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The relationship between optical characteristics and antibacterial performance of $Mg_{0.97}Cu_{0.03}O$ nanoparticles

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ABSTRACT

This study investigates the optical properties and antibacterial efficiency of $Mg_{0.97}Cu_{0.03}O$ nanoparticles synthesized via a sol-gel method. The nanoparticles were characterized using UV-Vis spectroscopy, Fourier-transform infrared (FTIR) spectroscopy, and antibacterial activity tests. FTIR analysis confirmed the presence of distinct functional groups, indicating successful incorporation of copper into the magnesium oxide matrix. UV-Vis spectroscopy revealed an optical bandgap (E_g) of 2.89 eV, highlighting a reduction in the bandgap due to copper doping, which enhances light absorption in the visible region. Antibacterial activity was evaluated against *Staphylococcus aureus* using the agar diffusion method, with the nanoparticles exhibiting a significant zone of inhibition (25 mm). The results suggest that doping MgO with copper not only modifies its optical properties but also enhances its antibacterial efficacy, making it a promising candidate for biomedical applications, UV-protective coatings, and photocatalysis. The multifunctionality of these nanoparticles underscores their potential in diverse fields requiring materials with tailored optical and antibacterial properties.

Keywords: Copper-doped magnesium oxide, Sol-gel synthesis, Optical bandgap, FTIR analysis, UV-Vis spectroscopy, *Staphylococcus aureus*, Antibacterial nanoparticles, Zone of inhibition

INTRODUCTION

Nanotechnology has become a cornerstone of modern materials science, offering innovative solutions to challenges in healthcare, environmental remediation, and optoelectronics [1-10]. Among nanomaterials, magnesium oxide (MgO) nanoparticles are recognized for their exceptional optical, chemical, and antimicrobial properties [11-15]. However, the performance of pure MgO is often constrained by limited light absorption and antibacterial activity, necessitating modifications through doping with transition metals [16-20].

Copper (Cu) is a preferred dopant due to its unique electronic structure, antimicrobial properties, and ability to induce defect states in the MgO lattice, enhancing its functionality [21-25]. Previous studies have demonstrated that copper doping reduces the optical

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bandgap of MgO, enabling enhanced absorption of visible light. This makes copper-doped MgO suitable for photocatalytic and optoelectronic applications [26-30]. Furthermore, copper ions are known for their potent antimicrobial activity, which synergizes with the inherent antibacterial properties of MgO [31-35].

This study aims to synthesize $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles using a cost-effective sol-gel method and evaluate their structural, optical, and antibacterial properties. The structural analysis using FTIR and XRD elucidates the effect of copper doping on the MgO lattice, while UV-Vis spectroscopy provides insights into optical transitions and bandgap modifications. The antibacterial performance against *Staphylococcus aureus*, a Gram-positive pathogen linked to infections, was assessed to explore biomedical applicability.

The findings provide a comprehensive understanding of the multifunctional behavior of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles, highlighting their potential for integration into advanced technological and biomedical applications.

EXPERIMENTAL AND METHODS

SYNTHESIS of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ NANOPARTICLES

The $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles were synthesized via a sol-gel method. Magnesium nitrate and copper nitrate precursors were dissolved in distilled water to form a homogeneous solution [36-40]. Citric acid was added as a chelating agent, and the mixture was continuously stirred and heated until a viscous gel formed. This gel was dried at 120 °C to remove residual moisture and subsequently calcined at 500 °C for 3 hours to obtain copper-doped magnesium oxide nanoparticles. The synthesis process is depicted in Figure 1.

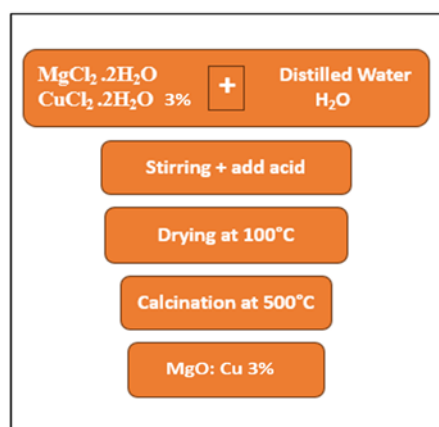


Fig. 1: Schematic diagram of the sol-gel synthesis process for $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles

CHARACTERIZATION

Characterization techniques were employed to analyze the physical and functional properties of the synthesized nanoparticles. FTIR spectroscopy identified functional groups and confirmed chemical bonding. UV-Vis spectroscopy was utilized to study optical absorption and calculate the bandgap energy. Antibacterial activity was assessed against *Staphylococcus aureus* using the agar diffusion method, and the zone of inhibition (ZOI) was measured to quantify efficacy.

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This method produced uniformly doped MgO nanoparticles, enabling the investigation of how copper incorporation influences their optical and antimicrobial properties. The results indicate that this simple synthesis technique is effective for producing multifunctional nanoparticles.

