

Structural and Optoelectronic properties of Cr doped Zinc Oxide Nanostructure Synthesized by chemical co-precipitation Process

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Abstract: Chromium-doped ZnO samples were prepared using a chemical co-precipitation method at ambient temperature. The structural, optical and morphological characteristics of the Cr-doped ZnO samples were examined using X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy, UV-Visible (UV-Vis) spectroscopy and Field Emission Scanning Electron Microscopy (FESEM). The X-ray diffraction (XRD) patterns indicate that the samples possessed a hexagonal wurtzite structure without any extra peaks, implying that Cr ions occupied the regular Zn sites within the ZnO crystal lattice. The lattice constants were determined through the analysis of X-ray diffraction data. This reveals that the lattice parameters increase with increase in the Cr content. The mean crystallite size was calculated using Scherrer's formula for both pure and chromium-doped ZnO samples. The crystallite size has been determined to be within the range of 12–13 nm. The band gap of the $\text{Zn}_{1-x}\text{Cr}_x\text{O}$ samples were assessed using UV-Vis spectroscopy. The band gap decreases as the Cr concentration increases, which may be ascribed to the interactions between s-d and p orbitals, as well as the increase in average crystallite size. This suggests that Cr ions were incorporated into the ZnO matrix and is significantly modifying the material property. The chemical species present in the grown crystals were identified using Fourier transform infrared spectroscopy (FTIR). The FTIR spectra revealed IR peaks corresponding to the Zn-O bands. FESEM reveals a shift from uniform nanoparticles to elongated columnar crystallite as the Cr concentration increases.

Key words: MnFe_2O_4 nanoparticles, Ca-doping, Spinel ferrite, Sol-gel auto-combustion.

1 Introduction

Studying the structural properties of Cr-doped Zinc Oxide (ZnO) nanoparticles is paramount to understanding their fundamental behaviour and optimizing them for various technological applications, particularly in the fields of spintronics and optoelectronics [1]. ZnO is a widely investigated II-VI semiconductor with a hexagonal wurtzite crystal structure, which is thermodynamically stable under ambient conditions [2]. Its intrinsic properties, such as a direct wide bandgap and large exciton binding energy, make it widely studied system [3]. When chromium (Cr) is introduced as a dopant into the ZnO lattice, it can significantly alter the properties of the host lattice. The chemical co-precipitation

method is a widely adopted synthesis route for producing Cr-doped ZnO nanoparticles. This technique is favoured because of its simplicity, cost-effectiveness, and ability to achieve homogeneous doping and control the particle size and morphology. Precise control over the synthesis parameters, such as pH, temperature, and precursor concentrations, is crucial in dictating the final structural characteristics of nanoparticles [4].

The intrinsic properties of ZnO can be customized or drastically altered by changing the crystallization conditions, adjusting the grain boundaries, or deliberately introducing specific impurities into its matrix. Doping with 3d transition metal (TM) ions (such as Mn, Fe, Co, Ni, and Cr) has

proved to be a highly effective approach to engineering the band structure, optical absorption edges, and magnetic profiles of ZnO nanostructures.

Replacing Zn^{2+} with open-shell transition metal ions converts the host material into a Diluted Magnetic Semiconductor (DMS). DMS systems utilize both the charge and spin of electrons, which is an absolute requirement for developing functional spintronic architectures like spin filters, non-volatile magnetic random-access memories (MRAM), and spin-polarized LEDs.

Chromium (Cr) is an exceptionally promising dopant candidate within the transition metal block. The ionic radius of chromium ions Cr^{3+} , approximately 0.061 nm or Cr^{2+} , approximately 0.073 nm is comparable to that of the host Zn^{2+} ion (0.074 nm), which favours smooth substitutional incorporation into the tetrahedral interstitial coordinates of the wurtzite lattice without triggering severe structural disintegration or clustering.

Furthermore, chromium introduces partially filled 3d electron shells that generate a unique interaction profile between the localized magnetic states and the free carriers of the semiconductor band. However, the exact structural alterations and the resulting optoelectronic trends—such as whether the band gap broadens or narrows upon chromium addition—continue to trigger debate, with results varying heavily based on synthesis pathways and crystalline defects. Here is a more polished, coherent, and publication-quality version suitable for a high-impact journal: Consequently, selecting a reliable, reproducible, and scalable synthesis strategy is essential for producing high-quality Cr-doped ZnO nanostructures with controlled physicochemical properties. Various preparation techniques, including sol-gel processing, hydrothermal synthesis, laser ablation, microwave-assisted methods, combustion synthesis, and chemical co-precipitation, have been employed to fabricate chromium-doped ZnO nanostructures. Among these, the chemical co-precipitation route is particularly attractive because it

