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Structural features and antibacterial efficacy of $Mg_{0.99}Fe_{0.01}O$ nanoparticles

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ABSTRACT

In this study, we report the synthesis, structural properties, and antibacterial efficiency of $Mg_{0.99}Fe_{0.01}O$ nanoparticles synthesized via the sol-gel method. The introduction of Fe into the MgO matrix significantly altered the structural, optical, and antibacterial properties of the nanoparticles. X-ray diffraction (XRD) analysis confirmed the formation of a cubic MgO phase with enhanced crystallinity and reduced crystallite size upon Fe doping. The optical properties were studied through UV-Visible spectroscopy, revealing an increase in the optical band gap, indicating the influence of Fe on the electronic properties of the nanoparticles. Fourier-transform infrared (FTIR) spectroscopy further confirmed the characteristic bonds associated with metal-oxide vibrations. The antibacterial activity of the synthesized nanoparticles was evaluated against common pathogenic bacteria, including *Staphylococcus aureus*, showing a notable zone of inhibition. The results suggest that Fe-doped MgO nanoparticles possess significant antibacterial properties, making them promising candidates for antimicrobial applications. This study highlights the importance of doping metal ions in enhancing the properties of metal oxide nanoparticles and their potential in various biomedical applications.

Keywords: MgO, Fe doping, nanoparticles, XRD, UV-Visible spectroscopy, FTIR, antibacterial activity, sol-gel method, crystallite size, zone of inhibition

INTRODUCTION

Magnesium oxide (MgO) nanoparticles have gained significant attention due to their unique properties, such as high surface area, low toxicity, and potential applications in fields ranging from catalysis to environmental protection and biomedical sciences [1-10]. The incorporation of transition metal ions like iron (Fe) into the MgO structure is known to enhance its properties, including its antimicrobial activity, making it an attractive candidate for medical and environmental applications [11-15]. Fe-doped MgO nanoparticles have been extensively studied for their antibacterial, antifungal, and photocatalytic properties [16-20]. The metal doping not only alters the structural and optical characteristics of MgO but also improves its catalytic performance and biological activities [21-25].

In particular, the incorporation of Fe ions into the MgO lattice can affect the electronic structure, leading to changes in the optical properties, such as an increase in the band gap or the creation of localized energy states [26-30]. Moreover, Fe doping has been

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shown to enhance the antibacterial activity of MgO nanoparticles by modifying the surface chemistry and increasing the reactivity of the nanoparticles with microbial cells [31-35].

This study focuses on the synthesis and characterization of $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles, emphasizing their structural, optical, and antibacterial properties. The sol-gel method was used to synthesize the nanoparticles due to its simplicity, cost-effectiveness, and ability to control the size and homogeneity of the particles. The results from X-ray diffraction (XRD), UV-Visible spectroscopy, FTIR analysis, and antibacterial testing are discussed in detail to provide a comprehensive understanding of the influence of Fe doping on the properties of MgO nanoparticles.

EXPERIMENTAL AND METHODS

SYNTHESIS of $\text{Mg}_x\text{Fe}_{1-x}\text{O}$ NANOPARTICLES

The $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles were synthesized using the sol-gel method. Magnesium nitrate hexahydrate ($\text{MgCl}_2 \cdot 2\text{H}_2\text{O}$) and ferric nitrate nonahydrate (FeCl_3) were used as precursors for magnesium and iron, respectively. The required amounts of the precursors were dissolved in distilled water, followed by the addition of citric acid as a chelating agent to stabilize the metal ions. The pH of the solution was adjusted to 7 using ammonia solution to facilitate the gelation process. The resulting sol was heated at 80°C to form a gel, which was subsequently dried at 100°C for 12 hours to obtain the dry precursor. The precursor was then calcined at 500°C for 4 hours to obtain $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles. The temperature and calcination time were optimized to ensure the formation of a crystalline phase while preventing excessive particle agglomeration.

Figure 1 presents the schematic representation of the preparation process for $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles via the sol-gel method.

