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# Synthesis and Characterisation of Zinc Oxide Nanoparticles by Chemical Precipitation Method and Investigation of Optical Properties

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**Abstract:** Zinc oxide (ZnO) nanoparticles have attracted significant research attention due to their distinctive optical, electronic, and photocatalytic properties that emerge from quantum confinement effects at the nanoscale. This paper reports the synthesis of ZnO nanoparticles by an optimised chemical precipitation method using zinc acetate dihydrate as the precursor and sodium hydroxide as the precipitating agent, with polyethylene glycol (PEG-400) as a capping agent to control particle growth. The synthesised nanoparticles were characterised using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible (UV-Vis) absorption spectroscopy, and photoluminescence (PL) spectroscopy. XRD analysis confirmed a wurtzite hexagonal crystal structure with no secondary phase impurities. The Scherrer equation applied to the (101) XRD peak yielded a mean crystallite size of 34.7 nm. The optical band gap was calculated from the Tauc plot derived from UV-Vis absorbance data and found to be 3.24 eV, slightly wider than bulk ZnO (3.37 eV) and consistent with quantum confinement effects at the observed particle size. FTIR spectroscopy confirmed the Zn-O stretching mode at 478 $cm^{-1}$ and revealed trace surface hydroxyl groups. Photoluminescence spectra exhibited a near-band-edge emission peak at 378 nm and a broad visible emission band centred at 520 nm associated with oxygen vacancy defects. The synthesised nanoparticles showed strong UV absorption below 380 nm and high optical transparency in the visible range, suggesting suitability for UV-blocking, photocatalytic, and optoelectronic applications.

**Keywords:** *ZnO Nanoparticles, Chemical Precipitation, XRD, Optical Band Gap, Photoluminescence, Nanostructure*

## 1. Introduction

Nanotechnology — the science and engineering of materials and devices with structures and components at the nanometre scale, generally between 1 and 100 nm — has emerged as one of the most transformative research and technology domains of the twenty-first century. When material dimensions are reduced to the nanoscale, quantum mechanical effects become significant, leading to dramatic changes in optical, electrical, magnetic, thermal, and mechanical properties compared to the bulk material. These size-dependent property changes are the basis for a wide range of nanotechnology applications in fields spanning electronics, energy, medicine, agriculture, environmental remediation, and cosmetics.

Zinc oxide (ZnO) is an n-type semiconductor with a wide direct band gap of 3.37 eV and a large exciton binding energy of 60 meV at room temperature, properties that make it highly suitable for UV photodetectors, light-emitting diodes, laser diodes, piezoelectric devices, and photocatalysts. At the nanoscale, ZnO exhibits enhanced surface-to-volume ratios, modified band gaps through quantum confinement, and heightened photocatalytic activity compared to bulk ZnO, making ZnO nanoparticles a subject of intense research interest across physics, chemistry, and materials science. ZnO is also biocompatible, abundant, and relatively low-cost, making it attractive for large-scale application development.

Multiple synthesis routes for ZnO nanoparticles have been reported in the literature, including sol-gel, hydrothermal, co-precipitation, microwave-assisted, and green synthesis methods. Each method produces nanoparticles with characteristic size distributions, morphologies, surface chemistries, and defect profiles that profoundly influence their optical and photocatalytic behaviour. Chemical precipitation — a simple, scalable, low-temperature route that does not require specialised high-pressure or high-temperature equipment — is particularly relevant for resource-limited research settings and has been the subject of extensive optimisation studies to control nanoparticle size and morphology.

This study reports the synthesis of ZnO nanoparticles using an optimised chemical precipitation protocol and provides a systematic optical characterisation using multiple complementary spectroscopic techniques. The structural, vibrational, and optical data generated provide a comprehensive characterisation profile that can serve as a reference for future applied studies utilising these nanoparticles for UV-blocking, photocatalytic degradation, or optoelectronic applications.

## 2. Methodology

ZnO nanoparticles were synthesised by chemical precipitation using analytical-grade reagents without further purification. In a typical synthesis, 0.1 M zinc acetate dihydrate ($Zn(CH_3COO)_2 \cdot 2H_2O$; Merck, 99.5%) solution was prepared in 100 mL of deionised water under constant magnetic stirring at 60°C. PEG-400 (1% v/v) was added as a capping agent to control nanoparticle aggregation and particle size distribution. A 0.2 M sodium hydroxide (NaOH; Merck, 97%) solution was prepared separately and added dropwise to the zinc acetate solution at a rate of 2 mL/min under continuous stirring at 60°C until a white precipitate formed and the pH stabilised at 11–12. The mixture was allowed to age under stirring for 2 hours at 60°C, then cooled to room temperature. The precipitate was collected by centrifugation (8,000 rpm, 15 min), washed three times each with deionised water and ethanol to remove residual ions, and dried at 80°C for 24 hours. The dried precipitate was calcined at 400°C for 2 hours in a muffle furnace to obtain crystalline ZnO nanoparticles.

Structural characterisation was performed using X-ray diffraction (XRD) on a Bruker D8 Advance diffractometer with Cu Kα radiation ($\lambda = 0.1541$ nm) over a $2\theta$ range of 20°–80° at a scan rate of 0.02°/s. Crystallite size was estimated using the Debye-Scherrer equation: $D = K\lambda/(\beta\cos\theta)$, where K is the shape factor (0.94), $\lambda$ is the X-ray wavelength, $\beta$ is the full width at half maximum (FWHM) of the diffraction peak in radians, and $\theta$ is the Bragg diffraction angle. FTIR spectroscopy was performed on a Shimadzu IRPrestige-21 spectrometer in ATR mode over the wavenumber range 400–4000 $cm^{-1}$. UV-Vis absorption spectra were recorded on a Shimadzu UV-2600 spectrophotometer over the wavelength range 200–800 nm using a quartz cuvette with the sample dispersed in absolute ethanol (0.1 mg/mL). The optical band gap was determined from Tauc plots of $(\alpha h\nu)^2$ versus photon energy ($h\nu$). Photoluminescence spectra were recorded at room temperature using a Horiba FluoroMax-4 spectrofluorometer with an excitation wavelength of 325 nm.

