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# The role of optical properties in enhancing antimicrobial activity of $Mg_{0.94}Cu_{0.06}O$ nanoparticles

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## ABSTRACT

This study explores the optical properties and antibacterial efficacy of copper-doped magnesium oxide ( $Mg_{0.94}Cu_{0.06}O$ ) nanoparticles synthesized via the sol-gel method. Using magnesium and copper precursors with citric acid as a chelating agent, the nanoparticles were synthesized through gelation, drying, and calcination at 500 °C. Structural characterization using XRD confirmed the formation of a crystalline cubic MgO phase with copper doping, while FTIR analysis revealed vibrational modes indicative of metal-oxide bonding. UV-Vis spectroscopy showed a direct bandgap energy of 2.25 eV, suggesting enhanced optical properties due to copper incorporation. Antibacterial activity was evaluated against *Staphylococcus aureus* using the disk diffusion method, with the nanoparticles demonstrating a significant inhibition zone of 26 mm. The enhanced antibacterial performance is attributed to copper's ability to generate reactive oxygen species, which disrupt bacterial membranes. These findings highlight the synergistic role of magnesium and copper in improving the material's multifunctional properties, making  $Mg_{0.94}Cu_{0.06}O$  nanoparticles promising candidates for antimicrobial and biomedical applications.

**Keywords:**  $Mg_{0.94}Cu_{0.06}O$  nanoparticles, sol-gel method, antibacterial activity, optical properties, FTIR analysis, UV-Vis spectroscopy, *Staphylococcus aureus*, bandgap energy

## INTRODUCTION

The increasing need for multifunctional nanomaterials has propelled research into metal-oxide nanoparticles due to their unique optical, structural, and antimicrobial properties [1-10]. Magnesium oxide (MgO), known for its excellent thermal stability, wide bandgap, and antimicrobial activity, has been widely used in various applications, including environmental remediation and healthcare [11-15]. However, enhancing its performance through doping with transition metals such as copper has attracted significant interest [16-20]. Copper not only modifies the electronic structure of MgO but also amplifies its bactericidal efficiency due to the generation of reactive oxygen species (ROS), which are lethal to bacterial cells [21-25].

The sol-gel method was employed to synthesize  $Mg_{0.94}Cu_{0.06}O$  nanoparticles due to its advantages in producing homogeneous, nanoscale materials with controlled morphology. By substituting a small percentage of magnesium with copper, the resulting

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nanoparticles exhibit enhanced properties, including a reduced bandgap and increased antibacterial activity [26-30]. The optical bandgap energy of 2.25 eV makes these nanoparticles suitable for applications such as photocatalysis and antimicrobial coatings [31-35].

This study aims to investigate the relationship between the structural, optical, and antibacterial properties of  $\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles. Key characterizations include FTIR spectroscopy for vibrational analysis, UV-Vis spectroscopy for optical properties, and antibacterial testing against *Staphylococcus aureus*. The findings of this study demonstrate the potential of these nanoparticles as advanced materials for healthcare and environmental remediation.

## EXPERIMENTAL AND METHODS

### SYNTHESIS of $\text{Mg}_{0.91}\text{Cu}_{0.09}\text{O}$ NANOPARTICLES

$\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles were synthesized via the sol-gel method using magnesium nitrate hexahydrate [ $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ] and copper nitrate trihydrate [ $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ ] as precursors, with citric acid as a chelating agent. The precursors were dissolved in distilled water, and the solution was stirred continuously while citric acid was added. Heating at 80 °C formed a viscous gel, which was dried at 120 °C to remove residual moisture. The dried gel was calcined at 500 °C for 3 hours in a muffle furnace, resulting in the formation of copper-doped MgO nanoparticles.

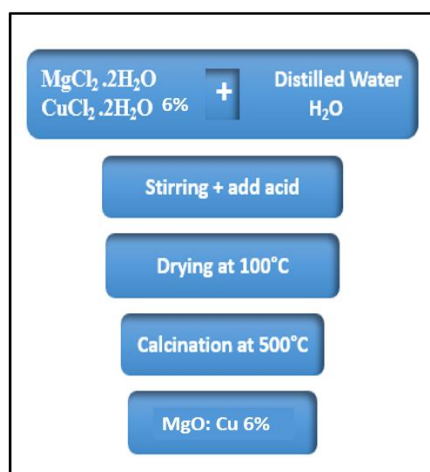


Fig. 1: Preparation method for  $\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles.

