SCHOLARLY PUBLICATIONS
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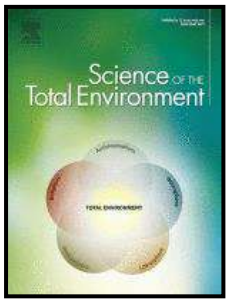
Journal Name: Science of the Total Environment **IF: 8.2**

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 (·OH) radicals, influencing the oxidation capacity of the atmosphere. We conduct a comprehensive investigation into the temporal dynamics of HONO, other gases (nitrogen oxides (NOx), ozone (O3), ammonia (NH3), sulphur dioxide (SO2), and nitric acid (HNO3)), particulate matter (PM2.5), 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 μg 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 μg m−3 compared to the average observed value of 7.00 μg m−3). The calculated production rates of HONO from observations for daytime to nighttime peaks are 3.10 μg m−3 h−1 (1.1 × 107 molecules cm3 s−1) and 2.00 μg m−3 h−1 (7.1 × 106 molecules cm3 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 ·OH formation rate of 9.4 × 107 molecules cm3 s−1 due to the photolysis of HONO, which is much higher than the production of HONO from the reaction of O1D with H2O. This underscores the predominant role of HONO photolysis as the primary source of ·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

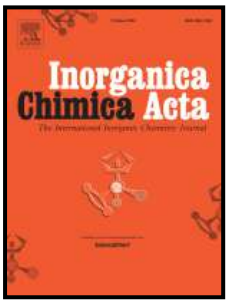
Journal Name: Inorganica Chimica Acta **IF: 6.9**

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, [PdCl4]2- solution. The Galvanic replacement reaction (GRR) starts instantaneously between less noble Ni0 nanoparticle i.e., zero valent nickel (ZVN) and more noble [PdCl4]2-. Thus ZVN is oxidatively etched out as soluble Ni2+ by more noble [PdCl4]2- depositing Pd0 onto the residual ZVN. Concurrently the Ni2+ ions move outwardly into the bulk solution and the Pd0enters 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.



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SCHOLARLY PUBLICATIONS
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Journal Name: **Journal of Materials Chemistry C** **IF: 5.7**

Title: Boosting the dielectric and electrical performance of perovskite materials by collaborative augmentation with reduced graphene oxide nanosheets for cutting-edge storage solutions

Author: Barik R.; Sahu P.; Sahoo S.; Bhuyan M.; Dhara S.; Sahoo D.

Details: August 2024

Abstract: This investigation delved into the dielectric properties of methylammonium lead iodide ($MAPbI_3$) nanoparticles and $MAPbI_3$@rGO nanocomposites, using a co-precipitation approach to synthesize a reduced graphene oxide (rGO)-doped $MAPbI_3$ nanocomposite with varying concentrations. The study adjusted the temperature, doping concentrations, and frequency range s to fully examine the dielectric characteristics, focusing on temperature range 25-60 °C, doping concentrations 0.5 wt%, 1 wt%, 5 wt%, and 7 wt%, and frequency range 10 Hz-4 MHz. The dielectric response analysis shows that the relative permittivity of $MAPbI_3$ (~870@10 Hz) is significantly enhanced (~5.8×10^5@10 Hz, ~500 times at ambient temperature) in the presence of rGO. The significant enhancement in dielectric permittivity in the $MAPbI_3$@rGO composites is due to numerous interfaces, ion migration, polar group reorientation, and nanocapacitor formation, which increases with temperature, thereby enhancing the relative permittivity. Nevertheless, at 60 °C and 10 Hz, the relative permittivity value for $MAPbI_3$@rGO composites reaches nearly 2.8×10^6 (2000 times), the highest reported $MAPbI_3$ composite to date. The composite material exhibited remarkable potential as a supercapacitor dielectric material, as evidenced by dielectric constant increases of up to 10^5 orders of magnitude following rGO injection at room temperature. Moreover, the AC conductivity at room temperature for $MAPbI_3$@rGO (7.9×10^{-3} s m^{-1}) is higher than that of pristine $MAPbI_3$ (1.01×10^{-3} s m^{-1}), possibly due to more charge conduction from the valence band to the conduction band. The conductivity is also increased as a function of temperatures for all composites ($\sigma_{max} = 15.3 \times 10^{-3}$ s m^{-1}@60 °C) due to the decrement of electronic resistance. The dielectric loss value exhibits a downward trend (for $MAPbI_3$ ~18 and $MAPbI_3$@rGO ~2.3, decreased by ~6 times), and the repair of the sp^2 network in the graphene sheet is approved by the higher AC conductivity in $MAPbI_3$@rGO NCs relative to $MAPbI_3$ NPs. Furthermore, $MAPbI_3$ augmented with rGO is predicted to be a promising material for energy storage capacitive devices in the electronic industry due to its superior NTCR behaviour.

