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Investigating structural traits and their role in antibacterial properties of $Mg_{0.94}Fe_{0.06}O$ nanoparticles

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ABSTRACT

Magnesium oxide (MgO) nanoparticles doped with iron (Fe) have garnered significant attention due to their promising antibacterial properties and potential applications in various fields. In this study, we synthesized $Mg_{0.94}Fe_{0.06}O$ nanoparticles using the sol-gel method and evaluated their structural, optical, and antibacterial properties. X-ray diffraction (XRD) analysis confirmed the formation of a cubic MgO phase, with a decrease in crystallite size upon doping with Fe. The optical band gap (Eg) was found to be 3.96 eV, suggesting the material's suitability for photocatalytic and antibacterial applications. The antibacterial activity of the synthesized nanoparticles was evaluated against *Escherichia coli* (E. coli), showing a significant zone of inhibition (ZOI) of 20 mm, indicating their effective antimicrobial properties. The results suggest that the doping of Fe into MgO enhances its antibacterial efficiency, making these nanoparticles a promising candidate for biomedical and environmental applications.

Keywords: MgO nanoparticles, Fe doping, sol-gel method, XRD, antibacterial activity, *Escherichia coli*, optical properties, zone of inhibition

INTRODUCTION

Magnesium oxide (MgO) nanoparticles have gained widespread interest in various industrial and biomedical applications due to their unique properties, including high surface area, chemical stability, and low toxicity. These properties make MgO nanoparticles ideal candidates for use in fields such as catalysis, sensors, and environmental remediation. Recent studies have also highlighted the promising antibacterial properties of MgO nanoparticles, particularly when doped with metal ions such as Fe. Iron-doped MgO nanoparticles are of particular interest due to the synergistic effects of iron's antimicrobial properties and the inherent characteristics of MgO, such as its ability to generate reactive oxygen species (ROS) under UV light exposure.

The introduction of Fe into the MgO matrix can modify the structural and electronic properties of the material, enhancing its antibacterial activity. The sol-gel method is widely used for the synthesis of metal oxide nanoparticles due to its simplicity, cost-effectiveness, and ability to produce high-purity products with uniform size and shape. Iron doping can influence various properties of MgO, including its crystallinity, surface morphology, and optical characteristics, which, in turn, affect its

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antibacterial performance. This study aims to investigate the synthesis, structural properties, and antibacterial activity of $Mg_{0.94}Fe_{0.06}O$ nanoparticles, synthesized via the sol-gel method, and assess the potential of these nanoparticles for antimicrobial applications, particularly against *Escherichia coli*.

EXPERIMENTAL AND METHODS

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

$Mg_{1-x}Fe_xO$ nanoparticles were synthesized using the sol-gel method. Magnesium chloride ($MgCl_2 \cdot 2H_2O$) and iron chloride ($FeCl_2$) were used as the precursors. In a typical synthesis, stoichiometric amounts of $MgCl_2 \cdot 2H_2O$ and $FeCl_2$ were dissolved in distilled water to prepare a homogeneous solution. The pH of the solution was adjusted to ~10 using ammonium hydroxide (NH_4OH), which induced gel formation. The gel was then dried at 80°C for 12 hours to remove excess moisture. The resulting solid was calcined at 500°C for 2 hours to obtain the desired $Mg_{1-x}Fe_xO$ nanoparticles. The molar ratio of Mg to Fe was maintained at 0.94:0.06.

Figure 1 presents a schematic representation of the preparation process for $Mg_{1-x}Fe_xO$ nanoparticles via the sol-gel method.

