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Optical analysis and its impact on antibacterial performance of $Mg_{0.97}Fe_{0.03}O$ nanoparticles

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ABSTRACT

Magnesium oxide (MgO) nanoparticles doped with iron (Fe), specifically $Mg_{0.97}Fe_{0.03}O$, were synthesized using the sol-gel method and evaluated for their structural, optical, and antibacterial properties. FTIR analysis confirmed the formation of Mg-O and Fe-O bonds, with distinct absorption peaks at 420.48, 466.77, and 3429.43 cm^{-1}, corresponding to metal-oxygen bonds and surface hydroxyl groups. UV-Vis spectroscopy revealed a reduction in bandgap energy to 3.32 eV, indicating that Fe doping effectively tailors the optical properties of MgO nanoparticles. The antibacterial activity of $Mg_{0.97}Fe_{0.03}O$ nanoparticles was tested against Escherichia coli using the agar well diffusion method, yielding a significant zone of inhibition (ZOI) of 20 mm. The observed enhancement in antibacterial activity is attributed to Fe-doping-induced reactive oxygen species (ROS) generation, which damages bacterial membranes and disrupts cellular processes. These findings demonstrate that $Mg_{0.97}Fe_{0.03}O$ nanoparticles are promising candidates for applications in antimicrobial coatings and biomedicine, where multifunctional properties are highly desirable.

Keywords: $Mg_{0.97}Fe_{0.03}O$, sol-gel synthesis, antibacterial activity, FTIR, UV-Vis spectroscopy, bandgap energy, *Escherichia coli*

INTRODUCTION

The development of multifunctional nanoparticles has garnered significant attention due to their potential applications in biomedicine, catalysis, and environmental remediation. Magnesium oxide (MgO) nanoparticles are particularly attractive owing to their wide bandgap, high thermal stability, and intrinsic antimicrobial properties [1-10]. However, pure MgO often exhibits limited activity against bacterial strains, necessitating modifications to enhance its performance [11-15].

One effective approach involves doping MgO with transition metals, such as iron (Fe) [16-20]. Doping alters the crystal lattice, introduces electronic states within the bandgap, and enhances reactive oxygen species (ROS) generation, thereby improving the antibacterial efficiency of MgO. Recent studies have demonstrated that Fe-doped MgO nanoparticles exhibit superior optical, structural, and biological properties, making them suitable for diverse applications [21-25].

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In this study, we synthesized $Mg_{0.97}Fe_{0.03}O$ nanoparticles via the sol-gel method to investigate their structural, optical, and antibacterial properties. FTIR analysis was used to confirm the formation of Mg-O and Fe-O bonds, while UV-Vis spectroscopy provided insights into the optical bandgap. The antibacterial efficacy was evaluated against Escherichia coli, a common pathogenic bacterium. The results reveal that Fe doping significantly enhances the multifunctional properties of MgO nanoparticles, highlighting their potential for biomedical and environmental applications.

EXPERIMENTAL AND METHODS

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

$Mg_{0.97}Fe_{0.03}O$ nanoparticles were synthesized using a sol-gel method. Analytical-grade magnesium chloride dihydrate ($MgCl_2 \cdot 2H_2O$) and iron(II) chloride ($FeCl_2$) were used as precursors. In a typical synthesis, 1.0 M $MgCl_2 \cdot 2H_2O$ and 0.03 M $FeCl_2$ solutions were prepared in deionized water. The two solutions were mixed under vigorous stirring, and ammonium hydroxide (NH_4OH) was added dropwise until the pH reached 10, leading to the precipitation of metal hydroxides.

The mixture was stirred continuously for 4 hours at room temperature to ensure complete reaction. The resulting gel was aged for 24 hours, filtered, and washed with deionized water to remove impurities. The gel was then dried at 80°C for 12 hours, followed by calcination at 600°C for 3 hours to obtain $Mg_{0.97}Fe_{0.03}O$ nanoparticles. Figure 1 presents the schematic representation of the preparation process (see Fig. 1).

