

Examining the Structural Characteristics and Antibacterial Efficiency of MgO pure Nanoparticles

Aasim Jasim Hussein^{1*}

¹ Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

* Aasim.jasim@uoanbar.edu.iq

ABSTRACT

This work examines the structural and antibacterial characteristics of sol-gel-synthesized pure magnesium oxide (MgO) nanoparticles for medicinal applications. A bandgap of 4.95 eV was found in UV-Vis and fluorescence spectroscopy of optical characteristics, including fluorescence absorption. XRD investigation validated the cubic crystal structure of MgO nanoparticles with a 13-nm crystallite size. Nanoparticles were biocompatible with human peripheral blood mononuclear cells and showed no cytotoxicity. Agar diffusion was used to test antibacterial activity against Gram-negative bacterium *Escherichia coli* (E. coli). A 13-mm zone of inhibition showed great antibacterial activity. MgO nanoparticles have antibacterial activity, making them a promising biomedical and antibacterial candidate. This study also reveals how nanoparticle size and surface area determine antibacterial activity, suggesting they might combat bacterial infections despite antimicrobial resistance.

Keywords: Medical applications, NPs, E. coli, zone of inhibition, antibacterial activity

INTRODUCTION

Antibiotic-resistant bacteria imperil global health, requiring innovative bacterial infection therapies. Nanotechnology, especially nanomaterials, may solve this. The large surface area to volume ratio and higher reactivity of nanoparticles make them effective against germs. Due to their capacity to destroy bacterial cell walls and produce ROS, magnesium oxide (MgO) nanoparticles are of interest.

Biocompatible, non-toxic, and eco-friendly MgO nanoparticles are suitable for wound healing and medicine administration. Many investigations have demonstrated MgO nanoparticles destroy Gram-positive and Gram-negative bacteria. Researchers have explored doping or enhancing manufacturing techniques to increase antibacterial efficacy and usage. Sol-gel-synthesized pure MgO nanoparticles are examined for structural and antibacterial characteristics. The sol-gel technique regulates nanoparticle size and form and is inexpensive. In this work, MgO nanoparticles' bandgap, fluorescence, and antibacterial activity against E. coli, a commonly studied Gram-negative bacterium, are evaluated. This study links the structural properties and antibacterial activity of MgO nanoparticles, suggesting their relevance in treating bacterial infections.

*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

MATERIALS AND METHODS

SYNTHESIS OF MgO NPs

Synthesis of sol-gel MgO NPs. Analytical-grade reagents, such as $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ and $\text{C}_6\text{H}_8\text{O}_7$, were acquired from Sigma-Aldrich and utilized without purification. Citric acid was added to a 100 mL solution of $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ in distilled water as a chelating agent. Heat to 80°C removed superfluous water from the mixture. The solution formed a thick gel with magnetic stirring. After drying at 120°C to eliminate moisture, the gel was calcined at 500°C for 3 hours to yield pure MgO nanoparticles. Sol-gel-synthesised MgO nanoparticles have good dispersion and crystalline shapes, making them promising candidates for antibacterial and medicinal applications.

As shown in Fig. 1, the synthesis method requires dissolving MgCl_2 and citric acid in distilled water, then heating to 80°C to eliminate moisture. After stirring to create a gel, the mixture is dried at 120°C and calcined at 500°C to produce magnesium oxide nanoparticles.

