SCHOLARLY PUBLICATIONS
School of Applied Sciences
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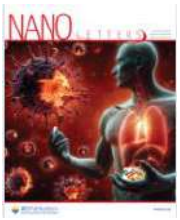
Journal Name: Nano Letters **IF: 9.6**

Title: Electrically Controlled Excitons, Charge Transfer Induced Trions, and Narrowband Emitters in MoSe2-WSe2 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 $MoSe_2$–WSe_2 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
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Journal Name: Journal of Alloys and Compounds **IF: 5.8**

Title: Effect of milling time on structural and electrical properties of thermomechanically synthesized of Ba0.1 (Bi0.45Na0.45)TiO3 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 $Ba_{0.1}(Bi_{0.45}Na_{0.45})TiO_3$ (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
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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

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

Title: Optimizing solvent mixtures to boost the electrochemical performance of BiOCl for supercapacitor applications

Author: Thakur Y.S.; Acharya A.D.; Sharma S.; Iqbal M.; Bisoyi S.; Amisha; Bhawna

Details: Volume 184, April 2025, Article number 113259

Abstract: The physical and morphological features of materials play a key function in the electrochemical performance of supercapacitor electrodes, prompting extensive research into optimizing electrode material morphology. This investigation explores the effects of various solvents ethylene glycol (EG), diethylene glycol (DEG), and triethylene glycol (TEG) on the fabrication of BiOCl using a solvothermal method, focusing on the electrochemical, structural, and morphological characteristics of the resulting nanostructures. Notably, the BiOCl electrode synthesized with triethylene glycol (BT) exhibits a marigold flower-like morphology adorned with nanosheets, improving surface area and enriching electrical conductivity. Consequently, BT demonstrates a superior specific capacity of 665 C/g at 0.5 A/g, alongside impressive rate competence. In addition, a supercapacitor device using a BT//BT configuration was erected, showcasing an extreme energy density of 15.6 Wh/kg at 838 W/kg power density. The device maintained commendable cyclic stability, retaining approximately 78 % of its specific capacity and 83 % of its coulombic competence after 5000 cycles. Practical application was validated by powering a red LED, underscoring the potential of BT electrodes for energy storage applications. This study offers an effective synthesis method for high-performance BiOCl electrodes and emphasizes the influence of solvents on morphology and charge storage mechanisms. These findings provide valuable insights for future advancements in BiOCl and other metal oxide materials for energy storage applications.

URL: https://www.sciencedirect.com/science/article/pii/S0025540824005877?via%3Dihub

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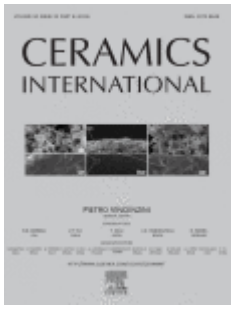
Journal Name: **Ceramics International** **IF: 5.1**

Title: Design and electromagnetic shielding of Bi0.5Na0.5TiO3 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 Bi0.5Na0.5TiO3 (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 µm. 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 ∼ −23.65 dB, SEA ∼ −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.



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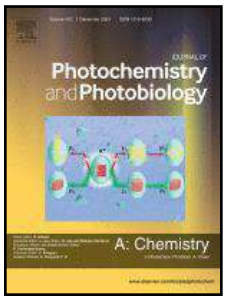
Journal Name: Journal of Photochemistry and Photobiology A: Chemistry **IF: 4.7**

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)]2O3 (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 Fe2O3 are investigated. The presence of pure α-Fe2O3 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 α-Fe2O3 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−1 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.



