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The influence of structural properties on antibacterial potential of $Mg_{0.95}Fe_{0.03}O$ nanoparticles

Mohammed RASHEED [1, 2], Habiba K. Aity [3, 4, 5], Ketam K. Khudair [6], Ruqaya Shaker Mahmood [1], Farqad A. Rashid [3], Zahraa Abbas [3], Areej A. Hateef [3], Ahmed RASHID [7], Taha Rashid [7, 8, *]

[1] Applied Sciences Department, University of Technology- Iraq, Baghdad, Iraq.
[2] Laboratoire Moltech Anjou Universite d'Angers/UMR CNRS 6200, 2, Bd Lavoisier, 49045 Angers, France
[3] Authority of Scientific Research, Ministry of Higher Education and Scientific Research, Baghdad, Iraq
[4] Laboratoire de Physique Appliquée, Faculté des Sciences, Université de Sfax, Tunisie
[5] bI3N and Physics Department, University of Aveiro, Aveiro 3810-193, Portugal
[6] Department of medical laboratory techniques, Kufa Technical Institute, Al-Furat Al-Awsat Technical University31001, Kufa, Al-Najaf, Iraq
[7] College of Arts, Al-Iraqia University Baghdad, Iraq.
[8] School of Electrical Engineering, Universiti Teknologi Malaysia, UTM Johor Bahru, 81310, Johor Bahru, Malaysia

[*] tsiham95@gmail.com

ABSTRACT

Magnesium ferrite nanoparticles ($Mg_{0.97}Fe_{0.03}O$) were synthesized using the sol-gel method to investigate their structural, optical, and antibacterial properties. The study aims to explore the effect of Fe doping on MgO nanoparticles and their efficiency as antibacterial agents. X-ray diffraction (XRD) confirmed the crystalline structure, with the crystallite size calculated to be 10.88 nm. UV-Vis spectroscopy revealed an optical bandgap (Eg) of 3.32 eV, indicative of the material's semiconducting nature. The antibacterial activity of $Mg_{0.97}Fe_{0.03}O$ nanoparticles was evaluated against *Staphylococcus aureus*, demonstrating a zone of inhibition (ZOI) of 15 mm. The results suggest that Fe doping enhances both the structural stability and antibacterial efficiency of MgO nanoparticles, making them suitable for applications in biomedicine and environmental remediation. This study highlights the potential of $Mg_{0.97}Fe_{0.03}O$ nanoparticles as multifunctional materials with promising properties for various industrial and healthcare applications.

Keywords: $Mg_{0.97}Fe_{0.03}O$ nanoparticles, sol-gel synthesis, antibacterial activity, structural properties, optical bandgap

INTRODUCTION

Magnesium oxide (MgO) is a widely studied material due to its excellent thermal, optical, and antibacterial properties. However, incorporating transition metals like iron (Fe) into the MgO matrix can enhance its functional properties, including structural stability, electronic conductivity, and antibacterial efficiency. $Mg_{1-x}Fe_xO$ nanoparticles have gained attention for their potential applications in biomedicine, water purification, and environmental remediation due to their semiconducting nature and ability to interact with bacterial cell membranes.

Fe doping in MgO modifies its structural and electronic properties, enabling fine-tuning for specific applications. The addition of Fe creates localized defects in the MgO lattice, which can influence optical absorption, bandgap energy, and surface reactivity. These changes can significantly enhance the material's bactericidal activity by facilitating reactive oxygen species (ROS) generation, which damages bacterial cell walls.

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

This study focuses on synthesizing $Mg_{0.97}Fe_{0.03}O$ nanoparticles using the sol-gel method, a cost-effective and scalable approach that ensures homogeneity and controlled particle size. We analyze the structural properties using X-ray diffraction (XRD). The optical properties are studied using UV-Vis spectroscopy to determine the bandgap energy. The antibacterial efficacy is assessed against *Staphylococcus aureus*.

The findings provide insights into the structural and functional enhancements imparted by Fe doping, demonstrating the material's potential for multifunctional applications. The study contributes to the growing body of research on doped metal oxides, paving the way for advanced materials with tailored properties.

EXPERIMENTAL AND METHODS

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

$Mg_{0.97}Fe_{0.03}O$ nanoparticles were synthesized via the sol-gel method. Magnesium chloride dihydrate ($MgCl_2·2H_2O$) and ferrous chloride ($FeCl_2$) were used as precursors for Mg and Fe, respectively. Citric acid acted as a chelating agent to enhance homogeneity.

