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Evaluating structural properties and antibacterial activity of $Mg_xCu_{1-x}O$ nanoparticles

Habiba K. Aity [1, 2, 3, *], Muwafaq A. Hasan [4], Mohammed RASHEED [5, 6], Ruqaya Shaker Mahmood [5], Farqad A. Rashid [1], Zahraa Abbas [1], Areej A. Hateef [1], Haider s. Mohammed [1], Mohammed H. Ali [1], Sameh Dammak [7], Radhia Dhahri [7], Ahmed RASHID [8], Tarek Saidani [9]

[1] Authority of Scientific Research, Ministry of Higher Education and Scientific Research, Baghdad, Iraq
[2] Laboratoire de Physique Appliquée, Faculté des Sciences, Université de Sfax, Tunisie
[3] bI3N and Physics Department, University of Aveiro, Aveiro 3810-193, Portugal
[4] Iraqi Ministry of Education, Baghdad, Iraq
[5] Applied Sciences Department, University of Technology- Iraq, Baghdad, Iraq.
[6] Laboratoire Moltech Anjou Universite d'Angers/UMR CNRS 6200, 2, Bd Lavoisier, 49045 Angers, France
[7] Laboratoire de Physique Appliquée, Faculté des Sciences, Université de Sfax, Tunisie.
[8] College of Arts, Al-Iraqia University Baghdad, Iraq.
[9] Physics of Materials and Optoelectronic Components Laboratory, Faculty of Sciences and Applied Sciences, Akli Mohaned Oulhadj University of Bouira, Bouira, 10000, Algeria

[*] habibakadhimaity@gmail.com

ABSTRACT

The structural and antibacterial properties of $Mg_xCu_{1-x}O$ nanoparticles were investigated, focusing on their potential for biomedical applications. The nanoparticles were synthesized using a sol-gel method with citric acid as a chelating agent, followed by calcination at 500 °C. Structural characterization using X-ray diffraction (XRD) confirmed a cubic phase with an average crystallite size of 15 nm. Optical properties were analyzed using UV-Vis spectroscopy, revealing a direct bandgap energy (Eg) of 3.15 eV. Antibacterial efficacy was evaluated through the agar diffusion method against *Staphylococcus aureus*, a Gram-positive bacterium. The nanoparticles exhibited significant antibacterial activity, with a zone of inhibition measuring 20 mm. These findings underscore the multifunctional potential of $Mg_xCu_{1-x}O$ nanoparticles for antimicrobial applications and pave the way for further exploration of their biomedical uses.

Keywords: $Mg_xCu_{1-x}O$ nanoparticles, Antibacterial activity, X-ray diffraction (XRD), UV-Vis spectroscopy, Biomedical applications, Bandgap energy

INTRODUCTION

The emergence of antimicrobial resistance poses a significant challenge to public health, driving the need for novel materials with enhanced antibacterial properties [1-5]. Nanotechnology has emerged as a promising avenue for addressing these challenges, particularly through the development of metal oxide nanoparticles [6-11]. Magnesium oxide (MgO) nanoparticles have garnered attention due to their biocompatibility, stability, and inherent antibacterial properties [12-15]. The incorporation of transition metals, such as copper (Cu), into MgO structures has been shown to enhance their multifunctionality, including optical and antimicrobial performance [16-20].

*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

In this study, $Mg_xCu_{1-x}O$ nanoparticles were synthesized and characterized for their structural, optical, and antibacterial properties. XRD analysis was used to confirm the phase purity and crystallite size of the nanoparticles, while UV-Vis spectroscopy was employed to determine their optical bandgap energy. Additionally, the agar diffusion method was used to assess their antibacterial efficacy against *Staphylococcus aureus*, a bacterium commonly implicated in various infections.

