielectric, impedance, and conductivity properties of layered perovskite type compound; NaYSnO<sub>4</sub>

**Author:** Panda R.; Sekhar Hota S.; Panda D.; Biswal L.; Joshi S.; Shukla A.; Nanda J.; Naresh Prasad Choudhary R.

**Details:** Volume 170, December 2024

**Abstract:** In this paper, the structural study of NaYSnO<sub>4</sub> (NYSO), a layered perovskite ceramic oxide, was done using an X-ray diffractometer (XRD) to identify the phase and determine the composition of NYSO. The microscopic structure of the sample seen by Scanning Electron Microscopy (SEM) was found to be polycrystalline and a mixture of large and small grains, which indicate the anisotropic nature of the sample. A FTIR spectroscopic behaviour of the material was used to identify the formation of different bonds in the material, and the XPS study gives an idea of the binding energy of each element in NYSO. A thorough analysis of the impedance, dielectric constant, dielectric loss, modulus and AC conductivity properties concerning temperature and frequency displays the electronic device characteristics. The complex impedance spectra were studied at temperatures range between 25 and 500°C and frequency of 100 Hz to 1 MHz range. Nyquist plots reveal the charge conduction mechanism of the grain and well-defined grain boundaries that correspond to the resistive and capacitive phenomena of the material. Furthermore, the activation energy has been estimated to investigate the charge transportation mechanism. This article concludes by discussing future possibilities and scientific challenges in NTCR thermistors using NYSO.



**URL:** <https://www.sciencedirect.com/science/article/pii/S1387700324012097?via%3Dihub>





**SCHOLARLY PUBLICATIONS**  
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**Journal Name:** *Molecules*

**IF:** 4.2

**Title:** Degradation of Decabromodiphenyl Ether Dispersed in Poly (Acrylo-Butadiene-Styrene) Using a Rotatory Laboratory Pilot Under UV-Visible Irradiation

**Author:** Benmammam R.K., Bouberka Z., Malas C., Carpentier Y., Haider K.M., Mundlapati V.R., Ziskind M., Focsa C., Khelifi S., Poutch F., Laoutid F., Suptot P., Foissac C., Maschke U.

**Details:** Volume 29, Issue 21, November 2024

**Abstract:** The growing volume of plastics derived from electronic waste (e-waste) underscores the imperative for environmentally sustainable strategies for the management of this waste. In light of the paramount importance of this issue, a pilot demonstrator for the decontamination of polymers containing Brominated Flame Retardants (BFRs) has been developed. The objective is to investigate the potential for decontaminating BFR-containing polymers from e-waste via UV-visible irradiation using a rotatory laboratory pilot operating under primary vacuum conditions. This report focuses on binary model blends composed of 90 weight% (wt%) poly(Acrylo-Butadiene-Styrene) (ABS) pellets and 10 wt% Deca-Bromo-Diphenyl Ether (DBDE), which is one of the most toxic BFRs. The efficiency of the irradiation process was evaluated as a function of pellet diameter and irradiation time using Fourier Transform InfraRed spectroscopy (FTIR) and High-Resolution Laser Desorption/Ionization Mass Spectroscopy (HR-LDI-MS). As a consequence, ABS + DBDE achieved a decontamination efficiency of 97% when irradiated with pellets of less than 1 mm in diameter for a period of 4 h. Additionally, the thermal behavior of the irradiated samples was investigated through thermogravimetric analysis and differential scanning calorimetry. It was thus established that the application of UV-visible irradiation had no significant impact on the overall thermal properties of ABS.



**URL:** <https://www.mdpi.com/1420-3049/29/21/5037>





## SCHOLARLY PUBLICATIONS School of Applied Sciences KIIT Deemed to be University

**Journal Name:** European Journal of Medicinal Chemistry Reports

**IF:** 4.0

**Title:** Combinational delivery of berbamine and 5-fluorouracil in cerium oxide nanoparticles for colon cancer therapy: Insights from in vitro and in silico studies

**Author:** Satpathy S.S.; Mishra S.; Pattnaik S.; Mohanty C.

**Details:** Volume 12, December 2024

**Abstract:** Colon cancer is traditionally treated by an antimetabolite drug 5-fluorouracil (5FU) but has been linked to several drawbacks and systemic toxicity. To overcome drug associated toxicity, combination therapy is a promising strategy that synergistically enhances the therapeutic effects of co-delivered drugs while minimizing administration doses. Therefore, the current study aims to investigate the anti-colon cancer potency of 5FU co-delivered with a phytochemical i.e., berbamine (BERB) in a Cerium oxide nanoparticles (CONPs) delivery system. CONPs loaded 5FU (5FU-CONPs) and BERB (BERB-CONPs) were prepared and characterized using different analytical techniques. Successful entrapment of both drugs into CONPs formulations was detected under X-ray diffraction (XRD) observations. Drug-loaded CONPs in combination showed effective anti-oxidant activity by preventing reactive oxygen species (ROS) generations and had superior cytotoxic effects on HT-29 cell lines compared to treatment with native drugs singly or in combination. They also triggered apoptosis through p21, p53, Bax upregulation, and Bcl-2 downregulation, as confirmed by Western blot studies. Additionally, in silico analysis was performed using molecular docking and molecular dynamics simulation (MDS) to validate the in vitro results. Results of the study suggest that 5FU and BERB CONPs in combination could be taken as a possible therapeutic approach for colon cancer treatment.



**URL:** <https://www.sciencedirect.com/science/article/pii/S2772417424000967?via%3Dihub>