In a typical synthesis, stoichiometric amounts of $MgCl_2·2H_2O$ and $FeCl_2$ were dissolved in deionized water under constant stirring. Citric acid was added in a molar ratio of 1:2 (metal ions to citric acid), and the pH was adjusted to 7 using ammonia solution. The solution was heated to 80°C to form a gel, which was then dried at 100°C overnight. The dried gel was calcined at 500°C for 3 hours to obtain crystalline $Mg_{0.97}Fe_{0.03}O$ nanoparticles.

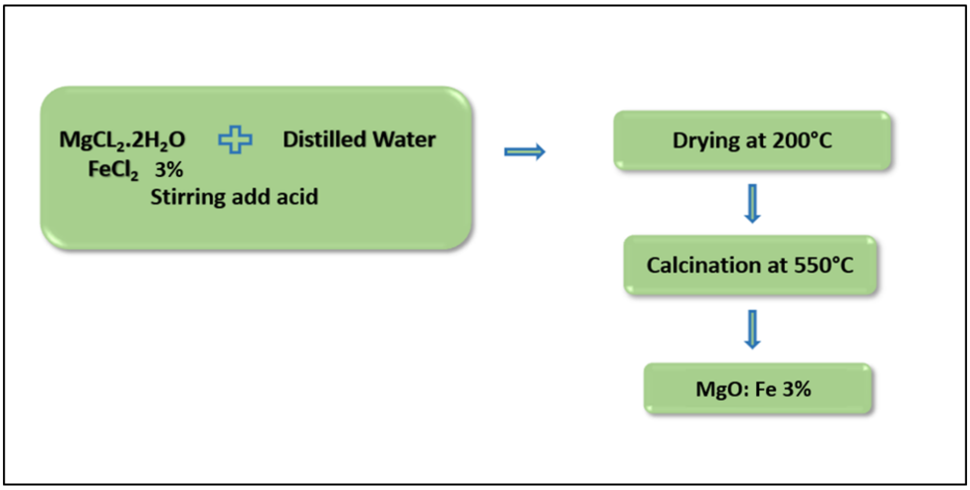


Figure 1: Schematic representation of the preparation process for $Mg_{1-x}Fe_xO$ nanoparticles via the sol-gel method

CHARACTERIZATION

The structural properties of the nanoparticles were analyzed using XRD to determine phase composition, crystallite size, and lattice parameters. UV-Vis spectroscopy was employed to study the optical properties and calculate the bandgap energy. Antibacterial activity was assessed using the agar diffusion method against *Staphylococcus aureus*.

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

RESULTS AND DISCUSSION

XRD ANALYSIS

The X-ray diffraction (XRD) analysis of $Mg_{0.97}Fe_{0.03}O$ nanoparticles confirmed the formation of a single-phase cubic structure, characteristic of the MgO lattice. The diffraction peaks were well-matched with the standard pattern for MgO (JCPDS No. 89-7746), confirming the absence of any secondary phases. This result suggests that Fe ions were successfully incorporated into the MgO lattice, replacing Mg ions without significantly altering the crystal structure. Such substitution typically occurs due to the comparable ionic radii of Mg^{2+} and Fe^{2+}.

The crystallite size was estimated using the Debye-Scherrer formula applied to the most prominent diffraction peak corresponding to the (200) plane. A crystallite size of 10.88 nm was calculated, indicating the nanometer-scale dimension of the particles. The incorporation of Fe may also have induced slight lattice distortions, reflected in the full width at half maximum (FWHM) value of 0.717° for the (200) plane. Table 1 summarizes the key XRD parameters, including 2θ values, FWHM, d-spacing, and crystallite size.

The sharp and well-defined peaks in the XRD pattern reflect high crystallinity, which is advantageous for applications requiring stable structural properties, such as catalysis and antimicrobial coatings. Additionally, the successful doping of Fe into the MgO lattice is expected to influence other properties, such as electronic and optical behavior, enhancing the multifunctionality of the nanoparticles. Figure 2 illustrates the XRD spectrum, highlighting the well-defined peaks corresponding to the cubic MgO phase and confirming the absence of impurities or secondary phases.