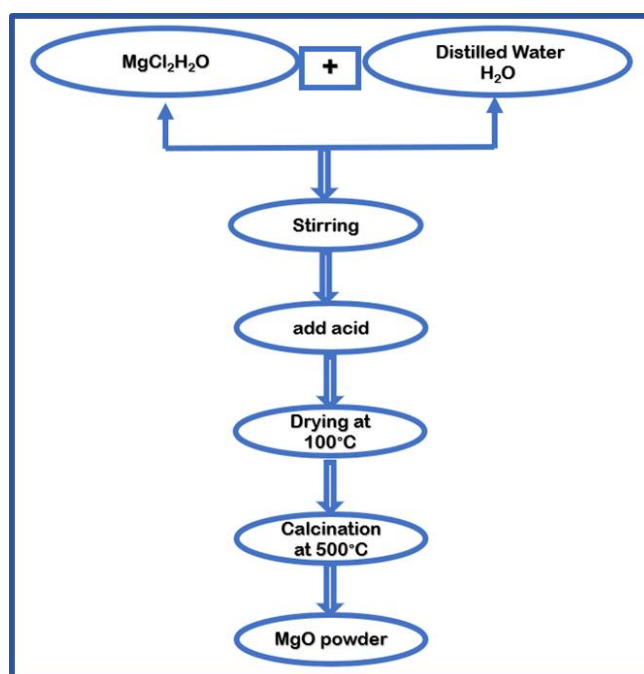


Fig. 1. MgO NPs preparation

CHARACTERIZATION

X-ray diffraction (XRD) confirmed the crystal structure and estimated particle size, UV-Vis and fluorescence spectroscopy examined optical properties, and agar diffusion assessed antibacterial activity of the synthesized nanoparticles. To determine biocompatibility for biomedical applications, human peripheral blood mononuclear cells were tested for nanoparticle cytotoxicity. The antibacterial capabilities were evaluated against Gram-negative bacterium *Escherichia coli* (*E. coli*), which causes illness.

*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

RESULTS AND DISCUSSION

XRD PATTERN OF MgO NANOPARTICLES

XRD measurement revealed MgO nanoparticles' crystalline structure. Pure MgO nanoparticles' XRD pattern showed face-centered cubic (FCC) structural peaks. The cubic phase of MgO is shown by the diffraction peaks at 37.007° , 42.857° , 68.307° , 74.457° , and 78.557° , which correspond to the (111), (200), (220), (311), and (222) crystal planes. The diffraction pattern showed significant nanoparticle crystallinity.

From the peak in the (200) plane, Scherrer's equation estimated the nanoparticles' average crystallite size. The computed crystallite size was 13 nm, showing nanoparticles are nanoscale, which supports their improved antibacterial activities. Sharp and well-defined XRD peaks indicated extremely crystalline nanoparticles.

The large surface area and reactivity of MgO nanoparticles allow them to interact with bacterial cells, increasing their antibacterial efficacy. XRD examination validated the fabrication of pure MgO nanoparticles with a well-defined crystalline structure, making them appropriate for antibacterial and biological applications (see Fig. 2).

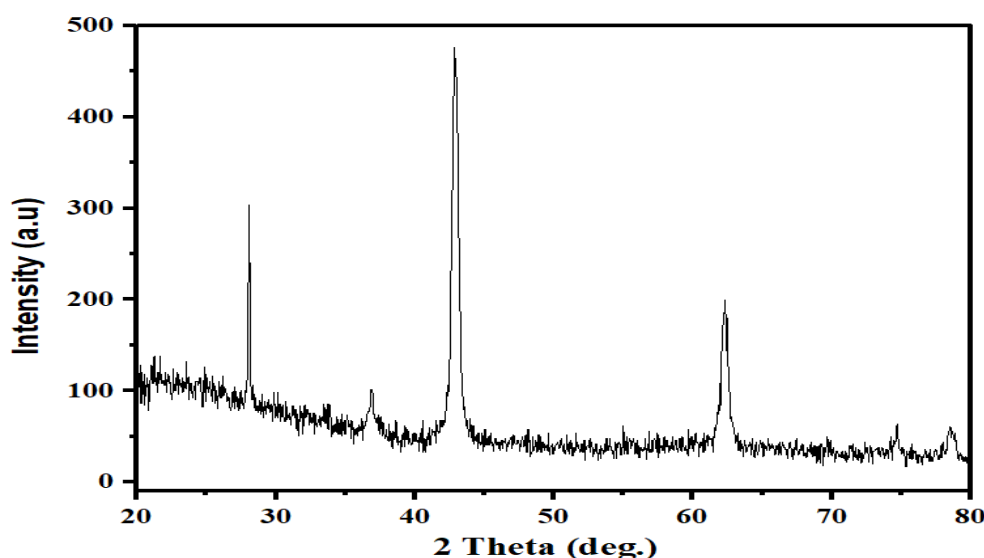


Fig. 2. MgO XRD diffractograms

Scherer's approach in Eq. 1 determined the average size of pure and doped nanoparticles from the (200) XRD peak [15].