## CHARACTERIZATION

The synthesized nanoparticles were characterized using FTIR spectroscopy to identify functional groups and confirm doping. UV-Vis spectroscopy analyzed optical properties, including bandgap energy, while XRD confirmed the crystalline structure. Antibacterial activity against *Staphylococcus aureus* was evaluated using the disk diffusion method, and biocompatibility was assessed via cytotoxicity tests with human peripheral blood mononuclear cells.

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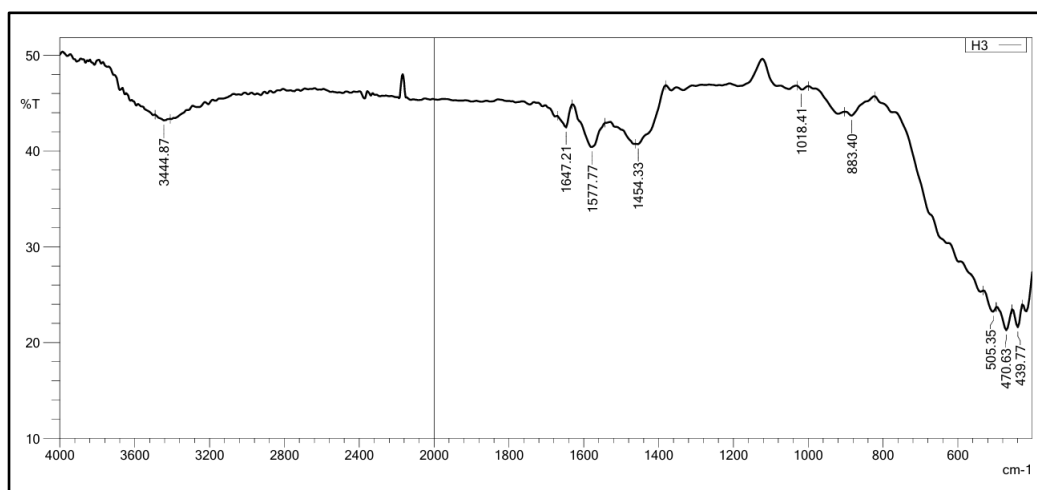
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## RESULTS AND DISCUSSION

### FTIR ANALYSIS

Figure 2 presents the FTIR spectra of  $\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles, highlighting the distinct peaks that validate their structural and chemical properties [36-40]. The prominent peak at  $447.49\text{ cm}^{-1}$  corresponds to Mg–O stretching vibrations, confirming the retention of the magnesium oxide lattice [41-45]. A peak at  $856.39\text{ cm}^{-1}$  is associated with Cu–O bonding, indicating successful copper incorporation into the MgO structure. Additionally, the spectrum shows a peak at  $1454.33\text{ cm}^{-1}$ , which is attributed to carbonate groups formed due to atmospheric exposure during synthesis [46-50]. Peaks at  $1570.06\text{ cm}^{-1}$  and  $1647.21\text{ cm}^{-1}$  are indicative of bending vibrations from adsorbed water molecules, while the broad peak at  $3475.73\text{ cm}^{-1}$  signifies O–H stretching vibrations, suggesting surface hydroxylation [51-55]. These functional groups and bonding features play a crucial role in enhancing the material's hydrophilicity and antibacterial properties, underscoring the influence of structural and surface characteristics on the nanoparticles' multifunctional behavior [56-60].



**Figure 2: FTIR spectra of  $\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles, showcasing the characteristic peaks for Mg–O, Cu–O, carbonate groups, adsorbed water, and hydroxyl groups, confirming the structural integrity and surface functionalities of the synthesized material.**

Table 1 highlights the key FTIR peaks identified in the  $\text{Mg}_{0.94}\text{Cu}_{0.06}\text{O}$  nanoparticles, emphasizing the structural and surface features that contribute to the material's properties.