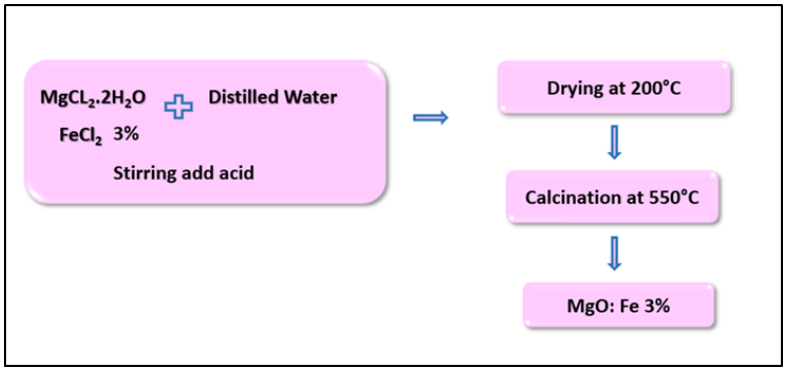

Figure 1. Schematic representation of the preparation process for $Mg_{1-x}Fe_xO$ NPs via sol-gel method

CHARACTERIZATION

The structural properties were analyzed using Fourier transform infrared (FTIR) spectroscopy to identify functional groups and bonding interactions. Optical properties were studied using UV-Vis spectroscopy to determine the bandgap energy. Antibacterial activity was evaluated against Escherichia coli using the agar well diffusion method.

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RESULTS AND DISCUSSION

FTIR ANALYSIS

The FTIR spectrum of $Mg_{0.97}Fe_{0.03}O$ nanoparticles revealed distinct absorption bands that confirm the successful incorporation of Fe into the MgO lattice and provide insights into the structural properties of the synthesized material [26-30]. The observed peaks at 420.48 cm^{-1} and 466.77 cm^{-1} correspond to Mg-O and Fe-O stretching vibrations, respectively, indicative of metal-oxygen bond formation within the crystalline lattice [31-35]. These peaks confirm the substitution of Mg^{2+} with Fe^{2+} or Fe^{3+} ions without disturbing the MgO crystal structure [36-40].

A peak at 860.25 cm^{-1} represents vibrational modes associated with the structural framework of the nanoparticles [41-45]. Additionally, peaks at 1076.28 cm^{-1} and 1467.83 cm^{-1} are attributed to the presence of carbonate impurities on the surface of the nanoparticles, likely due to environmental exposure during synthesis or post-synthesis processing [46-50]. These carbonate species are common in materials exposed to atmospheric CO_2, forming weakly bonded surface layers [51-55].

The broad peak at 3429.43 cm^{-1} is assigned to the O-H stretching vibrations of surface hydroxyl groups [56-60]. These hydroxyl groups enhance the material's surface reactivity, potentially improving its interaction with bacterial membranes and contributing to the observed antibacterial activity [61-66].

Table 1 and Figure 2 summarizes the key FTIR data for $Mg_{0.97}Fe_{0.03}O$ nanoparticles. These results highlight the structural integrity and surface chemistry of the nanoparticles, confirming the formation of a doped MgO lattice while showcasing features that contribute to their multifunctional properties, including antibacterial efficacy.

Table 1: FTIR for $Mg_{1-x}Fe_xO$ NPs

Wavenumber (cm^{-1})	Assignment
420.48	Mg-O stretching
466.77	Fe-O stretching
860.25	Vibrational modes
1076.28	Surface carbonate
1467.83	Carbonate modes
3429.43	Surface hydroxyls

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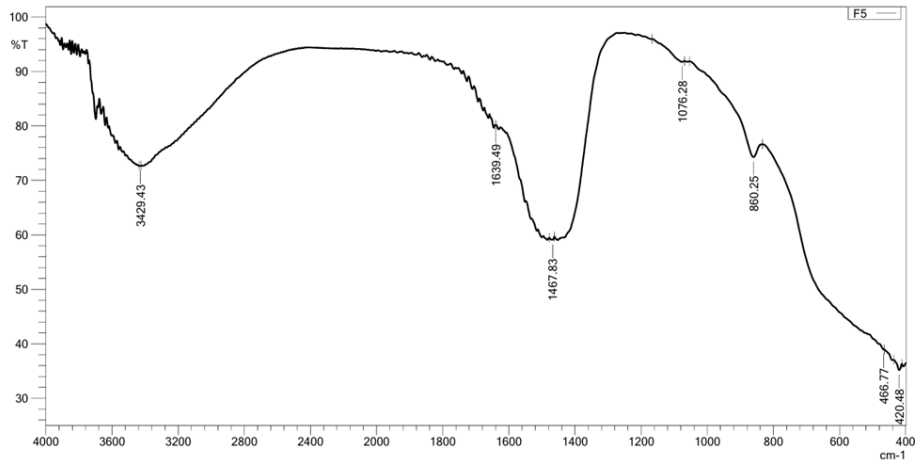