$$D_{sc} = \frac{0.9 \cdot \lambda}{\beta \cdot \cos \theta} \quad (1)$$

where particle size (Dave), full width at half maximum (FWHM), Bragg angle of (200) peak (θ), and wavelength (λ) are the factors. Table 1 shows that MgO averages 18 nm and MgO averages 13 nm.

Table 1. MgO XRD parameters

2Theata	FWHM	hkl	d-Spacing (A)	Crystallite size (nm)
42.9113	0.53460	200	2.10591	13.8304

*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

Antibacterial activity of MgO nanoparticles depends on their structure. MgO nanoparticles interact well with bacteria due to their high surface area to volume ratio. varied synthesis methods produce varied MgO nanoparticle morphologies and efficiency. Spherical, rod-shaped, or flower-like MgO nanoparticles are typical. Their antibacterial efficacy depends on particle size. Researchers found that smaller particle sizes had more surface area and reactivity, making them more antimicrobial.

OPTICAL PROPERTIES

UV-Vis spectroscopy was used to evaluate magnesium oxide (MgO) nanoparticle absorption throughout 190–1100 nm. This spectral range helps observe UV and visible areas, revealing materials' electronic transitions and optical properties.

MgO nanoparticles' UV-Vis absorption spectra showed different absorption peaks, usually in the UV region, due to electronic transitions from the valence band to the conduction band. The broad bandgap of MgO, roughly 4.95 eV for bulk MgO, explains its UV absorption, especially below 400 nm. However, particle size, morphology, and surface flaws may affect nanoparticle absorption, which may change the bandgap somewhat compared to bulk material.

Quantum size effects affect UV absorption spectra, which alter somewhat depending on MgO nanoparticle size. Due to the higher bandgap energy caused by smaller particles, the absorption edge typically shifts blue.

UV-Vis spectra may also be used to compute nanoparticle optical bandgap (E_g) using the Tauc plot approach, which assumes a straight transition model. This data is useful for photocatalysis, sensors, and antimicrobial coatings, where optical characteristics are crucial to performance.

Fig. 3 shows MgO nanostructures with energy band gaps (E_g) calculated using mathematical formulae (2). Equations are underneath:

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

For Eq. 2, E_g represents the optical bandgap, $h\nu$ represents photon energy, B is an invariable, and α measures absorption.

