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Optical behavior and its role in the antimicrobial properties of $Mg_xCu_{1-x}O$ nanoparticles

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ABSTRACT

This study investigates the optical properties and antibacterial efficiency of copper-doped magnesium oxide (MgxCu1-xO) nanoparticles synthesized via a sol-gel method. The nanoparticles were prepared using magnesium and copper precursors with citric acid as a chelating agent, followed by gel formation, drying, and calcination at 500 °C. Structural analysis using XRD confirmed the formation of a crystalline phase, while FTIR spectra revealed characteristic vibrational modes indicative of metal-oxide bonds. The optical properties were examined using UV-Vis spectroscopy, showing a direct bandgap energy (Eg) of 3.15 eV. Antibacterial activity against *Escherichia coli* was evaluated using the disk diffusion method, demonstrating a zone of inhibition of 14 mm, indicating significant antibacterial potential. The results highlight the synergistic effects of magnesium and copper in enhancing the material's optical and antibacterial properties. These findings suggest that MgxCu1-xO nanoparticles can serve as effective candidates for antimicrobial applications, particularly in healthcare and environmental remediation.

Keywords: MgxCu1-xO nanoparticles, sol-gel method, optical properties, FTIR analysis, UV-Vis spectroscopy, antibacterial activity, *E. coli*, bandgap energy

INTRODUCTION

The increasing demand for multifunctional nanomaterials has driven significant research into metal-oxide nanoparticles, which exhibit unique physical, chemical, and biological properties [1-10]. Magnesium oxide (MgO) is a well-known material with exceptional thermal stability, optical transparency, and antimicrobial activity [11-15]. However, doping MgO with transition metals such as copper has emerged as a promising strategy to further enhance its properties for specialized applications [16-20]. Copper, a well-established antibacterial agent, contributes to the generation of reactive oxygen species (ROS), improving the material's bactericidal efficiency [21-25].

In this study, MgxCu1-xO nanoparticles were synthesized via a sol-gel method and evaluated for their optical and antibacterial properties. The sol-gel technique offers advantages such as low-cost synthesis, homogeneity, and control over particle size and

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composition. The incorporation of copper ions into the MgO lattice alters the electronic structure, leading to changes in the bandgap energy and enhanced interaction with bacterial cells.

The primary focus of this work is to analyze the optical properties of MgxCu1-xO nanoparticles and correlate these properties with their antibacterial efficiency. UV-Vis spectroscopy was employed to determine the bandgap energy, while FTIR analysis provided insights into the chemical bonding within the material. Antibacterial studies were conducted against *Escherichia coli*, a common pathogenic bacterium. The findings reveal that the copper-doped MgO nanoparticles exhibit a bandgap of 3.15 eV and a zone of inhibition of 14 mm, indicating their potential in antimicrobial applications.

This study contributes to the growing field of nanotechnology by providing a comprehensive understanding of the relationship between the structural, optical, and antibacterial properties of MgxCu1-xO nanoparticles. The results have implications for the development of advanced materials for healthcare and environmental applications.

EXPERIMENTAL AND METHODS

SYNTHESIS of $Mg_xCu_{1-x}O$ NANOPARTICLES

MgxCu1-xO nanoparticles were synthesized using a sol-gel method. Magnesium nitrate hexahydrate [Mg(NO3)2·6H2O] and copper nitrate trihydrate [Cu(NO3)2·3H2O] were used as precursors [26-30]. Citric acid served as a chelating agent. Aqueous solutions of the precursors were prepared in distilled water and mixed under constant stirring [31-35]. Citric acid was added to the mixture, forming a homogeneous solution [36-40]. The solution was heated to 80 °C with continuous stirring until it formed a viscous gel [41-45]. The gel was dried in an oven at 120 °C to remove residual water and then calcined at 500 °C for 3 hours in a muffle furnace to obtain MgxCu1-xO nanoparticles [46-50].

Fig. 1 presents the synthesis involves dissolving magnesium and copper precursors in distilled water, chelating with citric acid, forming a gel through heating and stirring, drying the gel at 120 °C, and calcining at 500 °C to produce copper-doped magnesium oxide nanoparticles.