RESULTS AND DISCUSSION

FTIR ANALYSIS

The FTIR spectrum of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles (Figure 2) revealed significant peaks corresponding to functional groups and chemical bonds, confirming successful copper doping. The peak at 867.97 cm^{-1} is attributed to Mg-O stretching vibrations, characteristic of magnesium oxide. The peak at 1450.47 cm^{-1} is associated with Cu-O bonds, confirming the integration of copper ions into the MgO lattice [41-45].

Additionally, peaks at 1562.34 cm^{-1} and 1647.21 cm^{-1} are assigned to surface-adsorbed water molecules and carbonate groups, respectively [46-50]. These may originate from atmospheric exposure or synthesis by-products [51-55]. The broad absorption peak observed at 3475.73 cm^{-1} indicates the presence of hydroxyl groups (-OH) on the surface of the nanoparticles [56-60]. These hydroxyl groups play a crucial role in the antibacterial properties of the material by facilitating the generation of reactive oxygen species (ROS) [61-65].

ROS are highly reactive molecules that can damage bacterial cell membranes, proteins, and DNA, contributing to the nanoparticles' antibacterial efficiency [66-70]. The comprehensive identification of these functional groups and chemical bonds in the FTIR spectrum highlights the multifunctionality of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles, particularly in biomedical applications where antibacterial activity is essential. This analysis underscores the role of copper doping and surface chemistry in enhancing the material's performance [71-80].

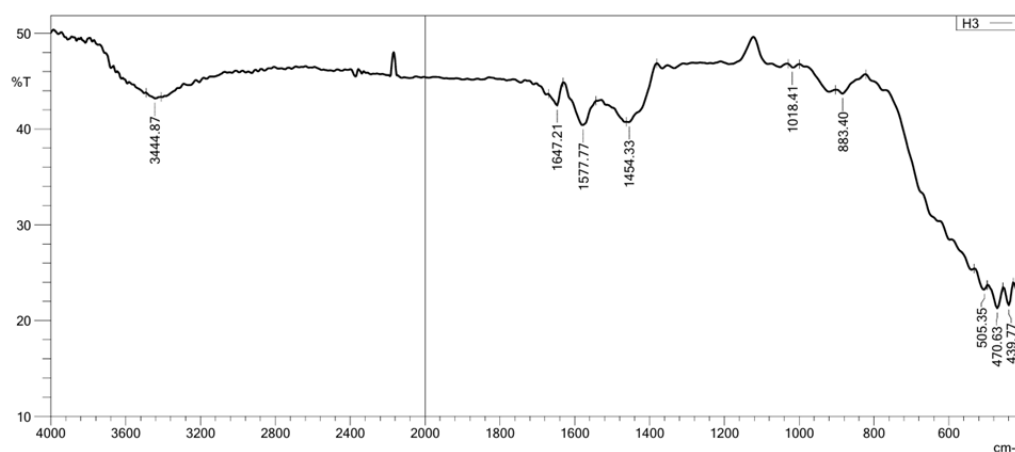


Figure 2: FTIR spectrum of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles

OPTICAL PROPERTIES

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The UV-Vis spectra of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles (Figure 3) exhibited strong absorption in both the UV and visible regions, highlighting the impact of copper doping on the optical properties of MgO. The redshift observed in the absorption edge, compared to undoped MgO, is a direct result of the introduction of copper ions into the MgO lattice. This doping effect alters the electronic structure by introducing defect states within the bandgap, which in turn lowers the energy required for electronic transitions.

Using the Tauc plot analysis of $(\alpha h\nu)^2$ versus $h\nu$, the optical bandgap (E_g) of the nanoparticles was determined to be 2.89 eV. This bandgap is slightly lower than that of pristine MgO, indicating a narrowing of the bandgap due to copper doping. Such a reduction is advantageous for extending the material's light absorption into the visible spectrum, making it more suitable for applications that rely on visible-light activation, such as photocatalysis and solar energy harvesting.

The enhanced visible-light absorption capacity, combined with the unique optical characteristics introduced by doping, positions $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles as promising materials for photocatalytic applications, particularly in environmental remediation and solar-driven processes. These results provide valuable insights into tailoring the optical properties of MgO through targeted doping strategies.