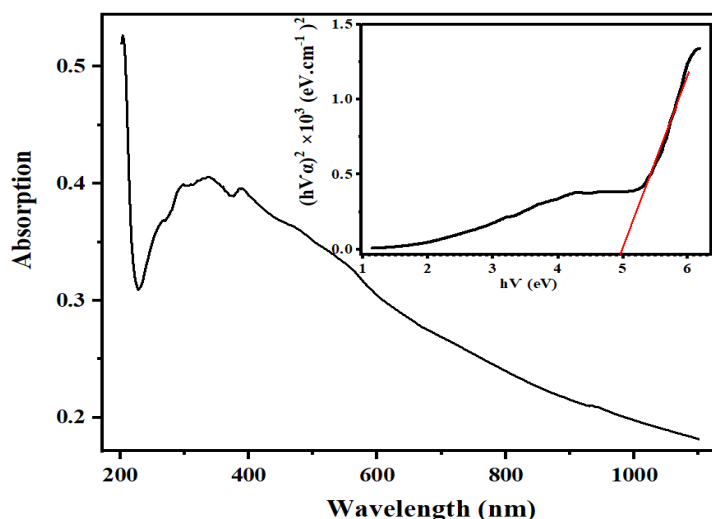


Fig. 3. MgO pure NPs absorption curve and $(\alpha h\nu)^2$ versus $(h\nu)$

*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

ANTIBACTERIAL PERFORMANCE

Agar diffusion was used to test the produced MgO nanoparticles' antibacterial activity. *E. coli*, a Gram-negative bacteria, was selected for this investigation because of its role in healthcare-associated illnesses. *E. coli* was put onto agar plates and MgO nanoparticles were added. For nanoparticle antibacterial effectiveness, the zone of inhibition (ZOI) width was assessed after 24 hours at 37°C. A ZOI of 13 mm surrounding nanoparticle-loaded wells indicated considerable antibacterial action.

MgO NPs attacking bacterial cells generate reactive oxygen species (ROS) when they interact with cell membranes. Microorganisms die when ROS destroy proteins, lipids, and nucleic acids. Nanoparticles' small size and huge surface area allow them to infiltrate bacterial cells, enhancing antibiotic action.

This study reveals that MgO nanoparticles are potent antibacterial agents, suggesting an antibiotic resistance treatment. MgO nanoparticles' biological applications' long-term stability, toxicity, and safety need more investigation (see Fig. 4).

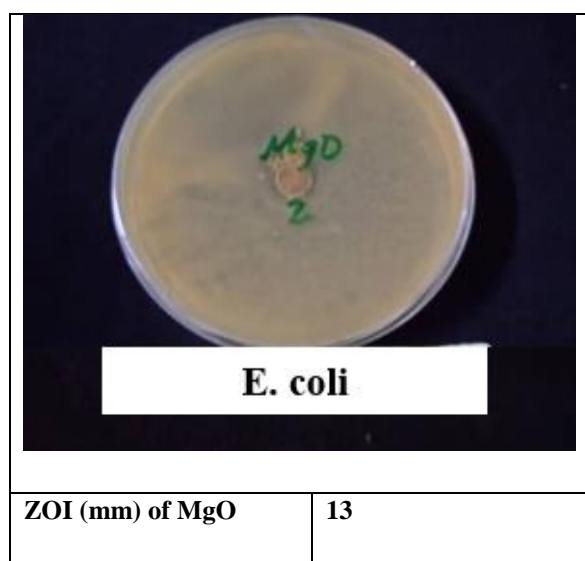


Fig. 4. Size of *E. coli* strain inhibitory zone and MgO NPs

CONCLUSION

In conclusion, this study demonstrates that magnesium oxide (MgO) nanoparticles synthesized via the sol-gel method exhibit significant antibacterial activity against *Escherichia coli*, a common Gram-negative bacterium. The XRD analysis confirmed the formation of highly crystalline MgO nanoparticles with a face-centered cubic (FCC) structure, and the crystallite size was determined to be approximately 13 nm. The optical properties, including a wide bandgap of 4.95 eV, suggest that the nanoparticles may have potential applications in photocatalytic and antibacterial treatments.

The results of the antibacterial tests showed a clear zone of inhibition of 13 mm, indicating that the MgO nanoparticles possess strong antibacterial properties. The mechanism of antibacterial activity is likely due to the generation of reactive oxygen species (ROS), which disrupt bacterial cell membranes and cause oxidative damage. The small particle size and high surface area of the nanoparticles further enhance their antibacterial efficacy.

Given their biocompatibility and strong antibacterial effects, MgO nanoparticles hold great promise for use in a wide range of biomedical applications, including drug delivery, wound healing, and as a component in antibacterial coatings. Further research is

*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

needed to optimize the synthesis process, evaluate the long-term stability and toxicity of MgO nanoparticles, and explore their potential for combating antibiotic-resistant bacterial infections.

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*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

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*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

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*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq

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*Corresponding author

Aasim Jasim Hussein,

Department of Biology, College of Education for Pure Sciences, University of Al-Anbar, Iraq

e-mail: Aasim.jasim@uoanbar.edu.iq