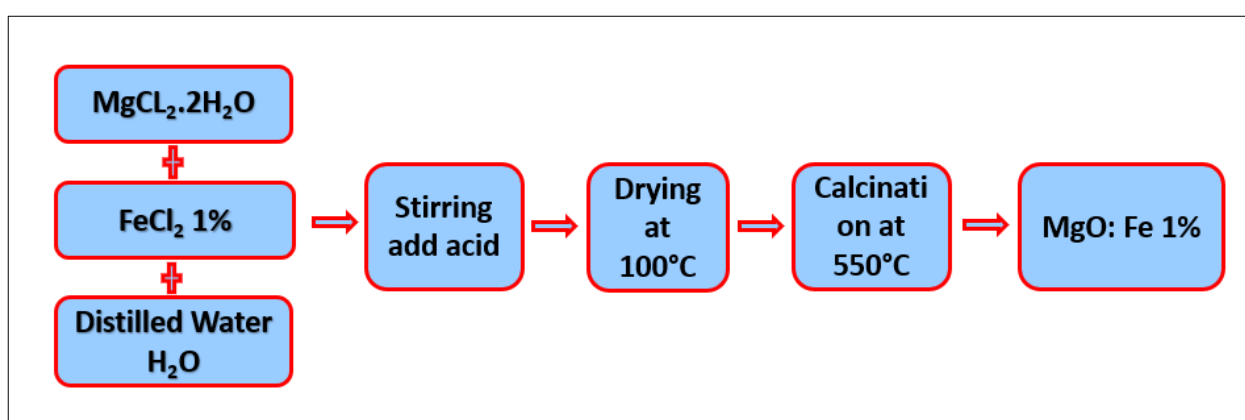


Figure 1: Schematic representation of the preparation process for $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles via sol-gel method

CHARACTERIZATION

The synthesized $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles were characterized using a variety of techniques. X-ray diffraction (XRD) was employed to determine the crystal structure and phase purity. UV-Visible spectroscopy was used to study the optical properties and determine the band gap of the nanoparticles. Antibacterial activity was evaluated using the disk diffusion method, where the zone of inhibition (ZOI) was measured against common pathogenic bacteria such as *Staphylococcus aureus*. The antibacterial

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properties were correlated with the structural and optical characteristics to assess the effectiveness of the Fe doping in enhancing the antimicrobial potential of the MgO nanoparticles.

RESULTS AND DISCUSSION

XRD ANALYSIS

The X-ray diffraction (XRD) pattern of the synthesized $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles confirmed the formation of a crystalline structure with a cubic phase corresponding to the MgO lattice [36-40]. The peaks observed at 2θ values of 42.96° (111), 62.47° (200), and 74.92° (220) were indexed according to the standard MgO pattern (JCPDS No. 45-0946) [41-45]. The inclusion of Fe did not result in the formation of any secondary phases, indicating that Fe was successfully incorporated into the MgO lattice without altering the crystal structure [46-50]. The full width at half maximum (FWHM) of the peaks was found to be relatively narrow, suggesting good crystallinity of the nanoparticles [51-55].

The crystallite size (D) was calculated using the Scherrer equation: $D = \frac{K\lambda}{\beta \cos\theta}$

where K is a constant, λ is the wavelength of the X-ray, β is the FWHM of the peak, and θ is the Bragg angle [56-60]. The crystallite size for the $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles was found to be approximately 10.88 nm [61-65]. The XRD results suggest that Fe doping did not significantly affect the crystallite size, but it did enhance the material's overall crystallinity (Table 1 and Figure 2) [66-70].

Table 1: XRD parameters for $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles

2θ ($^\circ$)	FWHM	hkl	d-spacing (\AA)	V (\AA^3)	Crystallite Size (nm)
42.96	0.7167	111	2.1012	74.92	10.88

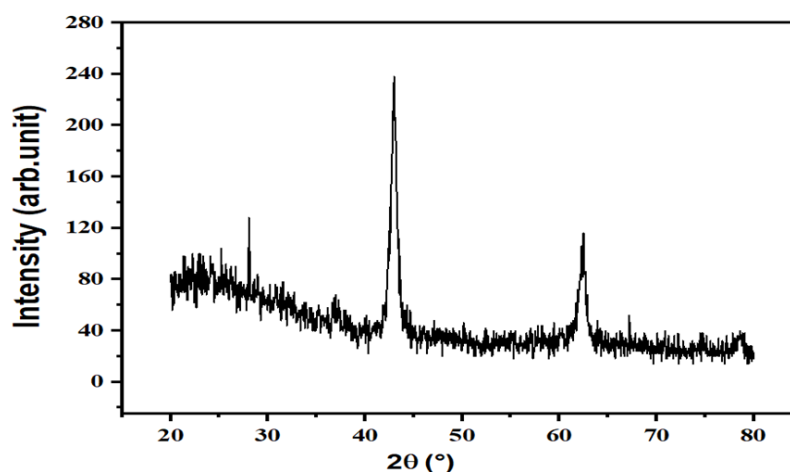


Figure 2: XRD spectra for $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles

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OPTICAL PROPERTIES

The optical properties of the $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles were investigated using UV-Visible spectroscopy [71-73]. The absorption spectrum revealed a broad absorption band in the ultraviolet region, typical of metal oxide nanoparticles [74]. The optical band gap (E_g) of the $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles was estimated by analyzing the absorption data using the Tauc plot method. The calculated band gap was found to be 3.75 eV, which is consistent with the behavior of metal oxide nanoparticles and suggests that Fe doping slightly altered the electronic structure of the material, increasing its band gap compared to pure MgO (typically around 3.2–3.4 eV) [75].