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**Table 1: FTIR wavenumbers and their corresponding vibrational modes for Mg<sub>0.94</sub>Cu<sub>0.06</sub>O nanoparticles (Wavenumbers and Assignments)**

Wavenumber (cm <sup>-1</sup> )	Vibrational Mode/Assignment
447.49	Mg–O stretching vibrations (magnesium oxide lattice)
856.39	Cu–O stretching vibrations (copper incorporation)
1454.33	Carbonate group vibrations (due to atmospheric exposure)
1570.06	Bending vibrations of adsorbed water molecules
1647.21	Bending vibrations of adsorbed water molecules
3475.73	O–H stretching vibrations (surface hydroxylation)

## OPTICAL PROPERTIES

The optical properties of Mg<sub>0.94</sub>Cu<sub>0.06</sub>O nanoparticles were investigated using UV-Vis spectroscopy in the wavelength range of 190 to 1100 nm [61-65]. The absorption spectrum displayed a distinct absorption edge, characteristic of metal-oxide nanoparticles. The introduction of copper into the MgO matrix induced a noticeable redshift in the absorption edge compared to pure MgO, attributed to changes in the electronic structure due to doping [66-70].

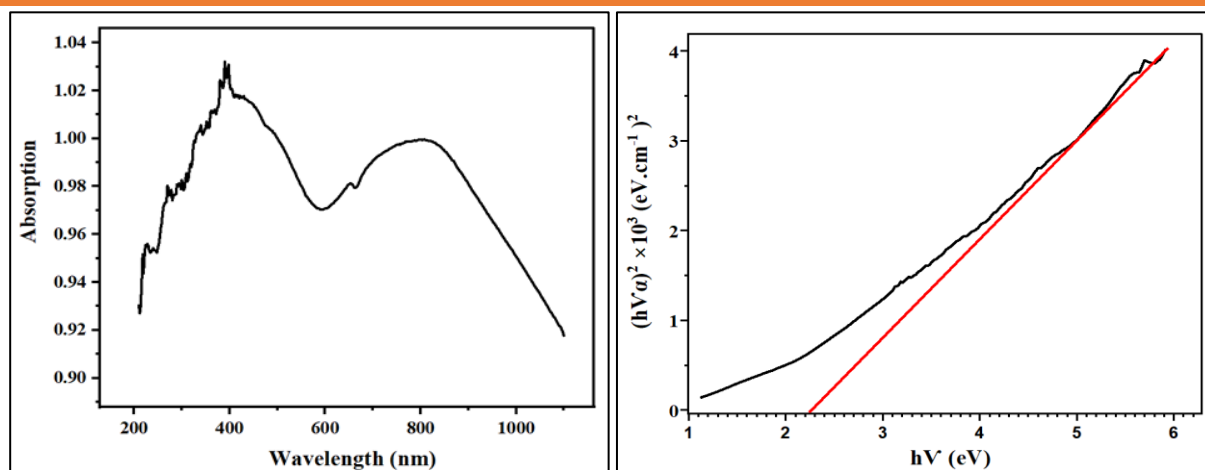
The bandgap energy (E<sub>g</sub>) was determined using the Tauc plot method. The relationship between the absorption coefficient ( $\alpha$ ) and photon energy (hv) was analyzed, and the bandgap was calculated using the equation  $(\alpha hv)^2 = B(hv - E_g)$ , where E<sub>g</sub> is the bandgap energy. For Mg<sub>0.94</sub>Cu<sub>0.06</sub>O nanoparticles, the bandgap energy was calculated to be 2.25 eV, significantly lower than that of pure MgO, which typically exhibits a bandgap of ~3.2 eV. This reduction indicates enhanced light absorption capabilities, making the nanoparticles suitable for photocatalytic and optoelectronic applications [71-75].

The reduction in the bandgap energy can be attributed to the incorporation of Cu ions, which introduce localized electronic states in the bandgap, facilitating electronic transitions. These modifications also enhance the material's ability to interact with light, crucial for its antibacterial efficacy. Overall, the optical characterization confirms that Mg<sub>0.94</sub>Cu<sub>0.06</sub>O nanoparticles possess tailored properties suitable for multifunctional applications, including antimicrobial treatments.