URL: https://pubs.rsc.org/en/content/articlelanding/2024/tc/d4tc03022b

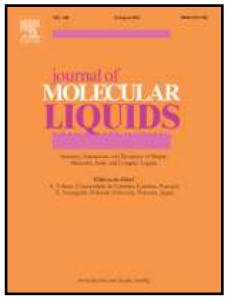
Journal Name: Journal of Molecular Liquids **IF: 5.3**

Title: Mechanistic exploration of Perfluorooctanoic Acid-Induced Hen egg white lysozyme aggregation at physiological Conditions: Spectroscopic and thermodynamic insights.

Author: Dudure, R; Pritam, P; Panda, AK; Ghosh, SK; Jadhao, M

Details: Volume 408 , 15 August 2024, Article No. 125255.

Abstract: Perfluoroalkyl substances (PFASs) have garnered attention in various scientific fields for their harmful effects on biological systems, including the endocrine, immune, and nervous systems. While research has delved into PFAS-protein binding, their impact on protein aggregation remains uncharted. In this study, we investigated the effect of perfluorooctanoic acid (PFOA) on the aggregation of Hen Egg White Lysozyme (HEWL), a model protein known to aggregate under harsh conditions. We uncovered compelling insights by employing an array of spectroscopic, computational and thermal techniques. Isothermal titration calorimetry (ITC), molecular docking, and fluorescence spectroscopy reveal strong PFOA-HEWL interactions via hydrogen bonding, hydrophobic forces, and ionic interactions. Moreover, techniques like synchronous fluorescence spectroscopy, circular dichroism, and FTIR demonstrates that PFOA induces substantial conformational changes in HEWL, profoundly affecting its secondary structure. Increased PFOA concentrations have been observed to lead to HEWL aggregation under physiological conditions (pH 7.4 and room temperature), verified through various assays and imaging techniques. This is the first comprehensive exploration of PFOA's influence on protein aggregation. Our findings provide valuable insights into the health risks of PFOA exposure from a protein aggregation perspective, advancing our knowledge in environmental ecology, toxicology, pathology, and life sciences.



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SCHOLARLY PUBLICATIONS
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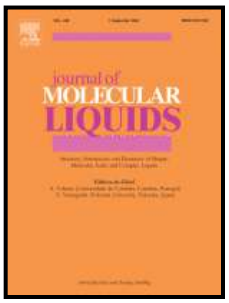
Journal Name: Journal of Molecular Liquids **IF: 5.3**

Title: Study of the perturbed hydrogen-bonded water structure of the hydration shell of N-Methyl-Acetamide by Raman multivariate curve resolution spectroscopy.

Author: Mishra, A; Mohapatra, H; Pradhan, M

Details: Volume 410, September 2024, Article number 125574.

Abstract: In this work, Raman scattering measurement combined with multivariate curve resolution (Raman-MCR) technique has been used to obtain the solute correlated spectra (SC) of N-methyl-acetamide (NMA) in an aqueous medium. The SC spectra is composed of NMA intramolecular vibrations and NMA induced-perturbations of water OH stretch vibrations. The SC spectra obtained for different mole-fractions of NMA reveal that as the mole-fraction of NMA increases the perturbed water interacting with the amide group is retained whereas it gets depleted from the hydrophobic hydration shell of the methyl group of NMA. The high wavenumber region of the OH spectrum shows that the fraction of the weakly hydrogen-bonded population is higher in the bulk water compared to perturbed water. The Raman spectra of perturbed OH spectral features due to hydration of the hydrophobic methyl group of NMA have been extracted from SC spectra obtained at low mole-fraction of NMA by the MCR technique. Its spectral feature resembles the SC-OH spectra of hydrophobic hydration of the methyl group of methanol.



