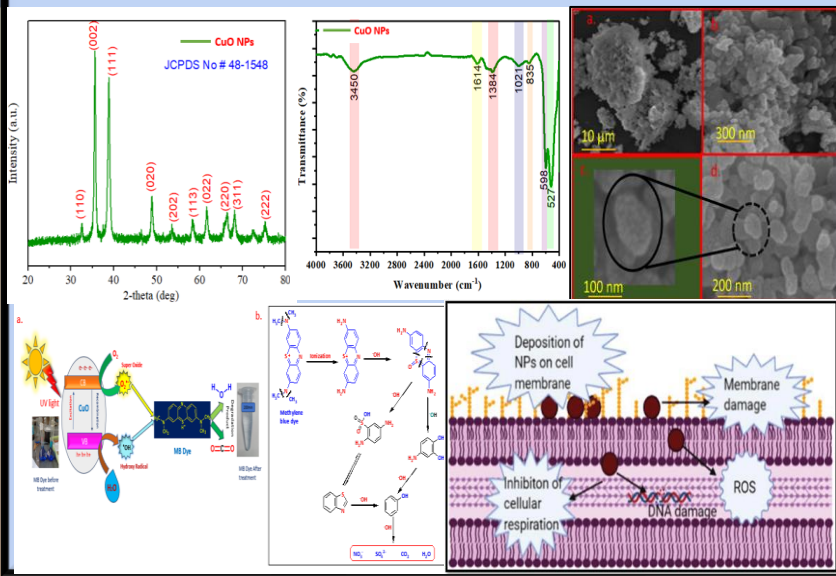


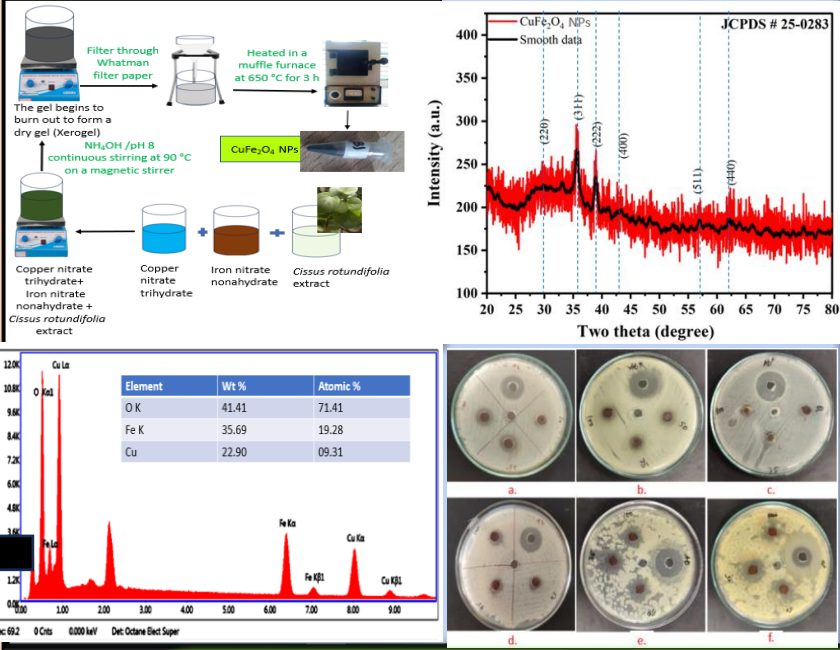
Thrust Area

1. Synthesis and characterization of Metal oxide-based nanoparticles and their nanocomposites, using the bottom-up approach.
2. Evaluation of Therapeutic and Environmental applications of the synthesized nanostructured materials