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SCHOLARLY PUBLICATIONS
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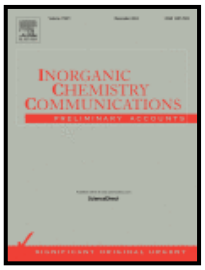
Journal Name: **Inorganic Chemistry Communications** **IF: 4.4**

Title: Investigation of structural, dielectric, impedance, and conductivity properties of layered perovskite type compound; NaYSnO4

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: n this paper, the structural study of $NaYSnO_4$ (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

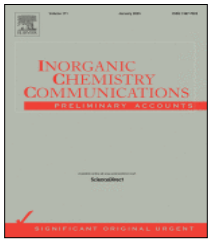
Journal Name: Inorganic Chemistry Communications **IF: 4.4**

Title: An extensive analysis of the impedance, dielectric, optical and structural properties of (Na0.5Bi0.5)SrTi2O6 ceramic

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

Details: Volume 172, February 2025, Article number 113738

Abstract: A stable solid solution of $0.5(Na_{0.5}Bi_{0.5})TiO_3$-$0.5(SrTiO_3)$ is prepared through a cost-effective high temperature solid state reaction route. The detailed structural phase analysis of the prepared compound is carried out using X-ray diffraction pattern and a comprehensive Raman analysis. Highly magnified FESEM images of the surface of sintered compound reveal the evolved microstructure of the compound. The chemical purity of the solid solution is verified through estimation of elements and their weight percentage utilizing EDX analysis. UV–visible spectroscopy technique is adopted to investigate the optical properties and band gap of the compound to find its suitability in opto-electronic devices. Dielectric and electrical properties are analyzed using the complex impedance spectroscopy (CIS) framework. The structure–property relationship, conduction mechanism, and other relevant aspects have been evaluated and investigated in a wide range of frequency (1 kHz–1 MHz) and temperature (25–500 °C). Electrical data analyzed through impedance and modulus formalism suggested dominating non-ideal bulk contribution to the overall electrical response and negative temperature coefficient of resistance (NTCR) behavior of the compound. The strong dependence of bulk resistance on temperature was exploited for possible application of compound as thermistor. The frequency-dependent ac conductivity data is modeled with the universal power law to know the conduction mechanism. Activation energies are determined from temperature dependent impedance data to figure out the type and nature of charge carriers involved in different electrical processes.



URL: https://www.sciencedirect.com/science/article/pii/S1387700324017283?via%3Dihub

Journal Name: Materials Chemistry and Physics **IF: 4.3**

Title: TiO2/graphene oxide-filled carboxymethyl cellulose/chitosan blend films

Author: Das M.; Fatma K.; Das B.; Kundu C.N.; Yadav M.; Tripathy J.

Details: Volume 332, 15 February 2025, Article number 130233

Abstract: This work focuses on the fabrication of TiO_2 nanoparticles and graphene oxide (GO) integrated carboxymethyl cellulose (CMC) and chitosan (CS) based nanocomposite films using a solvent casting approach. Structural and morphological characterizations using UV–Vis, FT-IR, XRD Raman spectroscopy, FE-SEM, EDS, elemental mapping, TEM and AFM verified the successful fabrication of the films. Incorporating graphene sheets and titanium dioxide nanoparticles (TiO_2) significantly enhanced the mechanical, barrier, thermal, and antibacterial properties of polymer nanocomposites. Upon the addition of GO and TiO_2, the light transmittance of the nanocomposite matrices was reduced by 54.49 % compared to the CMC/CS blend. Interestingly, the inclusion of TiO_2 and GO also resulted in a reduction of swelling and water vapor permeability (WVP) in the CMC/CS/TiO_2-GO nanocomposite films, with a WVP of 2.75×10^{-11} g m^{-2} s^{-1} Pa^{-1}. The antibacterial efficacy of the polymeric nanocomposite film was investigated through a well-known disc diffusion method as well as the growth inhibition assay. The CMC/CS/TiO_2-GO nanocomposites showed significant inhibition of bacterial cell growth. Further, the biocompatibility of fabricated nanocomposite films was ascertained through MTT assay.

URL: https://www.sciencedirect.com/science/article/pii/S0254058424013610?via%3Dihub

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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: Benmammar R.K., Bouberka Z., Malas C., Carpentier Y., Haider K.M., Mundlapati V.R., Ziskind M., Focsa C., Khelifi S., Poutch F., Laoutid F., Supiot 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

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