URL: https://www.sciencedirect.com/science/article/abs/pii/S0167732224016337?via%3Dihub

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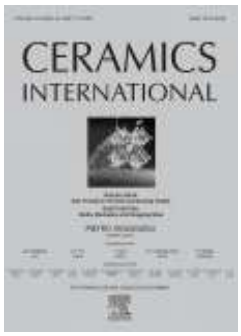
Journal Name: **Ceramics International** **IF: 5.1**

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.

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 solid-state reaction technique to prepare $Bi_{0.5}Na_{0.5}TiO_3$ (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 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 ($SE_T \sim -23.65$ dB, $SE_A \sim -18.91$ dB) at 9.2 GHz in the X-band (8.2–12.4 GHz). Meta-surface-based 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
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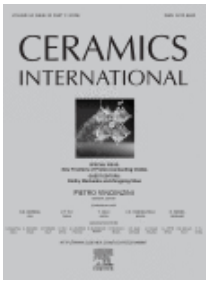
Journal Name: **Ceramics International** **IF: 5.1**

Title: Structural, optical and electrical properties study of (Na0.5La0.5)CaTi2O6 for possible industrial applications

Author: Priyadarshini L.; Biswal L.; Rout S.; Moharana K.; Parida A.K.; Behera B.

Details: August 2024

Abstract: An A site disordered rare earth-based perovskite-derived structured new compound is synthesized using low-cost solid-state reaction method. The phase formation of the desired compound is established through the X-ray diffraction technique. Rietveld analysis of the obtained XRD data confirmed that the compound exhibits orthorhombic symmetry with pbnm space group which is further supported through Raman spectroscopic analysis. The surface morphology and microstructure analysis of the synthesized compound is carried out using scanning electron microscopy approach. The optical properties study done through UV–Visible absorption spectroscopy suggests possible application in optoelectronic devices. The frequency and temperature dependence of dielectric properties are studied for the analysis of electric polarisation in the sample. Electrical properties study conducted through complex impedance spectroscopy approach disclosed the dominant contribution of grain to the electrical response of the material with temperature dependent relaxation process in the compound. The effect of temperature on the dc resistance is further analysed to find the suitability of the material for thermistor application. The frequency dependent data of ac conductivity follows Jonscher's power law. The temperature dependent ac conductivity graph was used to estimate the activation energy in order to identify the specific charge species engaged in the ac conduction process.



URL: https://www.sciencedirect.com/science/article/pii/S0272884224034795

SCHOLARLY PUBLICATIONS
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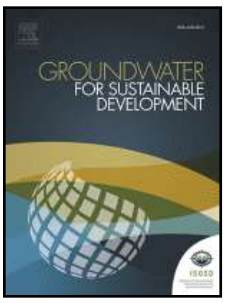
Journal Name: Groundwater for Sustainable Development **IF: 4.9**

Title: Microplastics and nanoplastics in environment: Sampling, characterization and analytical methods.

Author: Mahapatra, S; Maity, JP; Singha, S; Mishra, T; Dey, G; Samal, AC; Banerjee, P; Biswas, C; Chattopadhyay, S; Patra, RR; Patnaik, S; Bhattacharya, P

Details: Volume 26 , August 2024, Article No. 101267.

Abstract: Microplastics (MPs) and nanoplastics (NPs) have gained increasing attention in environmental research due to their ubiquitousness and potential impacts on natural environments and human health as per the UN Sustainable Development Goals (SDGs), particularly SDG-14 to address global threats where at least 12 SDGs, directly/indirectly impacts. Present review is undertaken to highlight the process of breakdown of diverse groups of plastic products in soil, surface water, and groundwater under the influence of different factors (UV, light, heat, microbe, etc.), which are mobilized as MPs/NPs to the surface water, groundwater, air, soil, and living organisms by different natural and anthropogenic processes. Review also highlights a comprehensive overview of the methodology for sampling, characterization, and analysis for these minuscule plastic particles (PPs) in various environmental samples, encompassing surface/subsurface water, sediments, soils, and biological organisms. The collection, extraction, and characterization of MPs/NPs, typically employ filtration processes, wherein a known volume of water is passed through a fine mesh to capture MPs/NPs from water samples. Sediment/soil samples require sieving and density separation techniques to isolate PPs from the surrounding matrix. Biological samples require digestion steps to remove organic matter, leaving behind plastics for analysis. Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy, and scanning electron microscopy (SEM) are commonly utilized to determine the polymer composition, size, shape, and surface characteristics of PPs. Quantification involves several approaches, visual counting, image analysis, and spectroscopic techniques. Abundance of MPs/NPs in the respective environmental samples (water, air, soil, etc.) can be determined by comparing the richness (i.e., number/mass) of plastics to the volume or weight of the original sample. Such comprehensive analytical methodologies contribute to understand the scope and magnitude of plastic pollution and its potential repercussions for ecosystems and human well-being, which are essential for developing the effective strategies to mitigate these pressing global environmental challenges for sustainable development.