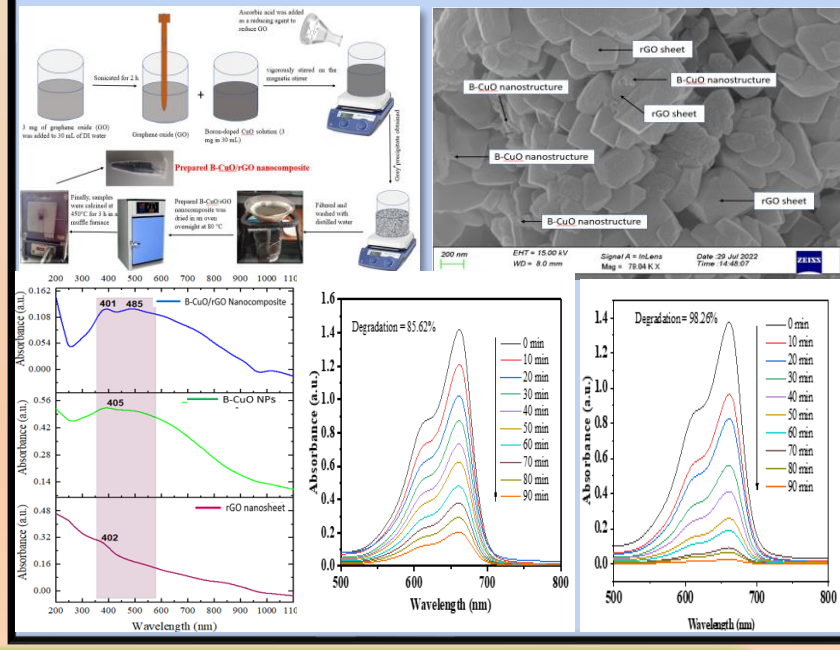
Green Synthesis of CuONPs from *Aloe Barbadensis* Miller: Antibacterial Activity, and Photocatalytic Dye Degradation



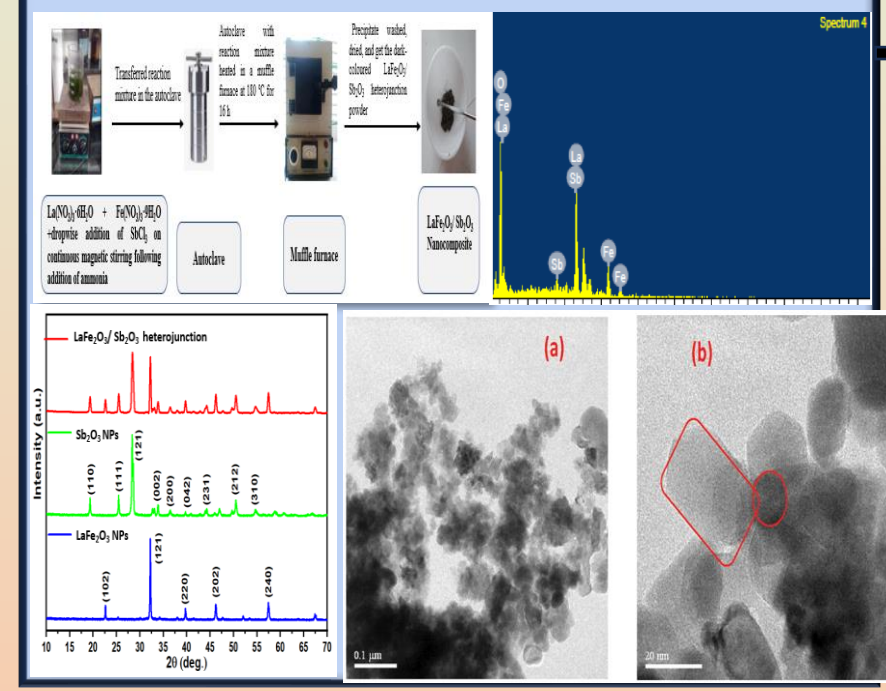
Green Synthesis of CuFe₂O₄ NPs from *Cissus Rotundifolia*: Antibacterial Activity, And Photocatalytic Dye Degradation



Chemical Synthesis Of B-CuO and B-CuO/rGO Binary Nanocomposite : Antibacterial Activity and Photocatalytic Dye Degradation



Chemical Synthesis of LaFe₂O₃/ Sb₂O₃ Heterojunction: Photocatalytic Dye Degradation



ACS OMEGA

Biogenic Synthesis of Copper Oxide Nanoparticles from *Aloe vera*: Antibacterial Activity, Molecular Docking, and Photocatalytic Dye Degradation