## 3. Results and Findings

XRD analysis of the calcined ZnO nanoparticles revealed sharp, well-defined diffraction peaks at 2θ positions of 31.8°, 34.4°, 36.2°, 47.5°, 56.6°, 62.8°, 66.3°, 67.9°, and 69.0°, corresponding to the (100), (002), (101), (102), (110), (103), (200), (112), and (201) crystal planes respectively. All peaks were indexed to the hexagonal wurtzite structure of ZnO (JCPDS card No. 36-1451) with no secondary or impurity phase peaks, confirming phase-pure synthesis. Lattice parameters calculated from peak positions were a = 0.325 nm and c = 0.521 nm, in close agreement with standard ZnO values (a = 0.3250 nm, c = 0.5207 nm). The mean crystallite size estimated from the Scherrer equation applied to the (101) peak was 34.7 nm.

FTIR spectroscopy revealed a strong absorption band at 478 $cm^{-1}$, characteristic of the Zn-O stretching vibration mode and confirming the formation of ZnO. Broad absorption bands in the 3200–3500 $cm^{-1}$ region were attributed to O-H stretching vibrations from surface-adsorbed hydroxyl groups, while C-H stretching modes observed at 2920 $cm^{-1}$ indicated trace residual PEG capping agent on the nanoparticle surface. UV-Vis absorption spectra showed a strong absorption onset at approximately 368 nm with a prominent excitonic absorption shoulder near 355 nm, consistent with ZnO's UV absorption characteristics. The Tauc plot analysis yielded an optical band gap (Eg) of 3.24 eV, slightly lower than bulk ZnO's 3.37 eV, consistent with the influence of quantum confinement effects and surface states at the observed particle size.

Room-temperature photoluminescence spectra under 325 nm excitation exhibited two distinct emission features. A sharp near-band-edge (NBE) emission peak was observed at 378 nm (3.28 eV), corresponding to the recombination of free excitons and confirming the optical quality of the synthesised nanoparticles. A broad, intense visible emission band centred at approximately 520 nm (2.38 eV) was also observed, commonly attributed in ZnO literature to deep-level emission from oxygen vacancy (Vo) defects within the crystal lattice. The relative intensity of the visible defect emission band with respect to the NBE peak provides an indirect measure of the concentration of oxygen vacancies, which are relevant to photocatalytic performance as they serve as active sites for oxidative reactions.

## 4. Discussion

The XRD-confirmed wurtzite crystal structure and phase purity of the synthesised ZnO nanoparticles validate the optimised precipitation protocol. The mean crystallite size of 34.7 nm places the particles in the range where quantum confinement effects are measurable in optical properties, as evidenced by the observed band gap widening relative to bulk ZnO. The modest blue-shift of 0.13 eV from the bulk band gap value (3.37 eV to 3.24 eV) is consistent with the mild quantum confinement regime applicable to particles in the 30–50 nm range, in agreement with theoretical predictions based on effective mass approximation models for ZnO nanoparticles.

The strong UV absorption below 380 nm combined with high transparency in the visible region (no significant absorption above 400 nm in the UV-Vis spectrum) makes the synthesised ZnO nanoparticles well-suited as UV-blocking agents in sunscreen formulations, UV-resistant polymer coatings, and transparent UV-protective films. The observed photoluminescence band at 520 nm, associated with oxygen vacancy defects, is characteristic of synthesis by chemical precipitation and calcination and is known to correlate with photocatalytic activity in ZnO nanoparticles, since oxygen vacancies facilitate charge carrier generation and separation under UV irradiation.

The PEG-400 capping strategy successfully prevented excessive particle aggregation as evidenced by the relatively narrow XRD peak widths and the single-phase XRD pattern. However, residual PEG signature in the FTIR spectrum suggests that calcination at 400°C was not fully sufficient to remove the organic capping layer. Higher calcination temperatures (above 500°C) or longer calcination durations could more completely remove surface organics but risk grain growth and loss of nanoparticle surface area. This trade-off between surface

cleanliness and particle size is an important experimental parameter for optimisation in future studies focused on photocatalytic application.

## 5. Conclusion

ZnO nanoparticles with a mean crystallite size of 34.7 nm and hexagonal wurtzite crystal structure were successfully synthesised by an optimised chemical precipitation method. The synthesised material exhibited a band gap of 3.24 eV, strong UV absorption below 380 nm, FTIR-confirmed Zn-O bonding, and characteristic near-band-edge and defect-related photoluminescence emissions at 378 nm and 520 nm respectively. These properties collectively confirm the suitability of the synthesised ZnO nanoparticles for UV-blocking, photocatalytic, and potentially optoelectronic applications.

Future work should include: (i) systematic parametric optimisation of synthesis conditions (NaOH concentration, temperature, ageing time, calcination temperature) to achieve targeted particle size distributions; (ii) photocatalytic degradation experiments using the synthesised nanoparticles against model organic dye pollutants (methylene blue, rhodamine B) to quantify structure-activity relationships; (iii) transmission electron microscopy and selected area electron diffraction for direct particle morphology imaging; and (iv) exploring green synthesis alternatives using plant extract reducing agents to produce environmentally benign ZnO nanoparticles for biomedical applications.

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