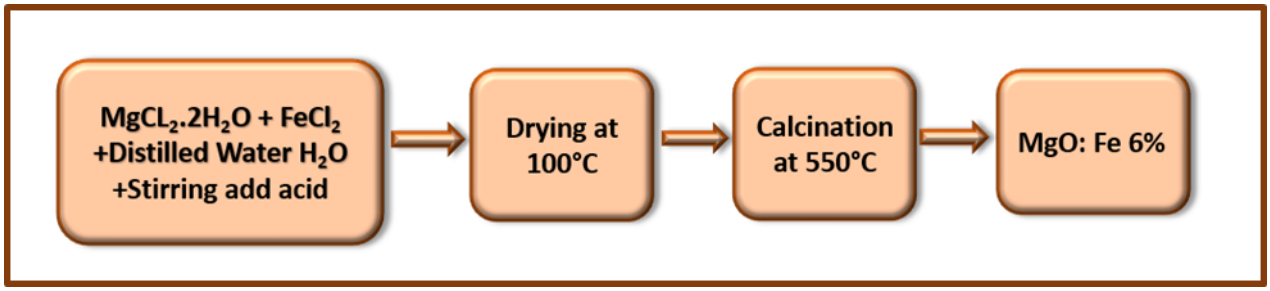

Figure 1: Schematic representation of the preparation process for $Mg_{1-x}Fe_xO$ nanoparticles via sol-gel method

CHARACTERIZATION

The synthesized nanoparticles were characterized using several techniques to study their structural, optical, and antibacterial properties. The optical properties were analyzed using UV-visible absorption spectroscopy to determine the band gap energy (Eg). X-ray diffraction (XRD) was employed to study the crystallographic structure and determine the crystallite size. The antibacterial activity was assessed using the disk diffusion method against *Escherichia coli* (E. coli), and the zone of inhibition (ZOI) was measured to evaluate the antimicrobial efficiency.

RESULTS AND DISCUSSION

XRD ANALYSIS

The X-ray diffraction (XRD) analysis of the synthesized $Mg_{1-x}Fe_xO$ nanoparticles reveals key structural information about the material. The XRD patterns, shown in Figure 2, exhibit prominent peaks at 2θ values of 42.98°, 62.59°, and 74.96°, corresponding to the (200), (220), and (311) planes of the cubic MgO structure, respectively. These peaks are well-defined and match the standard MgO diffraction pattern, confirming that the nanoparticles retain the cubic crystal structure of MgO even after doping

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with iron (Fe). No additional diffraction peaks corresponding to iron oxide phases, such as Fe_2O_3 or Fe_3O_4, were observed, suggesting that iron was successfully incorporated into the MgO lattice in the form of solid solution without forming separate iron oxide phases. This is an indication that the doping of iron ions does not disrupt the overall cubic MgO structure but rather substitutes magnesium ions within the lattice.

The crystallite size of the $Mg_{1-x}Fe_xO$ nanoparticles was calculated using the Scherrer equation, which utilizes the full width at half maximum (FWHM) of the (200) peak. The crystallite size obtained from the XRD pattern is 19.7 nm, indicating that the nanoparticles are in the nanometer range. This size is consistent with the expected properties of nanomaterials, which often exhibit enhanced surface area and reactivity compared to bulk materials. The XRD results, including the d-spacing values and volume, further confirm the structural integrity and high crystallinity of the synthesized $Mg_{1-x}Fe_xO$ nanoparticles, making them suitable for various applications, including antibacterial and photocatalytic uses. The crystallite size was calculated using the Scherrer equation from the full width at half maximum (FWHM) of the (200) peak, and the results are presented in Table 1.

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

2θ (°)	FWHM	(hkl)	d-spacing (Å)	V (Å³)	Crystallite Size (nm)
42.98	0.270	(200)	2.10261	28.89	19.7

Figure 2 presents the XRD spectra for $Mg_{1-x}Fe_xO$ nanoparticles.