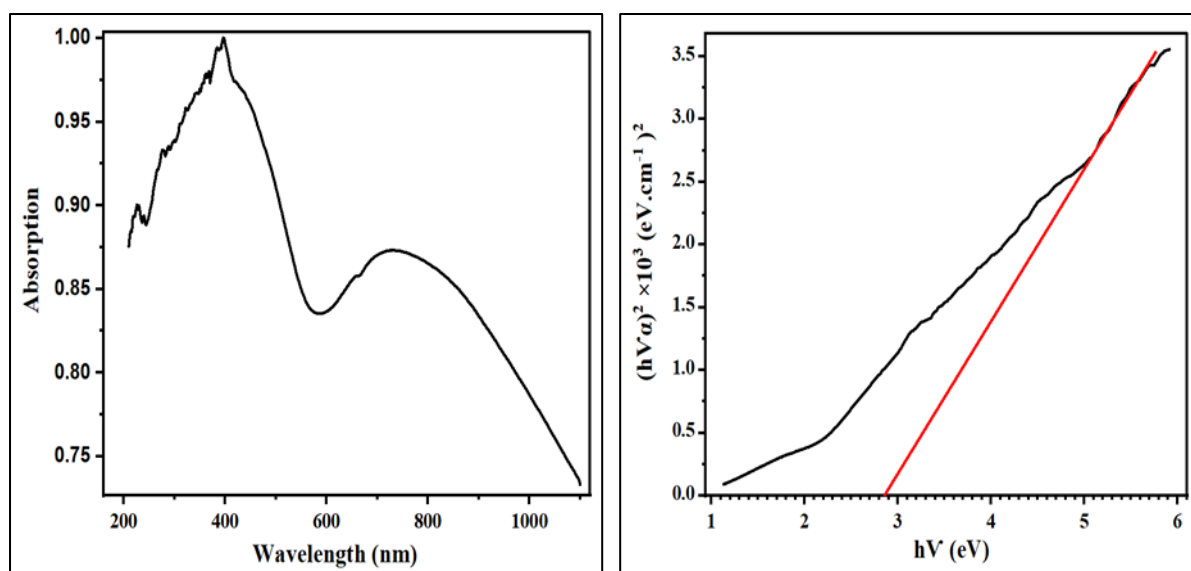


Figure 3: The UV-Vis spectra and E_g for $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ NPs

ANTIBACTERIAL ACTIVITY

The antibacterial activity of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles (NPs) was assessed using the agar diffusion method against *Staphylococcus aureus*, a Gram-positive bacterium commonly associated with infections (Figure 4). The synthesized nanoparticles demonstrated significant antibacterial efficacy, as evidenced by a 25 mm zone of inhibition (ZOI), shown in Figure 3. The notable antibacterial activity can be attributed to the synergistic effects of copper doping and the intrinsic properties of magnesium oxide. Copper ions (Cu^{2+}) are known to disrupt bacterial cell membranes by interacting with proteins and phospholipids, leading to structural damage and leakage of cellular contents. Additionally, MgO nanoparticles enhance this antibacterial effect by generating reactive oxygen species (ROS) under ambient conditions. These ROS, such as superoxide anions and hydroxyl radicals, cause oxidative stress, further damaging bacterial cells and inhibiting their growth.

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The combined mechanisms of membrane disruption by copper ions and ROS generation by MgO nanoparticles make $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ a highly effective antibacterial agent. The results suggest the potential application of these nanoparticles in biomedical fields, including wound dressings, coatings for medical devices, and antimicrobial packaging. This study highlights the importance of material engineering in enhancing antibacterial properties for targeted applications. Future investigations could explore the nanoparticles' efficacy against a broader spectrum of bacterial strains and their biocompatibility for practical applications.

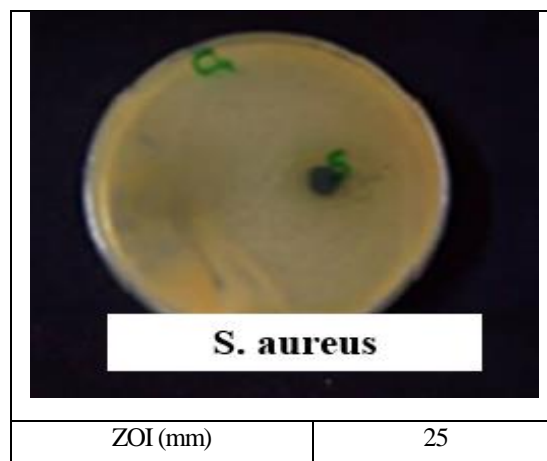


Figure 4: Antibacterial activity of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles against *Staphylococcus aureus*, demonstrating a 25 mm zone of inhibition (ZOI), indicating strong antibacterial efficacy

CONCLUSION

This study highlights the successful synthesis and characterization of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles, revealing significant enhancements in both optical and antibacterial properties due to copper doping. The reduction in bandgap energy to 2.89 eV enables the material to absorb visible light, enhancing its applicability in photocatalytic processes. This optical property improvement aligns with the growing demand for materials capable of utilizing solar energy effectively for environmental and biomedical applications.

The antibacterial evaluation using the agar diffusion method demonstrated a substantial zone of inhibition (ZOI) of 25 mm against *Staphylococcus aureus*. This enhanced antimicrobial activity can be attributed to the synergistic effects of copper ions and the generation of reactive oxygen species (ROS) by MgO. The interaction of ROS with bacterial membranes disrupts cell integrity, while copper's intrinsic antimicrobial properties further amplify the bactericidal effect. These characteristics position $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles as promising candidates for antibacterial coatings, wound dressings, and other biomedical applications.

The findings also emphasize the material's potential in photocatalysis for environmental remediation and disinfection under visible light conditions. Future studies could explore further optimization of doping levels and the incorporation of these nanoparticles into practical systems to enhance their effectiveness and applicability.

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The multifunctionality of $\text{Mg}_{0.97}\text{Cu}_{0.03}\text{O}$ nanoparticles—combining advanced optical properties and superior antibacterial activity—underscores their suitability for a range of applications, particularly in biomedicine and sustainable environmental technologies.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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