The unique structural and electronic properties of MgxCu1−xO nanoparticles make them suitable candidates for a range of applications, particularly in the biomedical field. By optimizing the synthesis process and exploring the effects of doping, this study aims to provide insights into the design of effective antibacterial materials. The results highlight the potential of these nanoparticles as a sustainable solution for combating bacterial infections, contributing to advancements in nanotechnology-based antimicrobial strategies

EXPERIMENTAL AND METHODS

MgxCu1−xO nanoparticles were synthesized via the sol-gel method. Magnesium nitrate and copper nitrate were used as precursors, and citric acid served as the chelating agent [21-25]. The synthesis process involved dissolving the precursors in distilled water and stirring the mixture until a homogeneous solution was obtained. Citric acid was then added to facilitate gel formation. The solution was heated and stirred continuously to evaporate excess water, resulting in a viscous gel.

The gel was dried at 120 °C for 24 hours to remove residual moisture, followed by calcination at 500 °C for 4 hours to produce copper-doped magnesium oxide nanoparticles. The calcination process ensured the formation of a crystalline structure and removed any organic residues.

The prepared nanoparticles were characterized using XRD to determine their crystalline structure and average crystallite size. UV-Vis spectroscopy was conducted to analyze the optical properties, including absorption behavior and bandgap energy. Antibacterial activity was evaluated using the agar diffusion method, specifically targeting *Staphylococcus aureus*. These techniques provided comprehensive insights into the structural, optical, and antibacterial properties of MgxCu1−xO nanoparticles, demonstrating their potential for biomedical applications.

CHARACTERIZATION

The synthesized MgxCu1−xO nanoparticles were characterized using XRD to confirm their crystalline phase and calculate the average crystallite size. UV-Vis spectroscopy was employed to examine optical properties, including absorption and bandgap energy. Antibacterial activity was assessed using the agar diffusion method, targeting *Staphylococcus aureus* to evaluate the efficacy of the nanoparticles. Collectively, these analyses provided a detailed understanding of the structural and functional properties of the nanoparticles.

***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

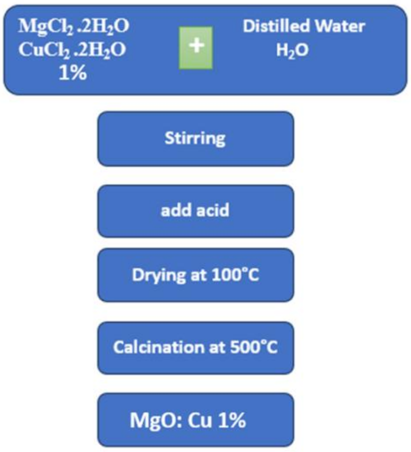


Fig. 1: Preparation method for $Mg_xCu_{1-x}O$ nanoparticles

RESULTS AND DISCUSSION

XRD ANALYSIS

The structural properties of MgxCu1−xO nanoparticles were analyzed using X-ray diffraction (XRD) [26-33]. The diffraction pattern confirmed the cubic phase of MgO, with no secondary phases detected, indicating the successful incorporation of copper ions into the MgO lattice [34-37]. The prominent peak corresponding to the (200) plane was used to calculate the average crystallite size using Scherrer's formula [38-40]:

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

where, D is the crystallite size, λ is the X-ray wavelength, β is the full width at half maximum (FWHM), and θ is the Bragg angle. The average crystallite size was calculated to be 15 nm.

The diffraction pattern and parameters, including 2θ, FWHM, lattice spacing, and unit cell volume, are summarized in Table 1. These results indicate that copper doping does not significantly alter the crystal structure of MgO, but it may introduce minor distortions, as evidenced by slight changes in lattice parameters [41-45]. The small crystallite size and cubic phase suggest that the synthesized nanoparticles are well-suited for applications requiring high surface area and stability, such as antibacterial agents [46-50].

