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Structural and Optical Properties of Zinc Oxide Nanoparticles for Rhodamine B Dye Degradation Under Visible Light

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Abstract
This research deals with the development and analysis of zinc oxide (ZnO) nanoparticles characterization by X-ray diffraction (XRD), FTIR, and UV-Vis absorption spectroscopy techniques. The X-ray analysis confirms the pure wurtzite phase structure, characterized by the space group $P6_3mc$. The values of lattice constant, lattice strain, and crystallite size were evaluated using the standard relation. The ZnO nanoparticles were also characterized by FTIR spectra, which reveal the presence of various functional groups such as O-H. The optical band gap, measured at approximately 3.04 eV, was determined using UV-Visible spectroscopy. The dye degradation of Rhodamine B was performed using ZnO NPs, indicating an efficiency of dye degradation of 80%.

Keywords: ZnO, XRD, FTIR, UV-Visible and dye degradation.

INTRODUCTION

Metal oxide semiconductors, represented by MO, are a prominent material found abundantly in nature with important characteristics. These semiconductors behave differently in comparison with the conventional organic semiconductors like Germanium, Silicon, which belong III-V group of compounds. The MO semiconductors belong to the II-VI group of compounds, exhibit very interesting properties such as carrier mobility, wide optical band gap, mechanical stress, etc.[1]. These distinct properties of MO semiconductors made them useful in many applications such as LED, Solar cells, Piezo electric devices, Sensors, Spintronic material, etc. Amongst the various MO, zinc oxides are one of the important oxides having a maximum band gap of the order 3.3 eV[2]**.** ZnO exhibits high electrical conductivity, optical transparency, etc., properties which are useful in optoelectronic devices. ZnO exhibits a wurtzite structure with space group $P6_3mc$. In the literature, a large number of papers are available on the synthesis on characterization of pure ZnO semiconductor as well as doped ZnO semiconductor for various applications. [3, 4]. However, the photocatalytic activity for various dye degradation was not systematically reported, though ZnO shows the highest band gap. In the present work, we report that ZnO nanoparticles were synthesized via a sol-gel auto combustion method and characterized by XRD, FTIR, and UV-Visible spectroscopy techniques. The photocatalytic activity was studied through the degradation of the Rhodamine B dye.

Experimental Work

A transparent solution was prepared by dissolving zinc nitrate hexahydrate in deionized water. Citric acid should be dissolved in deionized water in a different beaker. Generally speaking, zinc nitrate and citric acid were used in an equimolar ratio. To create a homogeneous solution, thoroughly mix the solutions of citric acid and zinc nitrate. Stirring the mixture is necessary until a clear solution is achieved. Stirring constantly, bring the solution to a moderate temperature of 80–90°C on a hot plate. The solution should be heated further until it converts to a gel. The exothermic nature of the nitrate-citrate will cause the gel to spontaneously burn. The combustion will produce a fluffy and porous centering precursor powder. Calcination was carried out in a furnace at a higher temperature, 800°C, for 5h. The synthesized zinc oxide nanoparticles are characterized by the X-ray diffraction (XRD) method, FTIR, and UV-visible spectroscopy (UV-Vis).

Results and Discussion

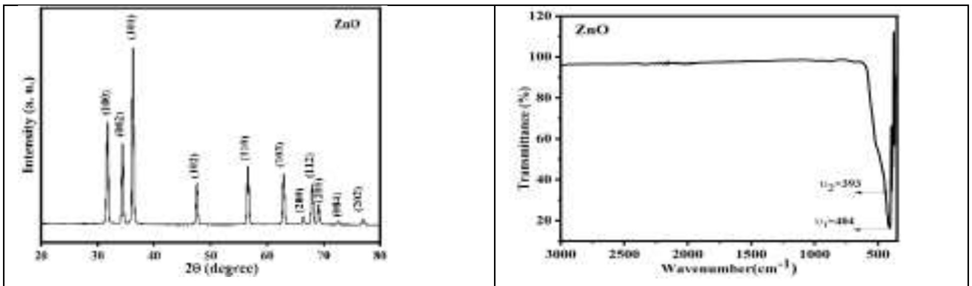
X-ray Diffraction

Figure 1(a) depicts XRD pattern of zinc oxide nanoparticles which show the reflections which are indexed by using Bragg's law as (100), (002), (101), (102), (110), (103), (200), (112), (201),(004) and (202) which closely matches with the JCPDS card number 01-079-0205[5]. The analysis of the XRD pattern suggests the wurtzite structure with space group $P6_3mc$. The value of lattice constant "a" and "c" has been calculated with the help of X-ray diffraction data and by the following relation. To find the unit cell volume (V) by the following relation: The other structural parameters, such as dislocation density and lattice strain, were also calculated using standard relations.

$$\frac{1}{d^2} = \frac{4}{3} * \left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2} \qquad \text{(i)}$$

$$V = \frac{\sqrt{3}}{2} a^2 c \qquad \text{(ii)}$$

$$t = \frac{0.9 * \lambda}{\beta * cos\theta} \qquad \text{(iii)}$$



(a) (b)

FIGURE 1 (a) XRD pattern and (b) FTIR spectra prepared ZnO NP.