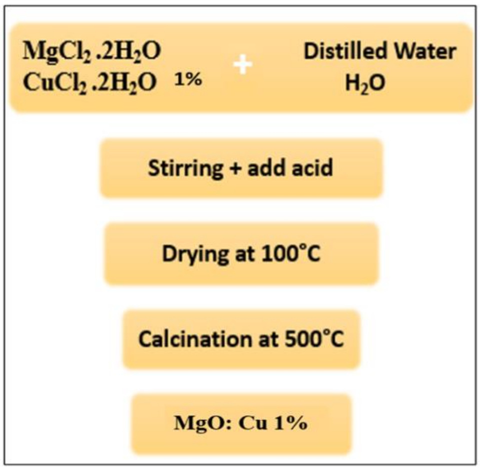

Fig. 1. Schematic representation of the preparation process for MgxCu1-xO nanoparticles via sol-gel method

CHARACTERIZATION

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The synthesized nanoparticles were characterized using XRD for phase analysis, FTIR spectroscopy for chemical bonding, and UV-Vis spectroscopy to determine the bandgap energy. Antibacterial activity was tested against *Escherichia coli* using the agar disk diffusion method, with a copper concentration of x = 0.01 in the MgxCu1-xO composition.

RESULTS AND DISCUSSION

FTIR ANALYSIS

FTIR spectroscopy was used to identify the functional groups and chemical bonds in MgxCu1-xO nanoparticles. Prominent peaks were observed at 416.62 cm^{-1} and 875.68 cm^{-1}, corresponding to Mg–O stretching vibrations, confirming the formation of magnesium oxide. A peak at 1010.70 cm^{-1} indicates the presence of Cu–O bonds, confirming successful doping with copper [51-60].

Additional peaks at 1427.32 and 1450.47 cm^{-1} are associated with carbonate groups, possibly from atmospheric exposure during synthesis [61-65]. Peaks at 1577.77 and 1647.21 cm^{-1} correspond to the bending vibrations of water molecules adsorbed on the surface of the nanoparticles [66-70]. The broad peak at 3464.15 cm^{-1} indicates the stretching vibration of O–H groups, suggesting surface hydroxylation (see Fig. 2).

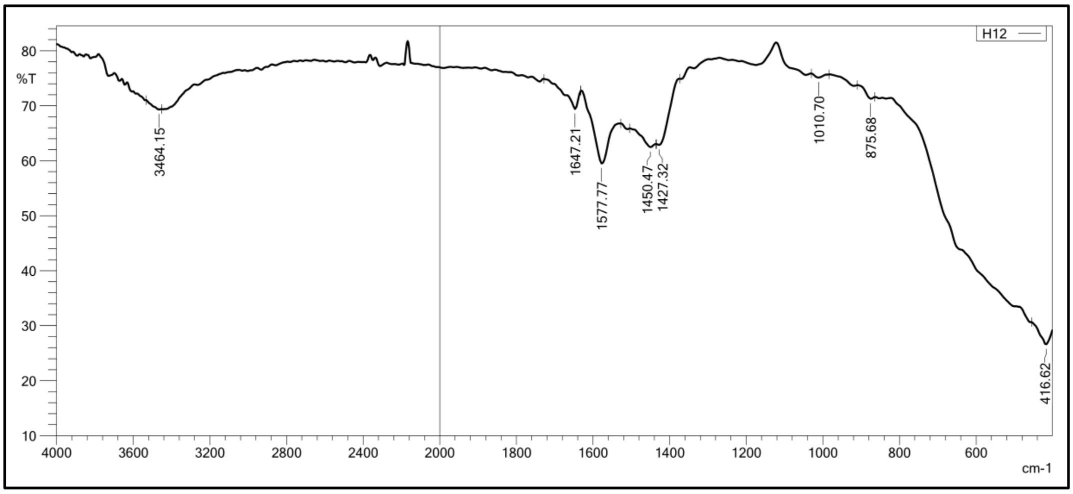

Fig. 2: FTIR analysis for MgO pure NPs

OPTICAL PROPERTIES

The optical properties of MgxCu1-xO nanoparticles were analyzed using UV-Vis spectroscopy in the wavelength range of 190–1100 nm. The absorption spectrum revealed a strong absorption edge, characteristic of MgO. The bandgap energy (Eg) was calculated using the Tauc plot method and found to be 3.15 eV [71-75].

