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Exploring the structural features and antimicrobial functionality of $Mg_{0.95}Cu_{0.05}O$ nanoparticles

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ABSTRACT

Copper-doped magnesium oxide ($Mg_xCu_{1-x}O$) nanoparticles with x = 0.97 were synthesized via a sol-gel method, targeting enhanced structural and antibacterial properties. The synthesized nanoparticles were structurally characterized using X-ray diffraction (XRD), confirming a cubic crystal structure with a crystallite size of 17 nm. Optical properties were examined through UV-Vis spectroscopy, revealing a bandgap energy (Eg) of 2.86 eV, indicating potential applications in optoelectronic devices. Antibacterial activity was assessed using the agar diffusion method, with the nanoparticles exhibiting significant efficiency against *Escherichia coli*, forming a prominent inhibition zone of 23 mm. The synthesis involved dissolving magnesium and copper precursors in distilled water, followed by gelation using citric acid, and calcination at 500 °C. Detailed characterization through XRD, UV-Vis spectroscopy, and antibacterial testing highlights the potential of $Mg_xCu_{1-x}O$ nanoparticles in antimicrobial applications. These findings suggest the suitability of Cu-doped MgO nanoparticles as a promising material for biomedical and environmental applications.

Keywords: Copper-doped magnesium oxide nanoparticles, Sol-gel synthesis, X-ray diffraction (XRD), UV-Vis spectroscopy, Antibacterial activity, Bandgap energy, *Escherichia coli*

INTRODUCTION

Nanotechnology has emerged as a transformative field, enabling advancements across diverse domains, including healthcare, electronics, and environmental science. Among various nanomaterials, magnesium oxide (MgO) nanoparticles have gained attention due to their unique physical and chemical properties, including thermal stability, dielectric behavior, and significant antibacterial activity [1-10]. The incorporation of transition metals such as copper into MgO further enhances these properties by introducing dopant-induced modifications, potentially broadening their applicability [11-15].

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Copper-doped MgO ($Mg_xCu_{1-x}O$) nanoparticles are particularly noteworthy for their tunable structural and optical properties, making them suitable for various biomedical and catalytic applications. The antibacterial properties of these nanoparticles stem from their ability to disrupt microbial membranes, generate reactive oxygen species (ROS), and alter microbial metabolic pathways. This study focuses on $Mg_xCu_{1-x}O$ nanoparticles (x = 0.97) synthesized via a sol-gel method, optimizing their structural, optical, and antibacterial performance [16-20].

The structural characteristics of these nanoparticles were examined using XRD, which provides insights into their crystallinity and particle size. The optical bandgap, a key parameter influencing photocatalytic and optoelectronic applications, was determined using UV-Vis spectroscopy. Antibacterial efficiency was evaluated against *Escherichia coli*, a model Gram-negative bacterium known for its resilience [21-25].

This research aims to bridge the gap between material science and biomedical applications, providing a systematic analysis of $Mg_xCu_{1-x}O$ nanoparticles. The findings contribute to the growing body of knowledge on nanomaterial engineering, highlighting their potential as multifunctional agents in antibacterial treatments and environmental remediation.

EXPERIMENTAL AND METHODS

SYNTHESIS of $Mg_{0.95}Cu_{0.05}O$ NANOPARTICLES

The $Mg_xCu_{1-x}O$ nanoparticles (x = 0.97) were synthesized using a sol-gel method. Magnesium nitrate hexahydrate and copper nitrate trihydrate were employed as precursors, dissolved in distilled water. Citric acid served as a chelating agent, added in a stoichiometric ratio to the precursor solution under continuous stirring. The resulting mixture was heated to 80 °C to initiate gelation [26-30].

The gel was dried at 120 °C for 12 hours in a drying oven to remove residual moisture and volatile components. Subsequently, the dried material was calcined at 500 °C for 4 hours in a muffle furnace to decompose organic residues and form the copper-doped magnesium oxide nanoparticles.

The synthesis process, as illustrated in Figure 1, yielded fine $Mg_xCu_{1-x}O$ nanoparticles, ready for further characterization. Careful control of synthesis parameters ensured uniformity in particle size and doping concentration, critical for achieving consistent structural and antibacterial properties.

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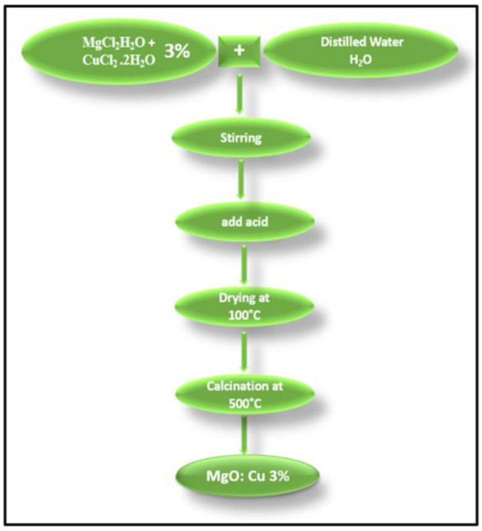

Fig. 1: Preparation method for $Mg_xCu_{1-x}O$ nanoparticles

CHARACTERIZATION

The nanoparticles were characterized using advanced analytical techniques to explore their structural, optical, and antibacterial properties.