is a simple, cost-effective, low-temperature process that requires minimal instrumentation, offers high product yield, and ensures excellent compositional homogeneity. Numerous studies have examined the structural, optical, and magnetic properties of Cr-doped ZnO nanoparticles synthesized by different methods. Sol-gel-derived Cr-doped ZnO has been reported to exhibit enhanced crystallinity, accompanied by variations in lattice parameters and a concentration-dependent decrease in the optical band gap, primarily attributed to defect generation and sp-d exchange interactions between the localized Cr 3d electrons and the ZnO band states [5,6]. Likewise, hydrothermal and combustion synthesis routes have demonstrated that chromium incorporation significantly influences crystallite size, surface morphology, and defect concentration, thereby modifying the optical and magnetic characteristics of ZnO nanostructures [7,8]. However, the reported results remain inconsistent. While some studies have observed lattice contraction accompanied by band-gap widening, others have reported lattice expansion together with band-gap narrowing. These discrepancies are generally attributed to variations in synthesis conditions, chromium oxidation state, dopant concentration, the possible formation of secondary phases, and the density of intrinsic defects, particularly oxygen vacancies.

Therefore, establishing a comprehensive relationship between the synthesis route, structural evolution, defect chemistry, and the resulting optoelectronic properties remains a significant scientific challenge. In this context, the present study employs a facile room-temperature chemical co-precipitation method to synthesize Cr-doped ZnO nanostructures and systematically investigates the influence of chromium incorporation on their crystal structure, crystallite size, morphology, and optical band-gap evolution.

This paper reports a detailed investigation into the structural and optoelectronic properties of $\text{Zn}_{1-x}\text{Cr}_x\text{O}$ nanostructures

synthesized via an ambient chemical co-precipitation route. The synthesized materials have been studied using XRD, FTIR, FESEM and U-V spectroscopy. The band gap is found to decrease with Cr- doping, which is directly linked with crystallite size. The paper provides an in-depth interpretation of lattice parameter variations, nanoscale crystallite sizing, morphology transformations, chemical bonding states, and electronic bandgap modifications dictated by the inter-orbital exchange interactions.

2 Experimental

2.1 Sample Preparation

The chemical co-precipitation technique was employed to synthesize Cr-doped ZnO nanoparticles ($\text{Zn}_{1-x}\text{Cr}_x\text{O}$: $x = 0.00$, and 0.04). In this procedure, raw chemicals $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ were employed for the synthesis of nanoparticles [9]. All raw materials were sourced from SRL and used without any additional alterations. All glassware were thoroughly cleaned with acetone to ensure the absence of impurities. The specified materials, in their stoichiometric proportions, were combined with 200 ml of deionized water in a beaker. A total of 500 mg of PVP was incorporated into the solution, which functions as a binding agent. The beaker containing the solution was placed on a magnetic stirrer and rotated at 700 rpm for 10 minutes to achieve a uniform mixture. Subsequently, NaOH was gradually introduced in droplet form to the solution, serving as a precipitating agent. The addition of NaOH droplets persisted until the pH of the solution reached 12, while maintaining the same rotational conditions. The

entire reaction occurred in a basic environment, resulting in precipitation. Furthermore, the precipitate was thoroughly washed multiple times with distilled water followed by ethanol to ensure that the pH was reduced to 7, achieving neutrality. The precipitate was then placed in a Petri dish and allowed to dry at room temperature [10]. The dried precipitate was then ground using a mortar and pestle. The synthesized pure ZnO and Cr-doped ZnO nanoparticles were analyzed using various techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and ultraviolet-visible spectroscopy (UV-Vis).

2.2 Characterisation

To explore the structural characteristics of both undoped ZnO and Cr-doped ZnO, X-ray diffraction (XRD) analyses were conducted using a Rigaku Mini Flex 600 spectrometer. To investigate the vibrational frequency modes and confirm the hexagonal structure, Fourier Transform Infrared (FTIR) spectroscopy was conducted on the synthesized $\text{Zn}_{1-x}\text{Cr}_x\text{O}$ ($x = 0.00$ and 0.04) samples using a Bruker Tensor 27 spectrometer.

Field Emission Scanning Electron Microscopy (FESEM) was employed to investigate the surface morphology using a SIGMA 300 instrument (Carl Zeiss Microscopy, Hamburg, Germany). The optical properties were examined using UV-Visible (UV-Vis) absorption spectroscopy with a PerkinElmer Lambda 950 spectrometer.