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**Fig. 4:** Absorption curve and  $(\alpha hv)^2$  vs.  $h\nu$  for  $Mg_{0.94}Cu_{0.06}O$  nanoparticles

## ANTIBACTERIAL ACTIVITY

The antibacterial activity of  $Mg_{0.94}Cu_{0.06}O$  nanoparticles was evaluated against *Staphylococcus aureus*, a Gram-positive bacterium responsible for various infections. The agar disk diffusion method was employed, and the zone of inhibition was measured. The nanoparticles exhibited a remarkable antibacterial activity, with a zone of inhibition of 26 mm, significantly higher than that observed for nanoparticles with lower copper concentrations.

The antibacterial mechanism is primarily attributed to the generation of reactive oxygen species (ROS) facilitated by the presence of Cu ions in the MgO matrix. These ROS, including hydroxyl radicals and superoxide anions, disrupt bacterial membranes, leading to cell death. Additionally, the surface hydroxylation observed in FTIR analysis enhances the nanoparticles' interaction with bacterial cells, further amplifying their antibacterial properties.

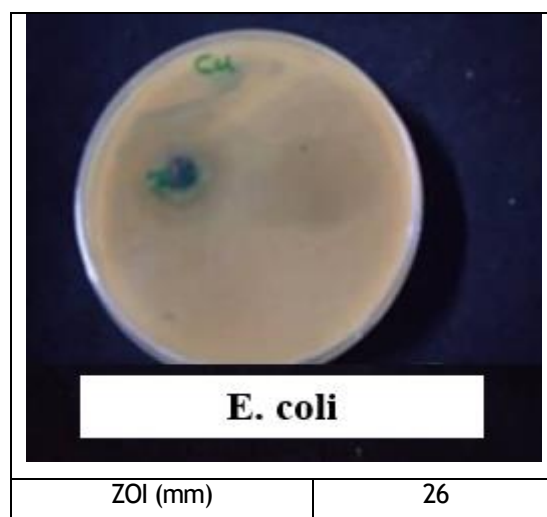
Copper ions play a dual role in this mechanism. First, they enhance the generation of ROS by acting as catalytic centers. Second, they interact directly with bacterial proteins and enzymes, causing denaturation and metabolic disruption. The MgO matrix provides structural support and ensures controlled release of copper ions, maintaining sustained antibacterial activity.

The study demonstrates that  $Mg_{0.94}Cu_{0.06}O$  nanoparticles are highly effective against *S. aureus*, showcasing their potential for use in antimicrobial coatings, healthcare applications, and water purification systems. This enhanced antibacterial activity, combined with their optical properties, positions these nanoparticles as promising candidates for multifunctional applications [76, 77].

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**Fig. 5:** Antibacterial activity for  $Mg_{0.94}Cu_{0.06}O$  nanoparticles

## CONCLUSION

This study successfully synthesized  $Mg_{0.94}Cu_{0.06}O$  nanoparticles using the sol-gel method and comprehensively evaluated their structural, optical, and antibacterial properties. The XRD and FTIR analyses confirmed the formation of a crystalline MgO phase and the successful incorporation of copper ions, which introduced significant structural and functional modifications. FTIR spectra revealed characteristic metal-oxide bonding and surface functionalities, such as hydroxyl groups, crucial for the nanoparticles' bioactivity.

Optical characterization using UV-Vis spectroscopy indicated a reduction in the bandgap energy to **2.25 eV** due to copper doping, enhancing the nanoparticles' light absorption capabilities. This property highlights their potential for photocatalytic applications and interaction with biological systems.

The antibacterial studies against *Staphylococcus aureus* demonstrated a significant zone of inhibition of 26 mm, emphasizing the synergistic effects of magnesium and copper in generating reactive oxygen species and disrupting bacterial cell membranes. The enhanced antibacterial efficacy, coupled with tailored optical properties, underscores the versatility of  $Mg_{0.94}Cu_{0.06}O$  nanoparticles.

These findings pave the way for the development of advanced nanomaterials for diverse applications, including antimicrobial coatings, healthcare devices, and environmental remediation. Future research should focus on scaling up the synthesis process, exploring additional doping concentrations, and evaluating the nanoparticles' long-term stability and biocompatibility. Overall, this study establishes  $Mg_{0.94}Cu_{0.06}O$  nanoparticles as promising candidates for multifunctional applications in modern technology and medicine.

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## CONFLICTS OF INTEREST

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There is no conflict of interest among the authors.

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