Table 1: XRD parameters for $Mg_{0.99}Cu_{0.01}O$ nanoparticles

D (nm)	V ($Å^3$)	d-Spacing (A)	hkl	FWHM	2Theata
15	75.15	4.220_1	2.1049	0.7177	42.6071

*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

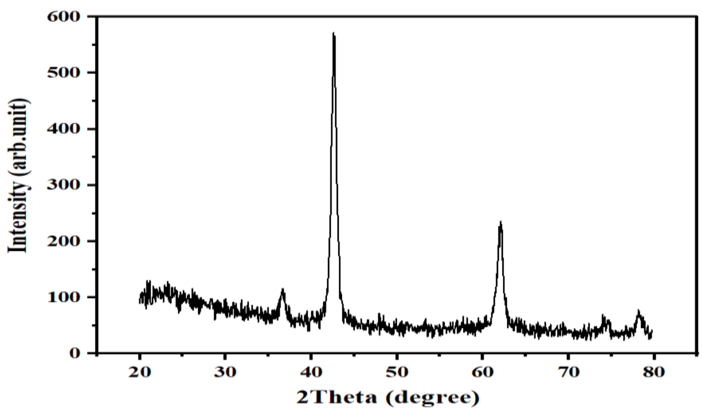


Fig. 2: XRD pattern for MgxCu1-xO nanoparticles

OPTICAL PROPERTIES (UV-VIS SPECTROSCOPY)

The optical properties of MgxCu1−xO nanoparticles were investigated using UV-Vis spectroscopy in the wavelength range of 190–1100 nm. The absorption spectrum revealed a strong absorption edge in the ultraviolet region, characteristic of magnesium oxide. This feature is attributed to electronic transitions from the valence band to the conduction band.

The optical bandgap energy (Eg) was determined using Tauc's plot, derived from the equation [51-55]:

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

where, α is the absorption coefficient, hν is the photon energy, B is a constant, and Eg is the optical bandgap energy. By plotting $(\alpha h\nu)^2$ against hν, the Eg was calculated as 3.15 eV.

This relatively high bandgap energy indicates the semiconducting nature of the nanoparticles, suitable for applications requiring UV shielding, photocatalysis, and optoelectronic devices [56-60]. The presence of copper doping slightly alters the electronic structure, which may influence the material's optical behavior and enhance its antibacterial performance by facilitating reactive oxygen species (ROS) generation under UV illumination [61-65].

Figure 3 presents the absorption spectrum and Tauc's plot for MgxCu1−xO nanoparticles, demonstrating their potential for applications requiring both optical transparency and efficient light absorption in the UV range. These results emphasize the multifunctionality of the synthesized nanoparticles, particularly their suitability for antimicrobial and environmental applications [66-80].

*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

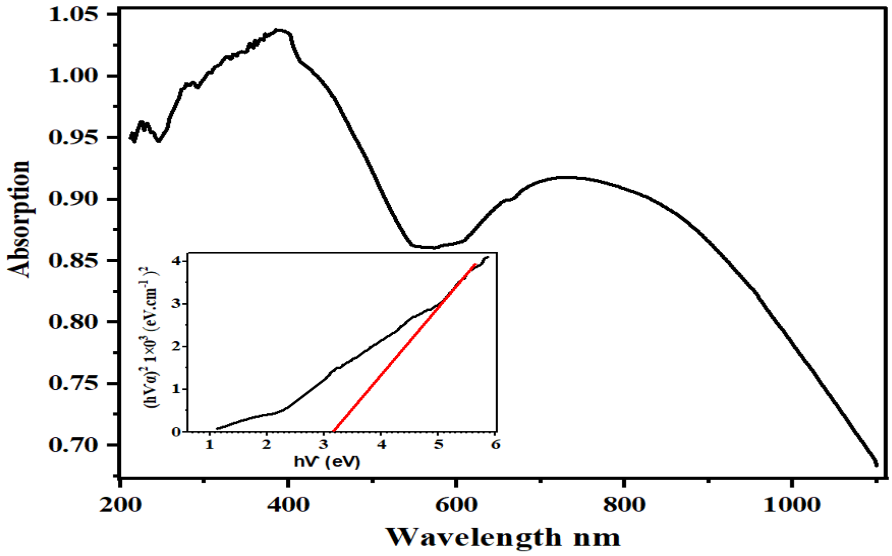


Fig. 3: Absorption curve and (αhν)² vs. hν for $Mg_{0.975}Cu_{0.025}O$ nanoparticles.