Table 1 gives the values of various structural parameters. It has been observed from Table 1 that the obtained lattice constant and other structural parameters are in close agreement with the literature data.

[6]. The Debye Scherrer formula was used to find crystalline size: An average crystallite size of about 25 nm was recorded.

FTIR ANALYSIS

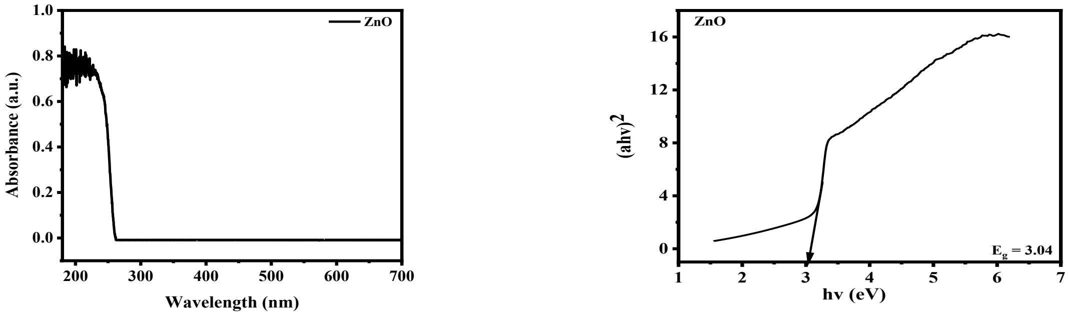
The wurtzite structure construction was confirmed by using the technique involving Fourier transform infrared spectra analysis, which was also utilised to gather data regarding the chemical bonding inside a material. It is employed to determine a material's basic components. FTIR spectra of pure ZnO nanoparticles are shown in **Figure 1(b)**. The Zn-O bond stretching vibration is identified by an absorption band at 404 cm^{-1}.

Optical Analysis

The UV-Visible absorption spectra of ZnO nanoparticles as recorded are shown in **Figure 2(a)**.The absorbance spectra were used to obtain (αhν). The band gap energy was calculated using the Tauc plot between $(\alpha h\nu)^2$ and hν, **Figure 2(b)**. The Tauc plot demonstrates the determination of the optical band gap, which is found to be of the order of **3.04 eV.**

Table 1: Values of Lattice constant (a), Crystallite size (t), Unit cell volume (V), Dislocation density (δ), Lattice strain (LS), and Energy band gap E_g for ZnO nanoparticles.

a and c (Å)	t (nm)	V ($Å^3$)	$\delta \times 10^{15}$ Lines/m^2	**LS**	E_g (eV)
a= b = 3.2506, c = 5.2039	25	47.61	1.56	0.00143	3.04



(a) (b)

FIGURE 2. (a) Absorption spectra and (b) Tauc plot of the ZnO NPs.

Photocatalytic Activity

ZnO nanoparticles were studied for photocatalytic activity under visible light-induced dye degradation of rhodamine B. The dye-containing distilled water solution absorption spectra reveal a peak at a wavelength of between 543 nm and 635 nm. The process of dye degradation was carried out with the produced ZnO nanoparticles at different time intervals. According to the data, the dye degradation process takes 210 minutes to finish with an 80% efficiency.

Conclusion

Sol-gel auto-combustion method was successfully employed to prepare zinc oxide nanoparticles in a single-phase wurtzite structure. All the structural parameters obtained from XRD data are well in agreement with the reported. FTIR spectrum also characterizes the ZnO nanoparticles and displays various functional groups. The band gap of the order of 3.08 eV was obtained through UV-Visible studies. The photocatalytic activity was tested to degrade the RB dye, which shows that the ZnO nanoparticles have 80% efficiency and require 210 min to degrade rhodamine B dye.

REFERENCE

1. Gulab, H., et al., *Advancements in zinc oxide nanomaterials: Synthesis, properties, and diverse applications.* Nano-Structures & Nano-Objects, 2024. **39**: p. 101271.
2. Biplob, M.M.H., *Preparation and Characterization of Mo-doped ZnO thin film by Spray Pyrolysis Method*. 2024, University of Rajshahi.
3. Saeed, M., et al., *Recent advances, challenges, and future perspectives of ZnO nanostructure materials towards energy applications.* The Chemical Record, 2024. **24**(1): p. e202300106.
4. Mutukwa, D., R.T. Taziwa, and L. Khotseng, *A Review of Plant-Mediated ZnO Nanoparticles for Photodegradation and Antibacterial Applications.* Nanomaterials, 2024. **14**(14).
5. Javed, U., et al., *Tuning of structural, magnetic, and optical properties of ZnO nanoparticles by Co and Cu doping.* Solid State Communications, 2024. **390**: p. 115616.
6. Birajdar, S.D., et al., *Effect of Co2+ ions on structural, morphological and optical properties of ZnO nanoparticles synthesized by sol–gel auto combustion method.* Materials Science in Semiconductor Processing, 2016. **41**: p. 441-449.