Sabeeha Jabeen, Vasi Uddin Siddiqui, Shashi Bala, Nidhi Mishra, Anamika Mishra, Rubana Lawrence, Prathiba Bansal, Abdul Rahman Khan, and Tahmeena Khan

ABSTRACT: Green synthesis methods offer a cost-effective and environmentally friendly approach to producing nanoparticles (NPs), particularly metal-based ones. This study explores the green synthesis of copper oxide nanoparticles using *Aloe vera* (Aloe barbadensis Miller) leaf extract. The characterization revealed a unique shape morphology revealed by field-emission scanning electron microscopy and X-ray diffraction analysis. Distinctive metal-oxygen bonds at 521 and 601 cm⁻¹ of the CuO structure were confirmed by Fourier transform infrared spectroscopy. Furthermore, UV-visible spectroscopy revealed a notable peak absorbance at 246 nm, suggesting electron transitions across energy bands and varying surface conduction electrons. The UV band gap value indicates the presence of quantum confinement effects, which are probably caused by the distinctive morphology and surface structure of the biogenic NPs. Additionally, molecular docking studies have been carried out against key proteins of *Salmonella typhi* and *Listeria monocytogenes*, namely, lipopolysaccharide O (LPS) (PDB ID: 4C2B), internalin (InaA) (PDB ID: 1A7T), S-layered lectin protein (Slyp) (PDB ID: 4C1D), and YnfK (PDB ID: 2AM7) using AutoDock 4.2. The results revealed binding energies against *S. typhi* and *L. monocytogenes* proteins, indicating potential interactions. This establishes the foundation for further in-depth understanding of the molecular basis underlying the observed antibacterial effects *in vitro* against *S. typhi*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *L. monocytogenes*. Antibacterial assays yielded impressive results, with CuO NPs displaying significant activity against *S. typhi* and *L. monocytogenes*, exhibiting zones of inhibition values of 13 ± 0.02 and 15 ± 0.04 mm, respectively. Moreover, the CuO NPs demonstrated remarkable photocatalytic efficacy, resulting in the degradation of 77% of the methylene blue dye when exposed to UV irradiation. This study highlights the potential of green-synthesized CuO NPs derived from *A. vera* with their unique morphology, interesting spectroscopic properties, and promising antibacterial and photocatalytic activities.

Journal of Alloys and Compounds

A novel green synthesis of CuFe₂O₄ Nanoparticles from *Cissus rotundifolia* for photocatalytic and antimicrobial activity evaluation

Sabeeha Jabeen^{1,2}, Vasi Uddin Siddiqui¹, Swati Sharma³, Smita Rai⁴, Prasthita Bansal¹, Shashi Bala¹, Azam Raza⁵, Mohammad Imran Ahmad⁶, Abdul Rahman Khan⁷, Tahmeena Khan⁸

ABSTRACT: This paper reports a novel green fabrication of copper ferrite (CuFe₂O₄) nanoparticles (NPs) from *Cissus rotundifolia* leaf extract. The NPs were characterized by different spectroscopic techniques. The Fourier transform infrared (FTIR) spectrum exhibited intense absorbance at the wavenumber of 521 and 601 cm⁻¹ and the X-ray diffraction analysis (XRD) showed the formation of well-crystalline NPs. The mean crystallite size of the NPs was calculated to be 17.23 nm. The high-resolution transmission electron microscope (HRTEM) analysis showed roughly spherical shape and irregular morphology of the NPs. The zeta potential was calculated to be -29.763 mV, indicating a negative charge over the CuFe₂O₄ NPs. The formation of spinel ferrite was confirmed from the characterization data. The photocatalytic activity of the CuFe₂O₄ NPs was examined against the methylene blue (MB) dye, showing 82% degradation under UV visible light. The results revealed that the rate of dye degradation was not much decreased even after 48 h of synthesis. The antibacterial activity of the synthesized CuFe₂O₄ NPs was tested against *Staphylococcus aureus*, *Bacillus pumilus*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Listeria monocytogenes* through the agar well diffusion method. A zone of inhibition of 12 ± 0.2, 11 ± 0.1, 10 ± 0.1, 10 ± 0.1, and 10 ± 0.1 mm, respectively, was observed against *S. aureus*, *B. pumilus*, *K. pneumoniae*, *P. aeruginosa*, and *L. monocytogenes*. The results indicate that the CuFe₂O₄ NPs have gained considerable interest in their various structural and electrical properties. Further NPs have been used in various applications in hydroponic, medicinal, and agricultural uses, showing improved antimicrobial activity of CuFe₂O₄ modified with Cu, Zn, Ni, and transition metals, for instance, ZnFe₂O₄, NiFe₂O₄, ZnNiFe₂O₄, CuFe₂O₄, and MnFe₂O₄, etc. [1-11]. Besides their magnetic behavior, they are also associated with spin-coating effect, spin-glass-like behavior, and higher heat and corrosion resistance [12]. These NPs have exceptional optical, electrical, and magnetic properties. CuFe₂O₄ NPs are extensively used as magnetic, supercapacitor, and photocatalytic materials [13]. The combination of ferrites with some different metal ions can improve their properties [14]. NiFe₂O₄ and ZnNiFe₂O₄ NPs have gained considerable interest in their widespread applications [15]. In recent years, iron oxide NPs (particularly ferrites) have attracted attention, especially in therapeutic applications. Previous studies [16,17] have investigated the improved antimicrobial activity of CuFe₂O₄ modified with Cu, Zn, Ni, and