Table 1: XRD parameters for $Mg_{1-x}Fe_xO$ nanoparticles

2θ (°)	FWHM	hkl	d-spacing (Å)	Crystallite Size (nm)
42.97	0.717	(200)	2.1012	10.88

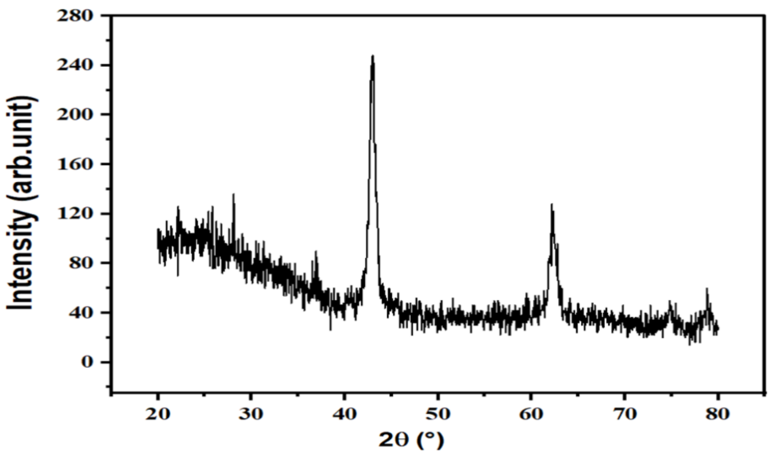


Figure 2: XRD spectra of $Mg_{1-x}Fe_xO$ NPs

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

Table 1: FTIR for the $Mg_xFe_{1-x}O$ NPs

Wavenumber (cm^{-1})	428.20	451.34	524.64	862.18	1076.28	1431.18	1483.26	3425.58
Vibrational Mode	Mg-O	Fe-O	Mg-O	Fe-O	Mg-O	Fe-O	Mg-O	O-H

OPTICAL PROPERTIES

The UV-Vis absorption spectrum of $Mg_{0.97}Fe_{0.03}O$ nanoparticles reveals a distinct absorption edge at approximately 375 nm, indicating their capacity to absorb ultraviolet light effectively. The bandgap energy (Eg) was determined using the Tauc plot method, yielding a value of 3.32 eV. This result classifies the nanoparticles as wide bandgap semiconductors, a characteristic that is critical for applications in optoelectronics, photocatalysis, and environmental remediation.

The slight reduction in Eg compared to pristine MgO (Eg ~ 3.4 eV) can be ascribed to the doping of Fe ions into the MgO lattice. This substitution introduces localized defect states within the bandgap, which facilitate electronic transitions at lower energy levels. Additionally, the incorporation of Fe modifies the electronic structure of MgO, enhancing its light absorption and potentially improving its photocatalytic efficiency under UV light.

The optical properties of these nanoparticles suggest that they possess enhanced light-harvesting capabilities, which could be leveraged in applications such as UV shielding, photocatalysis, and antimicrobial coatings. Figure 3 provides a graphical representation of the UV-Vis absorption spectrum and the Tauc plot used to determine the bandgap energy, illustrating the relationship between the optical behavior and the structural modifications induced by Fe doping.

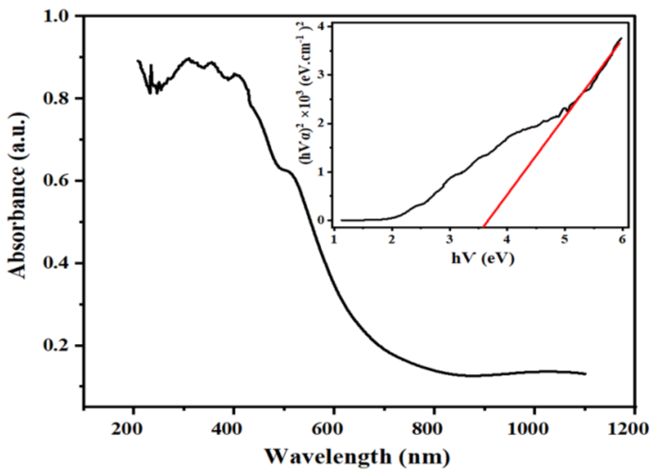


Figure 3: Absorption curve and Eg value for Mg1-xFexO NPs

ANTIBACTERIAL ACTIVITY

The antibacterial activity of $Mg_{0.97}Fe_{0.03}O$ nanoparticles was assessed against *Staphylococcus aureus* using the agar well diffusion method. The results revealed a prominent zone of inhibition (ZOI) measuring 15 mm, demonstrating substantial antibacterial