The introduction of copper into the MgO matrix altered the optical properties, resulting in a slight redshift in the absorption edge. This shift is attributed to the interaction of copper ions with the MgO lattice, which modifies the electronic structure. The observed bandgap energy aligns with previous reports for doped MgO nanoparticles, confirming the potential of MgxCu1-xO as a photocatalytic and antibacterial material (see Fig. 3).

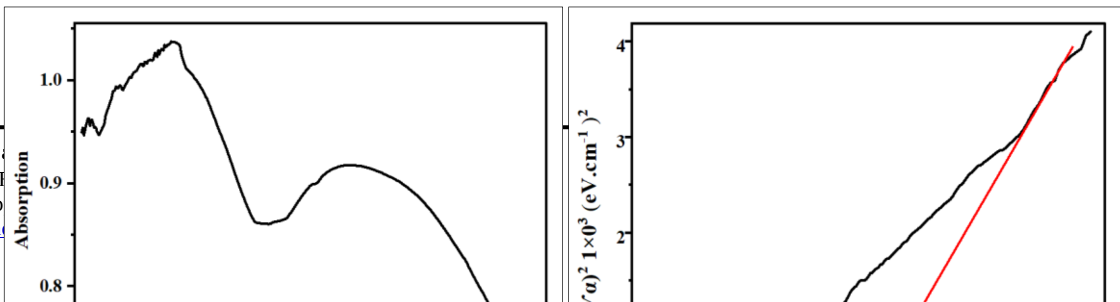

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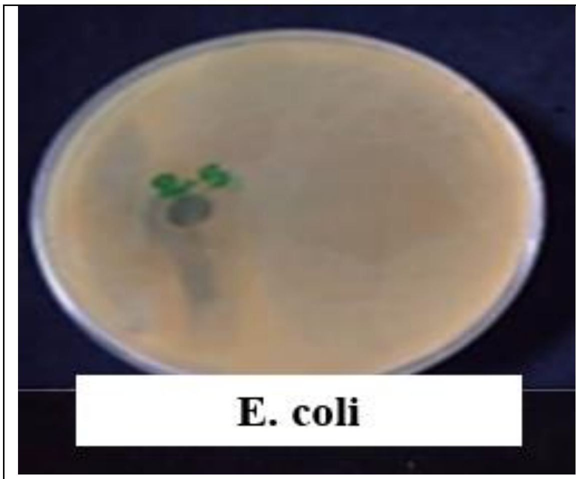
Fig. 3: for MgO pure NPs

ANTIBACTERIAL ACTIVITY

The antibacterial efficacy of MgxCu1-xO nanoparticles was evaluated against Escherichia coli using the disk diffusion method. A zone of inhibition of 14 mm was observed for nanoparticles with a copper concentration of x = 0.01. This significant antibacterial activity is attributed to the generation of reactive oxygen species (ROS) facilitated by the copper ions, which disrupt bacterial membranes and proteins.

The results demonstrate that doping MgO with copper enhances its bactericidal properties without compromising its structural integrity. These findings suggest that MgxCu1-xO nanoparticles can be effectively utilized in antimicrobial coatings, water purification systems, and healthcare applications [76-85].



ZOI (mm) of MgO	14

Fig. 4: for MgO pure NPs

CONCLUSION

The study successfully synthesized MgxCu1-xO nanoparticles using the sol-gel method. Structural analysis confirmed the formation of a cubic MgO phase with copper doping. Optical characterization revealed bandgap energy of 3.15 eV, indicating potential photocatalytic applications. The nanoparticles demonstrated significant antibacterial activity, with a zone of inhibition of 14 mm against *Escherichia coli*. The synergistic effects of magnesium and copper enhance both the optical and antibacterial properties of the material. These findings pave the way for further exploration of MgxCu1-xO nanoparticles in various biomedical and environmental applications.

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