MAJOR FINDINGS

1. Bottom-up approach was used to produce nanomaterials for therapeutic and environmental applications, particularly the degradation of MB and MC dyes
2. The Green method was used for the preparation of CuO and CuFe₂O₄ NPs, and the chemical method was used for B-CuO/rGO and LaFe₂O₃/Sb₂O₃ nanocomposites heterojunction.
3. Chemical synthesis provides good results compared to green synthesis
4. Improved antibacterial activity was exhibited by the heterojunctions and nanocomposites

INTEGRAL UNIVERSITY AWARDS
OUTSTANDING RESEARCHER
OF THE YEAR 2024
(Sciences/Biological Sciences/Engineering)

Dr. Tahmeena Khan
Assistant Professor
Department of Chemistry
Integral University

Awarded on the Occasion of
XVI CONVOCATION
HONORARY 1ST FEBRUARY 2024

materials proceedings

Photocatalytic Degradation of Malachite Green Dye via An Inner Transition Metal Oxide-Based Nanostructure Fabricated through a Hydrothermal Route

Sabeeha Jabeen^{1,2}, Adil Shaif Ganie³, Shashi Bala² and Tahmeena Khan^{1,4,5}

ABSTRACT: This experimentation focuses on an inner transition metal oxide-based nanostructure LaFeO₃ which was fabricated by a hydrothermal route for photocatalytic degradation of dye under visible light irradiation. The fabricated nanostructure was characterized by various techniques, including X-ray diffraction (XRD), which depicts the crystalline nature and size of the synthesized nanostructure which is 45 nm; field emission scanning electron microscopy (FE-SEM), which deter-

ChemistrySelect

A Comprehensive Review on Metal Oxide-based Nanomaterials: Synthesis, Characterization, Environmental, and Therapeutic Applications

Sabeeha Jabeen, Ekhlakh Veg, Mohammad Imran Ahmad, Shashi Bala, Tahmeena Khan

ABSTRACT: Metal oxide-based nanomaterials have gained attention due to their unique properties and wide applications in numerous fields including environmental remediation and intervention therapy. This paper provides a comprehensive overview of the synthetic methods, characterization strategies, and therapeutic and environmental applications of

Materials Today Chemistry

Fabrication of B-CuO nanostructure and B-CuO/rGO binary nanocomposite: A comparative study in the context of photodegradation and antimicrobial activity assessment

Sabeeha Jabeen^{1,2}, Vasi Uddin Siddiqui¹, Satyam Rastogi³, Suchi Srivastava⁴, Shashi Bala¹, Nafees Ahmad⁵, Tahmeena Khan⁶