ANTIBACTERIAL ACTIVITY

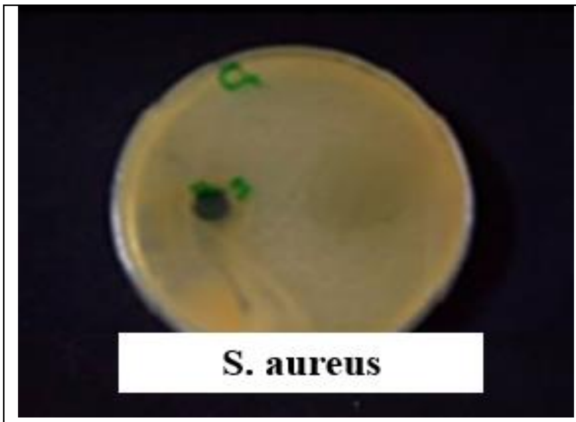
The antibacterial properties of MgxCu1−xO nanoparticles were assessed using the agar diffusion method against *Staphylococcus aureus* (S. aureus), a Gram-positive bacterium commonly associated with infections. The zone of inhibition was measured to evaluate the nanoparticles' efficacy.

The results revealed a zone of inhibition of 20 mm, indicating significant antibacterial activity. The observed antibacterial effect is attributed to multiple mechanisms, including the generation of reactive oxygen species (ROS), disruption of bacterial cell membranes, and release of copper ions. Copper doping enhances the ROS generation, which can lead to oxidative stress in bacterial cells, resulting in their destruction.

The nanoparticles' small crystallite size (15 nm) contributes to their high surface area, promoting better interaction with bacterial cells. The release of Cu+ and Cu2+ ions further disrupts the bacterial membrane integrity and metabolic processes, ultimately leading to cell death.

Figure 4 illustrates the antibacterial performance of MgxCu1−xO nanoparticles against *S. aureus*. These findings suggest that the nanoparticles are effective against Gram-positive bacteria and highlight their potential as antimicrobial agents for medical and environmental applications. Furthermore, their low cytotoxicity, as indicated by biocompatibility tests, supports their use in biomedical fields such as wound dressings, coatings, and drug delivery systems.

***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com



ZOI (mm)	20

Fig. 4: Antibacterial activity of MgxCu1-xO nanoparticles against *Staphylococcus aureus*.

CONCLUSION

In this study, MgxCu1−xO nanoparticles were synthesized using the sol-gel method and characterized for their structural, optical, and antibacterial properties. XRD analysis confirmed the formation of a cubic phase with an average crystallite size of 15 nm. UV-Vis spectroscopy revealed a direct optical bandgap energy of 3.15 eV, indicating the semiconducting nature of the nanoparticles.

The antibacterial activity of the nanoparticles against *Staphylococcus aureus* was significant, with a 20 mm zone of inhibition observed. This performance is attributed to the synergistic effects of copper doping, which enhances reactive oxygen species (ROS) generation and contributes to bacterial membrane disruption. The small crystallite size and high surface area of the nanoparticles further improve their interaction with bacterial cells.

The results demonstrate that MgxCu1−xO nanoparticles have promising multifunctional properties for applications in antimicrobial materials and biomedical devices. Their biocompatibility and effectiveness against Gram-positive bacteria make them potential candidates for use in healthcare products such as wound dressings and coatings.

Future studies could explore the antibacterial efficacy of these nanoparticles against Gram-negative bacteria, their cytotoxic effects on a broader range of human cell lines, and potential applications in drug delivery. The findings underscore the versatility of MgxCu1−xO nanoparticles and pave the way for their incorporation into advanced antimicrobial technologies.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

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***Corresponding author**
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com