3 Results and Discussion

3.1 X-ray Diffraction (XRD)

Figure 1 shows the XRD pattern of $\text{Zn}_{1-x}\text{Cr}_x\text{O}$ ($x = 0.00$ and 0.04) samples featuring distinct diffraction peaks corresponding to the (100), (002), (101), (102), (110), (103), (200), (112), and (201) lattice

planes of wurtzite hexagonal ZnO structure. The XRD patterns demonstrate that the peaks of ZnO shift towards higher angle with the incorporation of Cr ions in the ZnO sample. This shift in the XRD peaks in-

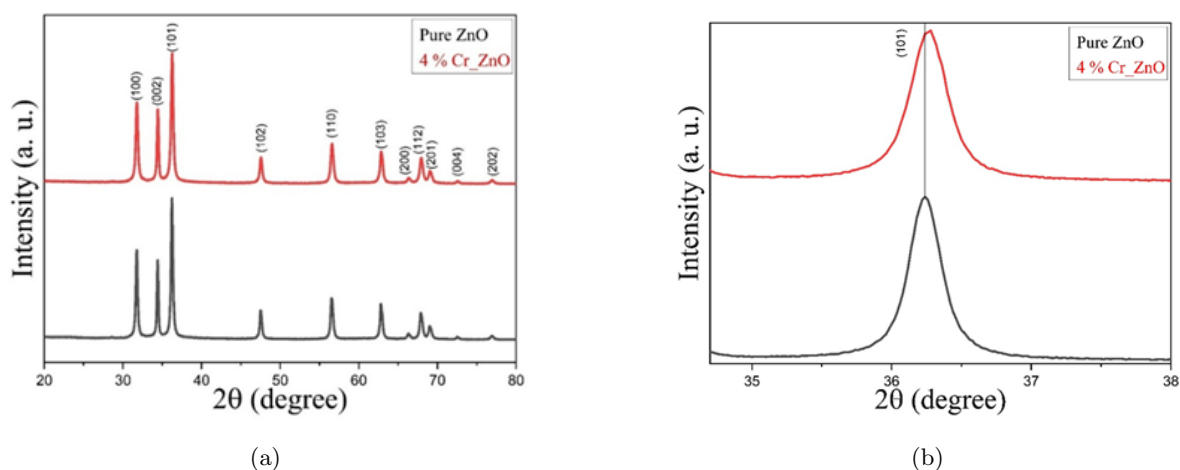


Figure 1: (a) XRD Pattern of undoped and Cr-doped ZnO. (b) XRD Pattern of shift most intense peaks relative to the corresponding peak of undoped ZnO.

dicating lattice expansion resulting from the substitution of Cr for Zn within the ZnO crystal lattice. This demonstrates a slight increase in the lattice constant as the Cr concentration increases. Table 1 shows that the lattice constant of ZnO increases with incorporation of Cr in ZnO host. A precise look at the lattice parameters reveals an interesting trend. The lattice dimensions a and c for the hexagonal cell were calcu-

lated using the standard crystallographic formula:

$$\frac{1}{d_{hkl}^2} = \left(\frac{4}{3}\right) \left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

The calculated values of the lattice parameters show that both the lattice parameters a and c expand with incorporation of chromium ion.

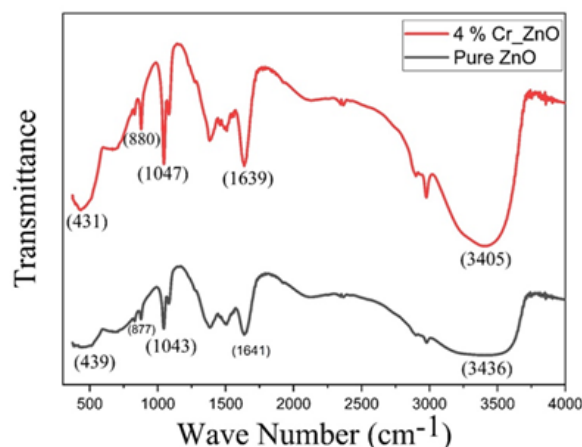


Figure 2: FTIR spectra of undoped and Cr-doped ZnO nanoparticles.

The observed structural expansion can be explained by the changes in the local lattice environment induced by chromium substitution. Although the ionic radius of six-coordinated Cr³⁺ (0.061 nm) is smaller than that of Zn²⁺ (0.074 nm), the incor-

poration of chromium ions into the ZnO lattice can generate local lattice distortions due to differences in valence state, bonding characteristics, and defect formation during room-temperature co-precipitation. These distortions may also be influenced by

Table 1: Crystalline parameters of undoped and Cr doped

Sl. no.	Cr-doping	b (rad)	Crystallite size (D) in nm	d-spacing (Å)	Lattice Parameter		Volume, $a^2 \times c$ (Å) ³	Microstrain (e)
					a=b (Å)	c (Å)		
1	00	0.0106	13.660 (±0.001)	2.475	3.2350 (±0.001)	5.2010 (±0.001)	47.136	8.63×10^{-3}
2	04	0.0120	12.070 (±0.001)	2.475	3.258 (±0.001)	5.2190 (±0.001)	47.974	9.81×10^{-3}

the possible presence of chromium in different oxidation states under the synthesis conditions.