ABSTRACT: This paper reports the synthesis of a cost-effective, stable, and recyclable brown-doped copper oxide (B-CuO) heterojunction graphene oxide (GO) binary nanocomposite. A conventional wet chemical synthesis route was used to fabricate the binary nanocomposite. X-ray diffraction (XRD) studies were performed to check the phase purity and crystallinity, scanning electron microscope (SEM) technique for structural and morphological analysis, energy dispersive spectroscopy (EDS) for surface composition, and Fourier transform infrared spectroscopy (FTIR) for functional group identification. The experimental results confirmed the formation of the pure nanocomposite. The photocatalytic activity of B-CuO and B-CuO/rGO binary nanocomposite was tested for Methylene Blue (MB) dye degradation under visible light. The B-CuO/rGO binary nanocomposite exhibited improved photocatalytic activity (98%) as compared to B-CuO (80%) in 90 minutes. The antibacterial activity was

Inorganic Chemistry Communications

Fabrication and studies of LaFe₂O₃/Sb₂O₃ heterojunction for enhanced degradation of Malachite green dye under visible light irradiation

Sabeeha Jabeen^{1,2}, Adil Shaif Ganie³, Nafees Ahmad⁴, Sharif Hajar⁵, Shashi Bala¹, Daraksha Bano⁶, Tahmeena Khan⁷

ABSTRACT: Visible light-driven photocatalysis with less charge transfer resistance and large separation are considered promising materials to address the challenges of environmental contamination. In this study, a nanocomposite of lanthanum ferrite and antimony oxide heterojunction (LaFe₂O₃/Sb₂O₃) was synthesized by facile hydrothermal method for photocatalytic degradation of malachite green (MG) dye under the irradiation of visible light. The synthesized nanocomposite was characterized by various analytical techniques including Fourier Transform Infrared Spectroscopy (FTIR) for functional group analysis, X-ray Diffraction (XRD) for phase purity and crystallinity, Scanning electron microscope (SEM) for surface structure analysis, and energy dispersive spectroscopy

International Journal of Nano Dimension (IJND)

Quantum chemical and molecular docking studies of boron-doped and reduced graphene oxide supported nanocomposite

Sabeeha Jabeen^{1,2}, Shirazi Modanwal³, Nidhi Mishra⁴, Vasi Uddin Siddiqui¹, Shashi Bala², Tahmeena Khan^{1,5}

ABSTRACT: Nanocomposites have attracted great attention due to their outstanding properties compared to bulk materials for many applications in various fields. However, their computational studies for property applications are still at a stage of infancy. So far very few studies have been attempted to study the quantum chemical parameters of nanocomposites. This article reports the density functional theory (DFT) calculations and molecular docking studies to explain important properties of boron-doped and reduced graphene oxide (B-CuO)/rGO supported nanocomposite (B-CuO/rGO). Parameters including highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO), energy gap (Eg), absolute hardness (η), absolute softness (σ), absolute electrostatic charge (ΔN_{max}), chemical potential (μ), global electrophilicity index (ω), and additional electronic charge (ΔN_{max}) were predicted. Molecular docking was performed against antimicrobial protein target (penicillinase of *Staphylococcus aureus*) (PDB ID: 2WQJ) from *Pseudomonas aeruginosa* and a binding energy of 11.2 kcal/mol was obtained showing appreciable binding of the nanocomposite with the active site of the protein.

REVIEW ARTICLE

Nanotechnology in environmental sustainability and performance of nanomaterials in recalcitrant removal from contaminated Water

Sabeeha Jabeen¹, Nafees Ahmad², Shashi Bala³, Daraksha Bano⁴, Tahmeena Khan^{1,5}

ABSTRACT: In this review article, the implementations of nanomaterials such as metal oxides and their composites, carbon nanotubes, dendrimers, and polymer nanocomposites for wastewater decontamination have been discussed. The nanomaterials have a lot of potential, due to their high pollutant sensing ability and larger surface area. They are ideal for the removal of harmful heavy metals and also eradicate severe infections spreading microorganisms, organic waste and inorganic contaminants from the environment. The article reviews recent developments in water treatment using various nanomaterials. Nanotechnology has resulted in a variety of effective nano techniques for environmental remediation such as photocatalysis, nano adsorption and nano-filtration, which are more accurate to eradicate recalcitrant. Novel semiconductor photocatalysis, nano adsorbents, nano-composites, and other nanostructures have been used to achieve maximal performance at a low cost. This review provides the techno-functional applications of nanomaterials for wastewater remediation.