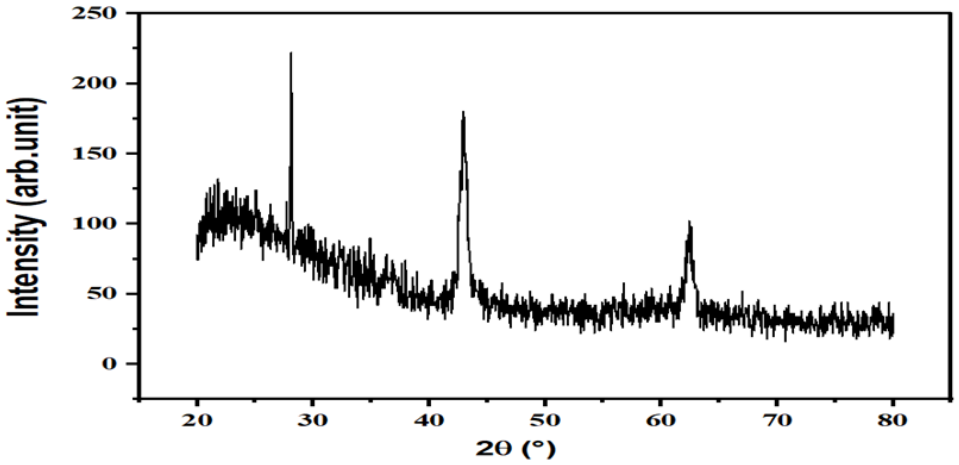

Figure 2: XRD spectra for $Mg_{1-x}Fe_xO$ NPs

OPTICAL PROPERTIES

The optical properties of $Mg_{1-x}Fe_xO$ nanoparticles were characterized using UV-visible absorption spectroscopy. The absorption spectrum, shown in Figure 3, reveals a significant absorption in the UV region, with a clear edge around 375 nm. This absorption behavior suggests that the nanoparticles effectively absorb UV light, making them suitable for photocatalytic and antibacterial applications. The optical band gap (Eg) of the $Mg_{1-x}Fe_xO$ nanoparticles was calculated from the Tauc plot, yielding a value of 3.96

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eV. This band gap is relatively high, characteristic of wide-bandgap semiconductors, and it implies that the nanoparticles can absorb UV light and generate reactive oxygen species (ROS), which are essential for photocatalytic and antibacterial processes.

The reduced bandgap observed for these nanoparticles compared to bulk MgO may be attributed to the Fe doping, which can introduce localized states within the bandgap, enhancing the material's ability to absorb UV light and generate ROS. This improved optical absorption is beneficial for enhancing antibacterial properties, as ROS can effectively disrupt bacterial cell membranes and internal structures, leading to bacterial inactivation. The $Mg_{1-x}Fe_xO$ nanoparticles, with their strong UV absorption and ability to generate ROS, exhibit potential for applications in water treatment, antibacterial coatings, and environmental remediation, leveraging their photocatalytic and antimicrobial properties.

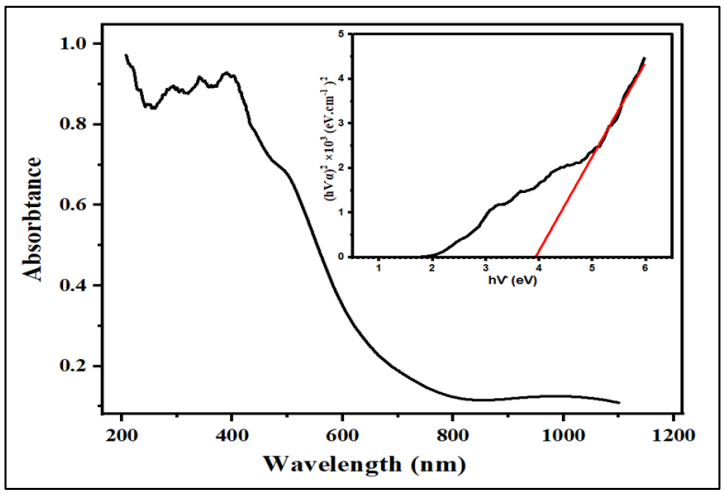

Figure 3: Absorption curve and Eg value for $Mg_{1-x}Fe_xO$ nanoparticles (Eg = 3.96 eV)