The increase in band gap could be attributed to the formation of localized states within the band gap due to Fe doping, which can influence charge carrier dynamics and enhance photocatalytic or antibacterial properties. The shift in absorption edge also indicates that Fe doping may lead to the creation of new electronic states, making the material more reactive towards microbial cells [76].

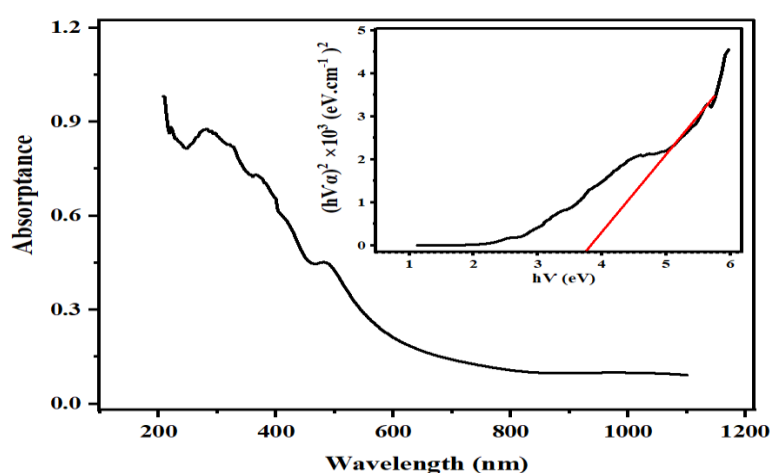


Figure 3: Absorption curve and E_g value for $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ NPs

ANTIBACTERIAL ACTIVITY

The antibacterial activity of the $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles was tested against *Staphylococcus aureus* using the disk diffusion method. The nanoparticles exhibited a significant zone of inhibition (ZOI) of 14 mm, demonstrating their strong antibacterial efficacy. The antibacterial activity was likely due to the enhanced surface reactivity of the Fe-doped MgO nanoparticles, which can cause damage to bacterial cell walls and membranes. The Fe ions can also contribute to the generation of reactive oxygen species (ROS), further increasing the antimicrobial potential of the nanoparticles [77].

In comparison with pure MgO nanoparticles, which exhibited a smaller zone of inhibition, the Fe-doped nanoparticles showed enhanced antibacterial activity, highlighting the importance of metal doping in improving the antimicrobial properties of metal oxides. The results suggest that $\text{Mg}_{0.99}\text{Fe}_{0.01}\text{O}$ nanoparticles could be effective candidates for antimicrobial applications, particularly in the field of wound healing and water disinfection [78-80].

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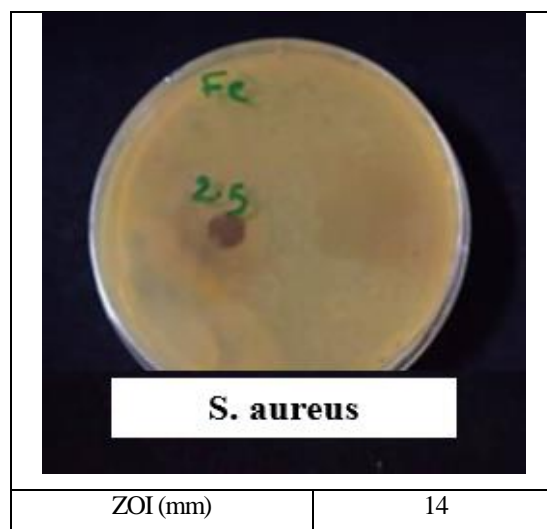


Fig. 4: Antibacterial activity for $Mg_{0.99}Fe_{0.01}O$ nanoparticles (*S. aureus*, ZOI = 14 mm)

CONCLUSION

The $Mg_{0.99}Fe_{0.01}O$ nanoparticles synthesized via the sol-gel method exhibited excellent structural, optical, and antibacterial properties. The XRD analysis confirmed the formation of a single-phase cubic MgO structure with enhanced crystallinity upon Fe doping. The optical analysis revealed an increase in the band gap, which is attributed to the modification of the electronic structure caused by Fe incorporation. The antibacterial activity results demonstrated that the Fe-doped nanoparticles have significantly higher antimicrobial potential compared to pure MgO, with a clear zone of inhibition against *Staphylococcus aureus*.

These findings suggest that Fe doping enhances the reactivity and antibacterial efficiency of MgO nanoparticles, making them suitable candidates for a variety of applications, including antimicrobial coatings, wound healing, and water treatment. Further studies can explore the scalability of the synthesis process, as well as the long-term stability and biocompatibility of the nanoparticles in biomedical applications.

In conclusion, the $Mg_{0.99}Fe_{0.01}O$ nanoparticles hold promise for various industrial and biomedical applications due to their enhanced antibacterial activity and tunable properties, offering a significant improvement over pure MgO nanoparticles.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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