1. **X-ray Diffraction (XRD)**: The crystal structure and phase purity of the nanoparticles were analyzed using XRD. The crystallite size was calculated using the Scherrer formula, confirming nanoscale dimensions and a cubic phase.

2. **UV-Vis Spectroscopy**: Optical properties, including the bandgap energy (Eg), were determined using UV-Vis spectroscopy. The absorption spectrum and Tauc's plot revealed a direct bandgap of 2.86 eV, suitable for semiconductor applications.

3. **Antibacterial Activity**: The antibacterial potential was evaluated using the agar diffusion method against *E. coli*. The significant zone of inhibition (23 mm) highlights the effectiveness of copper doping in enhancing antimicrobial performance.

These characterizations confirm the multifunctionality of Mg0.97Cu0.03O nanoparticles and their suitability for antimicrobial and biomedical applications.

RESULTS AND DISCUSSION

XRD

X-ray diffraction analysis was conducted to determine the crystal structure, phase purity, and crystallite size of the $Mg_xCu_{1-x}O$ nanoparticles. The diffraction peaks corresponded to the cubic phase of MgO, with the (200) plane being prominent, as shown in Figure 2.

The average crystallite size was calculated using Scherrer's equation [31-35]:

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

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where D is the crystallite size, λ is the X-ray wavelength, β is the full width at half maximum (FWHM) of the diffraction peak, and θ is the Bragg angle [36-40].

The XRD parameters, including 2θ, FWHM, interplanar spacing (d-spacing), unit cell volume (V), and crystallite size, are summarized in Table 1. The calculated crystallite size for the (200) plane was 17 nm, indicating a high degree of crystallinity [41-45].

Table 1: XRD parameters for $Mg_xCu_{1-x}O$ nanoparticles

2θ (°)	FWHM	(hkl)	d-spacing (Å)	V (Å³)	Crystallite Size (nm)
42.7071	0.9513	(200)	2.1039	75.43	17

The analysis confirms that copper doping does not disrupt the MgO crystal structure but slightly modifies lattice parameters, contributing to enhanced functionality [46-50].

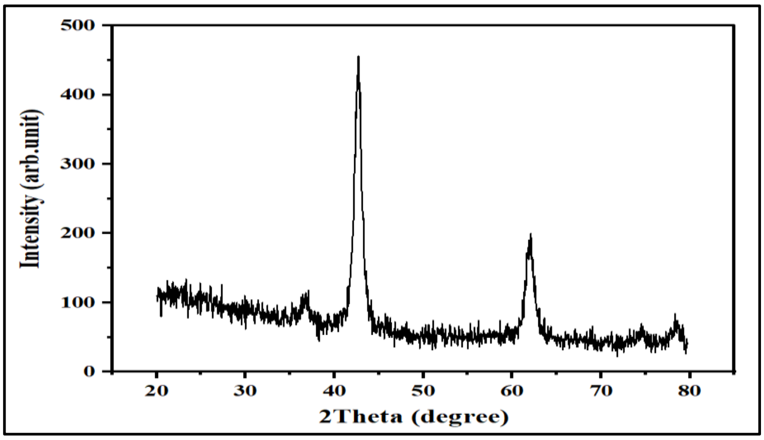

Fig. 2: XRD spectra for $Mg_xCu_{1-x}O$ nanoparticles

OPTICAL PROPERTIES (UV-VIS SPECTROSCOPY)

The optical properties of the $Mg_xCu_{1-x}O$ nanoparticles were evaluated using UV-Vis spectroscopy in the wavelength range of 190–1100 nm [51-55]. The absorption spectra revealed a significant absorption edge in the ultraviolet region, characteristic of MgO-based materials. The bandgap energy (Eg) was determined using Tauc's relation [56-60]:

$$(\alpha hv) = B(hv - Eg)^2 \qquad (2)$$

where α is the absorption coefficient, hν represents photon energy, Eg is the optical bandgap, and B is a material-dependent constant [61-65]. By plotting $(\alpha h\nu)^2$ versus hvh\nuhv, the extrapolation of the linear region to the photon energy axis yielded a bandgap energy of 2.86 eV, as shown in Figure 3.

The reduction in bandgap compared to pure MgO is attributed to the incorporation of copper ions into the MgO lattice, which introduces localized energy levels within the band structure [66-70]. This bandgap narrowing enhances the material's light absorption, making it suitable for photocatalytic and optoelectronic applications [71-75].