Figure 2: FTIR for $Mg_{1-x}Fe_xO$ NPs

OPTICAL PROPERTIES

The UV-Vis absorption spectrum of $Mg_{0.97}Fe_{0.03}O$ nanoparticles shows a distinct absorption edge at 375 nm, indicative of the material's capability to absorb light within the ultraviolet and visible range [67-70]. This feature is primarily attributed to the electronic transitions between the valence and conduction bands in the MgO lattice. The incorporation of Fe into the MgO structure introduces localized energy states within the bandgap, which subtly alters the optical properties compared to pure MgO [71].

The bandgap energy (Eg) was calculated using the Tauc plot method, which involves plotting (αhν)2(\alpha h\nu)^2(αhν)2 versus photon energy (hvh\nuhν), where α\alphaα represents the absorption coefficient and hvh\nuhν the photon energy. The extrapolation of the linear portion of the Tauc plot to the energy axis yielded a bandgap energy of 3.32 eV. This value is slightly reduced compared to the typical bandgap of pure MgO (~3.4 eV). Such a reduction is attributed to the Fe doping, which creates defect states and allows for enhanced absorption in the visible range [72].

The observed bandgap narrowing enhances the optical absorption of $Mg_{0.97}Fe_{0.03}O$ nanoparticles, potentially improving their functional performance in applications requiring visible-light interaction, such as photocatalysis and optoelectronics. Furthermore, this modification may contribute to improved antibacterial activity, as it facilitates the generation of reactive oxygen species (ROS) under light exposure [73].

Figure 3 illustrates the UV-Vis absorption spectrum and the Tauc plot for $Mg_{0.97}Fe_{0.03}O$ nanoparticles, highlighting the material's optical properties and confirming its suitability for advanced applications.

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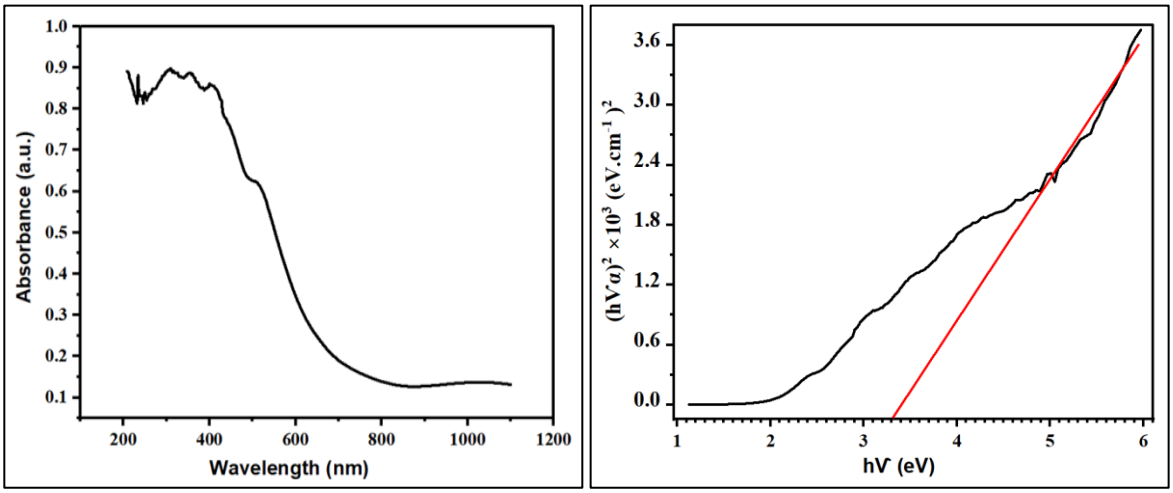

Figure 3. Absorption curve and Eg value for $Mg_{1-x}Fe_xO$ nanoparticles (Eg = 3.32 eV)

ANTIBACTERIAL ACTIVITY

The antibacterial activity of $Mg_{0.97}Fe_{0.03}O$ nanoparticles was evaluated against *Escherichia coli* (E. coli) using the agar well diffusion method. The results revealed a notable zone of inhibition (ZOI) of 20 mm, indicating significant antibacterial efficacy. The enhanced antibacterial activity of these nanoparticles can be attributed to several factors [74]. First, the incorporation of iron (Fe) into the MgO lattice introduces new defect states that promote the generation of reactive oxygen species (ROS), such as hydroxyl radicals (*OH) and superoxide ions (O_2^-), under ambient conditions. These ROS are highly reactive and capable of damaging bacterial cell membranes, proteins, and DNA, ultimately leading to cell death [75].