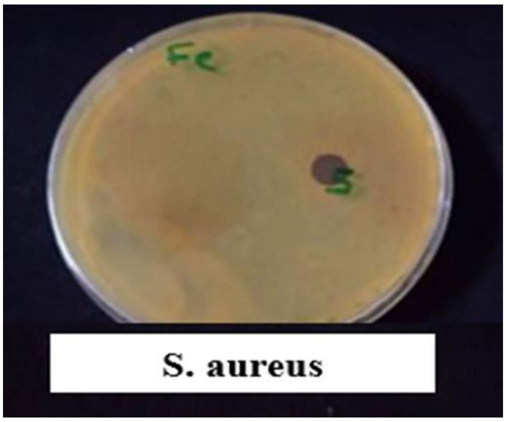
*Corresponding author
Mohammed RASHEED,
Department of Applied Sciences, University of Technology- Iraq, Baghdad, Iraq
e-mail: rasheed.mohammed40@yahoo.com

efficacy. The activity can be attributed to the synergistic effect of magnesium oxide (MgO) and iron (Fe) doping, which enhances the intrinsic antimicrobial properties of MgO.

One of the key mechanisms underlying this antibacterial activity is the generation of reactive oxygen species (ROS) at the nanoparticle surface. These ROS interact with the bacterial cell membrane, causing lipid peroxidation, protein denaturation, and DNA damage. The Fe ions incorporated into the MgO lattice further amplify ROS generation, owing to their ability to participate in redox reactions that facilitate electron transfer processes. This results in an elevated oxidative stress environment that is lethal to bacterial cells.

Additionally, the nanoparticles exhibit strong interactions with the bacterial cell wall due to their nanoscale dimensions and high surface area. The small size of the $Mg_{0.97}Fe_{0.03}O$ nanoparticles allows them to penetrate bacterial cells effectively, disrupting cellular integrity and function. The unique properties of Fe-doped MgO also contribute to enhanced ionic release, which can interfere with enzymatic activity in the bacteria.

Figure 4 visually represents the ZOI for $Mg_{0.97}Fe_{0.03}O$ nanoparticles against *S. aureus*. These findings highlight the potential of $Mg_{0.97}Fe_{0.03}O$ nanoparticles as an efficient antimicrobial agent for applications in biomedicine, coatings, and environmental disinfection, where robust antibacterial performance is crucial.



ZOI (mm)	15

Fig. 4: Antibacterial activity of $Mg_{1-x}Fe_xO$ nanoparticles (*S. aureus*, ZOI = 15 mm)

CONCLUSION

The $Mg_{0.97}Fe_{0.03}O$ nanoparticles synthesized via the sol-gel method demonstrate promising structural, optical, and antibacterial properties, making them suitable for multifunctional applications. X-ray diffraction (XRD) analysis confirmed the successful incorporation of Fe ions into the MgO lattice, resulting in a cubic structure with a calculated crystallite size of 10.88 nm. This incorporation led to slight lattice distortions, indicative of Fe substitution, without compromising the crystalline quality of the material.

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

Ultraviolet-visible (UV-Vis) spectroscopy showed a direct bandgap of 3.32 eV, slightly lower than pure MgO, reflecting the influence of Fe incorporation on the electronic structure. This bandgap adjustment highlights the potential of these nanoparticles in optoelectronic applications.

The antibacterial efficacy of the $Mg_{0.97}Fe_{0.03}O$ nanoparticles was evaluated against *Staphylococcus aureus*, a gram-positive bacterium. The zone of inhibition (ZOI) of 15 mm observed in the antibacterial assay signifies notable antibacterial activity, attributed to the synergistic effects of MgO and Fe. The mechanism likely involves reactive oxygen species (ROS) generation and membrane disruption, enhanced by the presence of Fe ions.

Overall, the results underscore the effectiveness of Fe doping in enhancing the structural stability, optical performance, and antibacterial properties of MgO nanoparticles. These findings open pathways for their use in diverse applications, including biomedicine, environmental remediation, and antimicrobial coatings, positioning $Mg_{0.97}Fe_{0.03}O$ as a versatile nanomaterial for advanced technological needs.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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

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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