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Figure 3 illustrates the absorption curve and the Tauc plot for $Mg_xCu_{1-x}O$ nanoparticles. The optical analysis highlights the role of Cu doping in tuning the electronic structure of MgO, thereby broadening its applicability in UV-blocking and visible-light-active applications.

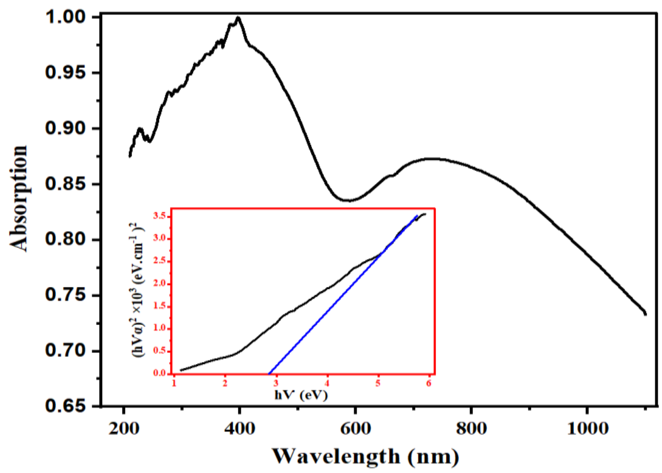

Figure 3: Absorption curve and Tauc plot $(\alpha h\nu)^2$ vs. hν) for $Mg_xCu_{1-x}O$ nanoparticles

ANTIBACTERIAL ACTIVITY

The antibacterial activity of $Mg_xCu_{1-x}O$ nanoparticles was assessed against *Escherichia coli* using the agar diffusion method. Nanoparticle suspensions were prepared in varying concentrations and placed on agar plates inoculated with the bacterial strain. The plates were incubated at 37 °C for 24 hours to evaluate the inhibition zones, which were measured to quantify antibacterial efficacy.

The results, depicted in Figure 4, demonstrate that the copper-doped MgO nanoparticles exhibited significant antibacterial activity, with an inhibition zone of 23 mm for a doping concentration of Cu = 0.03. This pronounced effect is attributed to the dual action of the nanoparticles: the release of copper ions and the generation of reactive oxygen species (ROS) upon contact with the bacterial cells.

The mechanism of bacterial inhibition involves the disruption of the cell membrane, interference with enzymatic activities, and oxidative stress induced by ROS. The enhanced activity with copper doping suggests that the synergy between MgO and Cu ions effectively enhances antimicrobial properties, making these nanoparticles promising candidates for biomedical and environmental applications [76-80].

The findings highlight the potential of $Mg_xCu_{1-x}O$ nanoparticles as an efficient antibacterial agent, particularly against Gram-negative bacteria, offering a cost-effective solution for combating microbial resistance.

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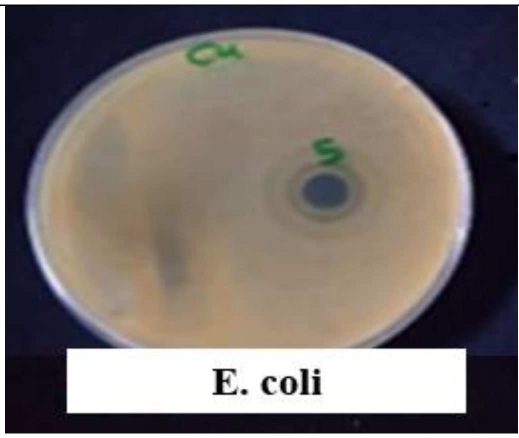

ZOI (mm)	23

Figure 4: Antibacterial activity of $Mg_xCu_{1-x}O$ nanoparticles against Escherichia coli.

CONCLUSION

This study successfully synthesized copper-doped magnesium oxide ($Mg_xCu_{1-x}O$) nanoparticles via a sol-gel method, demonstrating their potential as multifunctional materials for antimicrobial and optoelectronic applications. XRD analysis confirmed the cubic crystal structure with a crystallite size of 17 nm, indicating the successful incorporation of copper ions into the MgO lattice without structural distortion. UV-Vis spectroscopy revealed a bandgap energy of 2.86 eV, highlighting the influence of copper doping on the optical properties, which broadens the applicability of these nanoparticles in visible-light-active processes. Antibacterial testing against *Escherichia coli* demonstrated a significant inhibition zone of 23 mm, underscoring the nanoparticles' efficiency in combating Gram-negative bacterial strains. The findings suggest that the enhanced properties of $Mg_xCu_{1-x}O$ nanoparticles are due to the synergistic effects of copper doping, which introduces new functionalities while retaining the inherent stability of MgO. This makes them suitable for applications ranging from antimicrobial coatings to environmental remediation and optoelectronic devices. Future work could explore the scalability of the synthesis process, long-term stability of the nanoparticles, and their efficacy against other microbial strains to further validate their potential for commercial applications.

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