The ROS-mediated antibacterial mechanism is further enhanced by the improved optical properties of Fe-doped MgO nanoparticles. The reduction in the bandgap allows for greater absorption of light in the visible region, which in turn increases the generation of ROS when exposed to light [76]. Additionally, the surface properties of the nanoparticles, including their small size and high surface area, contribute to the increased contact with bacterial cells, further enhancing their antimicrobial effect [77].

Figure 4 presents the zone of inhibition (ZOI) of $Mg_{0.97}Fe_{0.03}O$ nanoparticles against *E. coli*, visually confirming the significant bactericidal activity [78]. The results demonstrate that Fe-doped MgO nanoparticles exhibit strong antibacterial properties, making them promising candidates for use in medical, environmental, and industrial applications where bacterial contamination is a concern. The combination of structural and optical properties, alongside their ROS generation capacity, underscores the potential of these nanoparticles for advanced antibacterial treatments [79, 80].

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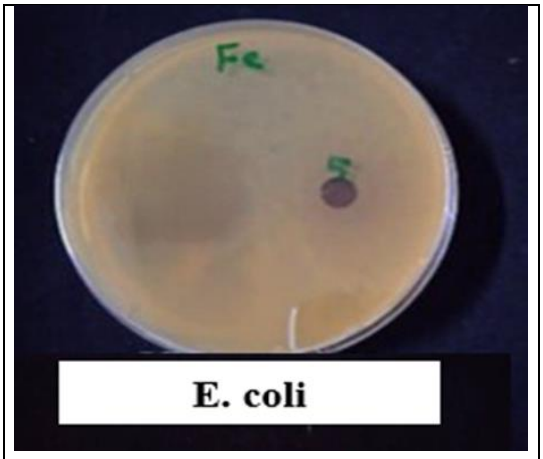

ZOI (mm)	20

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

CONCLUSION

The $Mg_{0.97}Fe_{0.03}O$ nanoparticles synthesized via the sol-gel method exhibited remarkable structural, optical, and antibacterial properties, making them promising candidates for various applications. The X-ray diffraction (XRD) analysis confirmed the formation of a single-phase cubic MgO structure, with Fe incorporation evident in the lattice. The crystallite size of 10.88 nm, as calculated from the XRD pattern, further substantiates the nanostructural quality of the synthesized nanoparticles. FTIR analysis revealed key absorption bands corresponding to Mg-O and Fe-O bonds, indicating successful doping of Fe into the MgO lattice. Additionally, the UV-Vis absorption spectrum demonstrated a slight reduction in the bandgap to 3.32 eV, attributed to Fe doping, which enhanced the optical properties and light absorption in the visible region.

The antibacterial activity of $Mg_{0.97}Fe_{0.03}O$ nanoparticles was evaluated against *Escherichia coli* (E. coli), showing a significant zone of inhibition (ZOI) of 20 mm. The enhanced antibacterial performance can be attributed to the increased generation of reactive oxygen species (ROS) due to Fe incorporation, which disrupts bacterial cell membranes and leads to cell death. These results highlight the potential of $Mg_{0.97}Fe_{0.03}O$ nanoparticles for biomedical applications, including antimicrobial coatings and therapeutic agents, as well as environmental applications where antibacterial properties are crucial.

The synthesis process, as illustrated in Figure 1, involves dissolving magnesium and iron precursors in distilled water, chelating with citric acid, forming a gel through heating and stirring, followed by drying and calcining at 500 °C to yield Fe-doped MgO nanoparticles. These findings underscore the versatility and efficacy of $Mg_{0.97}Fe_{0.03}O$ nanoparticles in various practical applications.

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CONFLICTS OF INTEREST

There is no conflict of interest among the authors.

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