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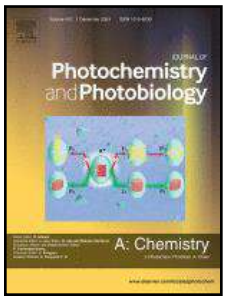
Journal Name: Journal of Photochemistry and Photobiology A: Chemistry **IF: 4.7**

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: **ACS Applied Polymer Materials** **IF: 4.4**

Title: 2D and 3D Printable Self-Healing Hydrogels Based on Polyacrylic and Tricarballylic Acids through a Double Network Strategy

Author: Sahoo S.D.; Prasad E.

Details: Volume 12, April 2024

Abstract: Mechanical and self-healing properties are desirable characteristics for engineering hydrogels for various practical applications. However, developing hydrogels that combine these attractive properties in a single material remains challenging. This work attempts to address this issue by designing and synthesizing a metallohydrogel using a double network (DN) strategy. The gel, composed of poly(acrylic acid), tricarballylic acid (TA), and Fe^{3+}, exhibits excellent mechanical strength (with a tensile strain of 3145% and tensile stress of 51 kPa) and high self-healing properties (with a HE of 93%) under ambient conditions without any external trigger. The modified hydrogel enables 3D printing structures, paving the way for future applications in diverse fields, ranging from soft robotics to energy storage. Furthermore, the required rheological properties, such as non-Newtonian and shear thinning behavior, are achieved for the ink by optimization of the composite concentration. More importantly, the prepared ink is able to print different structures with a high degree of accuracy.

URL: https://pubs.acs.org/doi/10.1021/acsapm.4c01541

SCHOLARLY PUBLICATIONS
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Journal Name: **Physics of Fluids** **IF: 4.1**

Title: Analytical study of electroosmotically driven shear-thinning flow in a non-uniform wavy microchannel

Author: Parida, SK; Sutradhar, A; Deb, D; Dev, AN

Details: Volume 36, Issue 9, September 2024

Abstract: n efficient mathematical model of electroosmotic blood flow in a non-uniform wavy microvessel is investigated. In the present study, the microvessel is considered as an impermeable microchannel in which the Herschel-Bulkley (H-B) model of shear-thinning character is chosen to represent the complex flow of blood. An external electric field is applied along the channel length. Due to the negative charge of the glycocalyx layer located at the inner s urface of the microchannel, an electric double layer is formed. As a result, an electric potential developed, which is described by the Poisson-Boltzmann equation. Eventually, the study analytically solves a boundary value problem to determine the axial velocity of H-B fluid flow by employing a long wavelength and low Reynolds number. Additionally, the analysis derives the volumetric flow rate in the microchannel across a single wavelength and stream function for the flow field. Using Mathematica symbolic software, graphs are plotted to visualize the impact of rheological features on the axial velocity, streamlines, and volumetric flow rate concerning various physical parameters such as H-B shear-thinning flow index, plug radius, Debye length, and Helmholtz-Smoluchowski velocity. It is found that the flow of blood becomes smoother as blood behaves more shear-thinning in nature, which is the key innovation of this work. Also, an increment in Debye length helps in increasing the size of fluid bolus remarkably, which adds the novelty of physics to this study. Such a model can have applications in canalicular flow, transport in human skin, fluid dialysis, and separation methods.

URL:https://pubs.aip.org/aip/pof/article-abstract/36/9/091901/3311198/Analytical-study-of-electroosmotically-driven?redirectedFrom=fulltext