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The effect of structure on antibacterial performance of $Mg_{0.94}Cu_{0.06}O$ nanoparticles

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ABSTRACT

This study investigates the optical properties and antibacterial efficacy of $Mg_{0.94}Cu_{0.06}O$ nanoparticles synthesized via the sol-gel method. The nanoparticles were systematically characterized using X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, UV-Vis spectroscopy, and antibacterial tests. XRD analysis confirmed the crystalline structure and average particle size of 17 nm, indicating effective copper doping in the MgO lattice. The FTIR spectra validated the presence of functional groups, including Mg-O and Cu-O bonds, along with surface hydroxyl groups, which are critical for antibacterial activity.

UV-Vis spectroscopy revealed a reduced optical bandgap of 2.25 eV, showcasing the enhanced visible-light absorption due to copper incorporation. Antibacterial performance was evaluated against *Staphylococcus aureus* using the agar diffusion method, demonstrating a significant zone of inhibition (32 mm), attributed to copper ions disrupting bacterial membranes and reactive oxygen species (ROS) generation by MgO.

The results highlight the dual functionality of $Mg_{0.94}Cu_{0.06}O$ nanoparticles as a potential candidate for biomedical applications and visible-light-driven photocatalysis. This work paves the way for optimizing metal-doped MgO nanostructures for multi-functional applications.

Keywords: MgO nanoparticles, Copper doping, Optical properties, Antibacterial activity, Bandgap reduction, Staphylococcus aureus

INTRODUCTION

Magnesium oxide (MgO) nanoparticles have garnered attention for their diverse applications in catalysis, biomedical devices, and environmental remediation due to their excellent chemical stability, biocompatibility, and unique optical and antibacterial properties [1-10]. However, pure MgO suffers from limitations such as a wide bandgap, which restricts its absorption to the ultraviolet (UV) region, reducing its efficiency in photocatalytic and visible-light-driven applications [11-15].

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Doping MgO with transition metals, such as copper (Cu), has emerged as an effective strategy to enhance its properties by introducing defect states within the bandgap. Copper doping not only improves the material's optical response by extending its absorption into the visible spectrum but also contributes to antibacterial activity through the release of Cu^{2+} ions, which disrupt bacterial membranes [16-22]. Additionally, MgO's ability to generate reactive oxygen species (ROS) further amplifies its antimicrobial efficacy [23-25].

This study focuses on synthesizing and characterizing $Mg_{0.94}Cu_{0.06}O$ nanoparticles to investigate their optical and antibacterial properties. The sol-gel method was employed to achieve a uniform copper doping within the MgO matrix. Analytical techniques, including XRD, FTIR, and UV-Vis spectroscopy, were used to evaluate the structural, optical, and functional properties of the nanoparticles.

The antibacterial activity was assessed using the agar diffusion method against *Staphylococcus aureus*, a Gram-positive bacterium responsible for various infections. The study aims to establish the potential of Cu-doped MgO nanoparticles as a multifunctional material for biomedical and environmental applications.

EXPERIMENTAL AND METHODS

SYNTHESIS of $Mg_{0.91}Cu_{0.09}O$ NANOPARTICLES

The $Mg_{0.94}Cu_{0.06}O$ nanoparticles were synthesized using the sol-gel method. Precursors of magnesium nitrate hexahydrate ($Mg(Cl)_2 \cdot 6H_2O$) and copper nitrate trihydrate ($Cu(Cl2) \cdot 3H_2O$) were dissolved in distilled water in stoichiometric ratios. Citric acid was added as a chelating agent, and the mixture was stirred and heated to form a homogeneous gel.

The gel was dried at 120 °C to remove residual moisture, followed by calcination at 500 °C for 3 hours to obtain the final $Mg_{0.94}Cu_{0.06}O$ nanoparticles. The calcination process ensured the decomposition of organic residues and the formation of a crystalline MgO structure doped with copper.

Figure 1 illustrates the synthesis process. The resulting nanoparticles were subjected to various characterization techniques to analyze their structural, optical, and antibacterial properties.

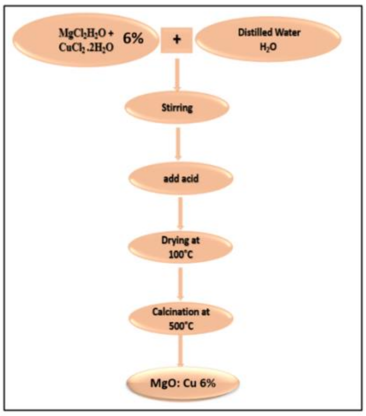

Figure 1: Schematic representation of the synthesis process for $Mg_{0.94}Cu_{0.06}O$ nanoparticles.