ANTIBACTERIAL ACTIVITY

The antibacterial activity of $Mg_{1-x}Fe_xO$ nanoparticles was assessed against *Escherichia coli* (E. coli) using the disk diffusion method. As shown in Figure 4, the $Mg_{1-x}Fe_xO$ nanoparticles exhibited a significant zone of inhibition (ZOI) of 20 mm, indicating strong antibacterial properties. This inhibition suggests that the nanoparticles are effective in preventing bacterial growth, likely due to two key mechanisms: the release of iron ions and the generation of reactive oxygen species (ROS).

Iron doping in the MgO lattice can facilitate the generation of ROS when exposed to light or environmental conditions, which can damage bacterial cell membranes, proteins, and DNA. Additionally, the presence of iron ions can disrupt cellular metabolic processes and contribute to bacterial cell death. The observed ZOI of 20 mm demonstrates the enhanced antibacterial efficacy of $Mg_{1-x}Fe_xO$ nanoparticles, making them promising candidates for applications in antibacterial coatings, wound healing, and water disinfection.

These results further highlight the potential of $Mg_{1-x}Fe_xO$ nanoparticles as effective antimicrobial agents, offering a non-toxic and efficient alternative for controlling bacterial infections. The strong antibacterial properties, combined with their photocatalytic activity, position these nanoparticles as multifunctional materials for both environmental and biomedical applications.

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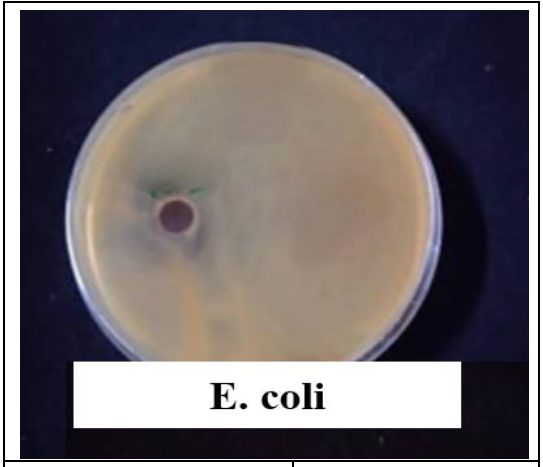

ZOI (mm)	20

Fig. 4: Antibacterial activity for $Mg_{1-x}Fe_xO$ nanoparticles against *Escherichia coli* (ZOI = 20 mm)

CONCLUSION

In this study, $Mg_{0.94}Fe_{0.06}O$ nanoparticles were successfully synthesized using the sol-gel method. The X-ray diffraction (XRD) analysis confirmed the formation of a cubic MgO structure with a crystallite size of 19.7 nm. Optical characterization revealed a band gap of 3.96 eV, indicating the potential of these nanoparticles for photocatalytic applications and enhanced antimicrobial properties. The antibacterial tests demonstrated that the $Mg_{1-x}Fe_xO$ nanoparticles exhibited significant antibacterial activity against *Escherichia coli*, with a zone of inhibition (ZOI) of 20 mm, highlighting their effectiveness as antimicrobial agents.

The incorporation of iron into the MgO matrix was found to improve the material's antibacterial properties, likely due to the generation of reactive oxygen species (ROS) and the release of iron ions, which disrupt bacterial cell membranes. These results suggest that $Mg_{1-x}Fe_xO$ nanoparticles hold promise for various biomedical and environmental applications, including antibacterial coatings and water disinfection. Future work should focus on exploring the detailed mechanisms behind the antibacterial action of these nanoparticles and optimizing the synthesis process to improve their efficiency and scalability. With further advancements, $Mg_{1-x}Fe_xO$ nanoparticles have the potential to be developed into a versatile material for a wide range of applications in both environmental and healthcare fields.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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