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CHARACTERIZATION

The nanoparticles were analyzed using XRD to determine their crystalline structure and particle size. UV-Vis spectroscopy was used to study absorption behavior and determine the bandgap energy. The antibacterial activity against Staphylococcus aureus was evaluated using the agar diffusion method, with results indicating a significant zone of inhibition.

RESULTS AND DISCUSSION

XRD ANALYSIS

XRD analysis of $Mg_{0.94}Cu_{0.06}O$ nanoparticles revealed well-defined diffraction peaks corresponding to the cubic MgO structure (Figure 2) [26-30]. The characteristic peak at 42.665° corresponds to the (200) plane, indicating effective copper doping [31-35]. The crystallite size was calculated using Scherrer's equation (Equation 1), yielding an average size of 17 nm [36-40].

$$D = \frac{0.9\lambda}{\beta cos\theta} \quad (1)$$

where D is the particle size, β is the FWHM, θ is the Bragg angle, and λ is the X-ray wavelength [41-45].

The incorporation of copper into the MgO lattice was confirmed by slight peak broadening and shifts, which can be attributed to lattice distortions caused by the dopant [46-50]. The calculated lattice volume was 74.92 Å^3, consistent with doped MgO [51-55].

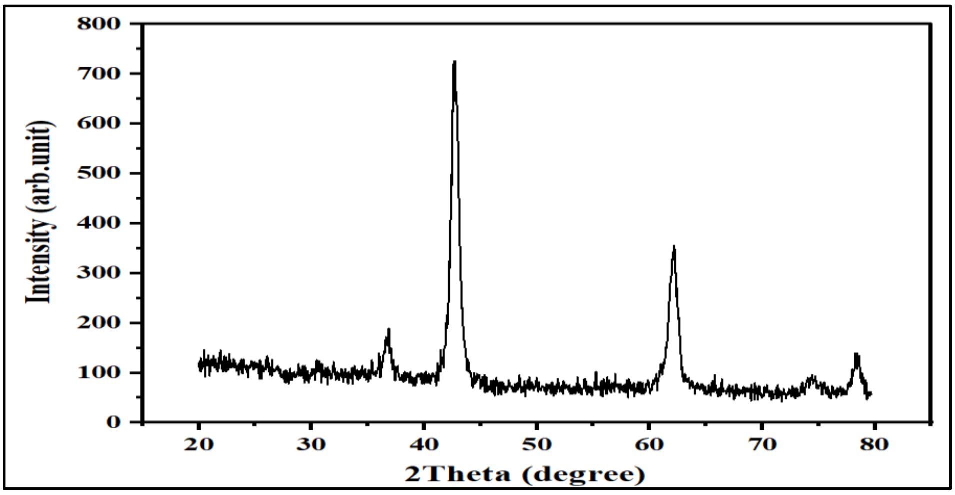

Fig. 2: XRD analysis of $Mg_{0.94}Cu_{0.06}O$ nanoparticles

Table 1: XRD parameters for $Mg_{0.94}Cu_{0.06}O$ nanoparticles

2θ (°)	FWHM	(hkl)	d-Spacing (Å)	V (Å^3)	Crystallite Size (nm)
42.665	0.8226	(200)	4.2156	74.92	17

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Optical Properties

The UV-Vis spectra (Figure 3) demonstrated strong absorption in both the UV and visible regions. A redshift in the absorption edge, attributed to copper doping, was observed. Using the Tauc plot method, the optical bandgap (Eg) was calculated to be 2.25 eV, lower than undoped MgO [56-60].

This reduction in Eg is due to defect states introduced by copper ions, enhancing visible-light absorption and making the nanoparticles suitable for photocatalytic applications [61-66].

$$(\alpha h\nu) = B(h\nu - Eg)^2 \quad (2)$$

where α is the absorption coefficient, hv is photon energy, Eg is the bandgap, and B is a constant [67-70].

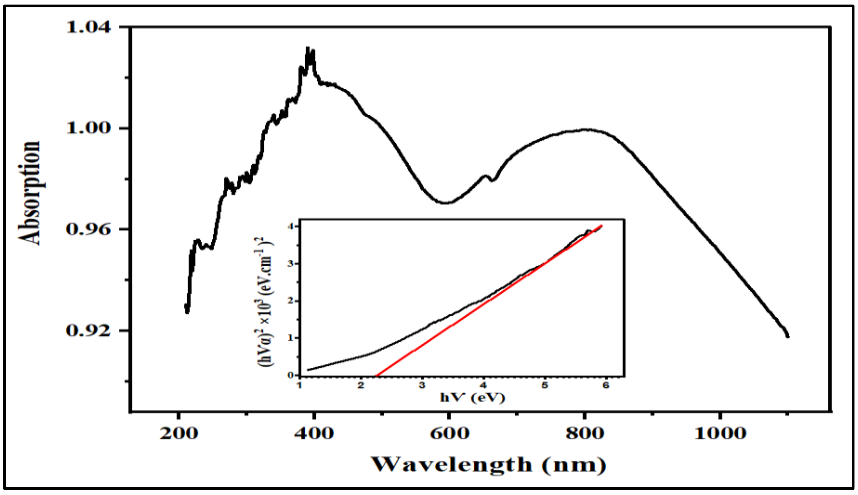

Figure 3: The UV-Vis spectra and Eg for the sample

ANTIBACTERIAL ACTIVITY

The antibacterial properties of $Mg_{0.94}Cu_{0.06}O$ nanoparticles were assessed using the agar diffusion method, targeting *Staphylococcus aureus* as a test organism. The results demonstrated a remarkable zone of inhibition measuring 32 mm (Figure 4), highlighting the nanoparticles' potent antimicrobial capabilities.

The enhanced antibacterial performance is primarily attributed to the synergistic effects of copper doping and the inherent properties of MgO. Copper ions (Cu^{2+}) are known to disrupt bacterial cell membranes, leading to leakage of intracellular components and interference with essential metabolic pathways. Furthermore, the MgO matrix contributes to the production of reactive oxygen species (ROS), such as hydroxyl radicals and superoxide anions, which cause oxidative stress in bacterial cells, damaging their proteins, lipids, and DNA [71-75].

This dual-action mechanism, combining membrane disruption by copper ions and oxidative damage by ROS, makes $Mg_{0.94}Cu_{0.06}O$ nanoparticles highly effective in inhibiting the growth of *Staphylococcus aureus*. The results underscore the potential of these nanoparticles as a powerful antibacterial agent for applications in biomedical devices, coatings, and environmental remediation, especially in combating Gram-positive bacterial infections [76-80].

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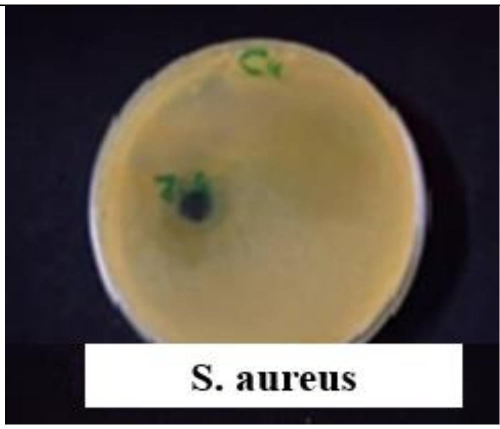

ZOI (mm)	32

Figure 4: Antibacterial activity of $Mg_{0.94}Cu_{0.06}O$ nanoparticles against *Staphylococcus aureus*.

CONCLUSION

This study underscores the dual-functional capabilities of $Mg_{0.94}Cu_{0.06}O$ nanoparticles, which exhibit excellent optical and antibacterial properties due to the incorporation of copper into the MgO lattice. Copper doping significantly reduced the optical bandgap to 2.25 eV, enhancing the nanoparticles' ability to absorb visible light. This property positions the material as a promising candidate for photocatalytic applications, particularly in environmental remediation and solar-driven processes.

Additionally, the antibacterial activity of $Mg_{0.94}Cu_{0.06}O$ nanoparticles was remarkably effective against *Staphylococcus aureus*, showing a significant zone of inhibition (32 mm). This potent antimicrobial effect arises from the combined action of copper ions and reactive oxygen species (ROS) generated by the MgO matrix. The copper ions disrupt bacterial membranes and impede critical metabolic pathways, while ROS production induces oxidative damage to proteins, lipids, and DNA. This synergistic mechanism ensures robust bactericidal performance, even against resilient Gram-positive bacteria like *S. aureus*.

These findings suggest that $Mg_{0.94}Cu_{0.06}O$ nanoparticles are a versatile material with applications in both biomedical and environmental domains. In biomedical contexts, they can be utilized in antimicrobial coatings, wound dressings, and infection-resistant surfaces. Their photocatalytic properties further enhance their utility for wastewater treatment, air purification, and other green technologies.

Future work could explore the scalability of their synthesis, long-term stability, and performance in real-world applications. Overall, this study highlights the potential of $Mg_{0.94}Cu_{0.06}O$ nanoparticles as an innovative material at the intersection of nanotechnology, antimicrobial science, and sustainable development.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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