The lattice expansion is primarily attributed to the redistribution of local charge density, the generation of point defects such as oxygen vacancies, and the resulting modification of interatomic interactions within the ZnO crystal structure. Chromium incorporation alters the local crystal field and internal lattice strain, producing a slight increase in the lattice parameters despite the smaller ionic radius of Cr³⁺.

The mean crystallite size D of the nanostructures was calculated using Scherrer's

standard equation:

$$D = \frac{K\lambda}{\beta \cos \theta}$$

The average crystallite size (D) of the synthesized nanostructures was determined using Scherrer's equation. The calculated crystallite sizes lie within the narrow range of 12–13 nm and exhibit a slight increase with increasing chromium concentration. This gradual increase in crystallite size suggests that chromium doping promotes crystal growth during thermal annealing, resulting in a modest enhancement of the average crystallite volume and improved crystallinity.

3.2 Fourier Transform Infrared (FTIR)

The FTIR spectra of both pure and Cr-doped ZnO nanoparticles are shown in Figure 2. The chemical species, local functional bonds, and structural defects in the grown nanostructures were analysed via Fourier Transform Infrared (FTIR) spectroscopy. The recorded spectra for both pristine and chromium-doped samples show a prominent, sharp absorption band located between 430 cm⁻¹ and 540 cm⁻¹ which represents the standard stretching vibration of the zinc-oxygen Zn-O bond in a tetrahedrally coordinated wurtzite lattice.

With chromium doping, this particular absorption peak shift toward different wavenumber, confirming the substitution of zinc by chromium ions and the resulting rearrangement of local bond strain. Zn-O peak shift from 439 cm⁻¹ to 431 cm⁻¹ due to 4% Cr-doping indicates weakening of the Zn-O bond due to lattice distortion and increased bond length after Cr- incorporation.

The wider absorption features observed near 3420 cm⁻¹ and 1615 cm⁻¹ are assigned to the stretching O-H and bending O-H vibrations of surface-absorbed water molecules and residual hydroxyl groups. The absence of other prominent organic bands confirms the high purity of the samples processed via co-precipitation.

The FTIR spectra of the pure sample in this study closely resembled those of the Cr-doped ZnO samples and aligned well with previously reported values [11-14].

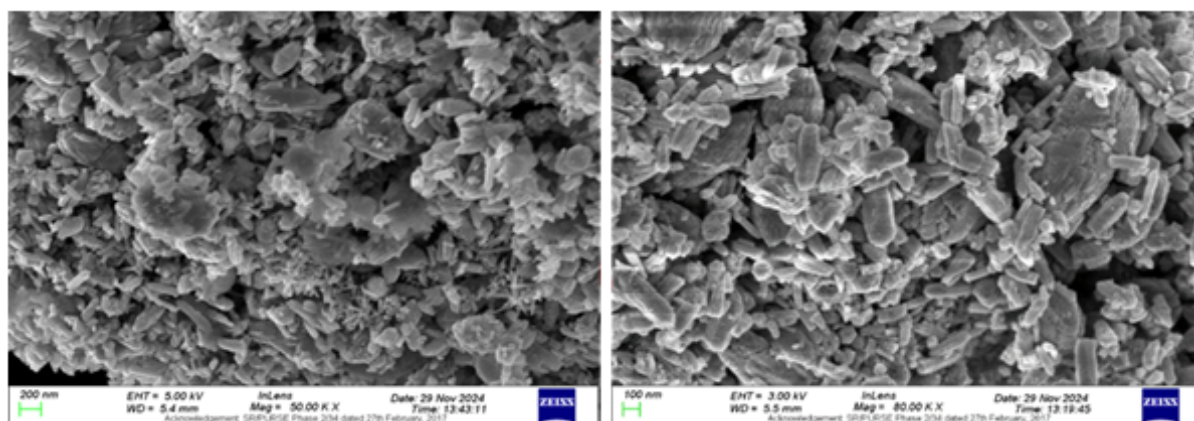


Figure 3: FESEM image of: Undoped ZnO and 4% Cr doped ZnO.

3.3 Field Emission Scanning Electron Microscopy (FESEM)

Field Emission Scanning Electron Microscopy (FESEM) images as shown in figure 3 reveal significant microstructural and morphological evolution in response to

chromium doping. Pure Zinc Oxide exhibits uniform, isotropic, closely packed spherical nanoparticles with minimal agglomeration. The individual particle dimensions match well with the grain metrics calculated via the Scherrer formula.

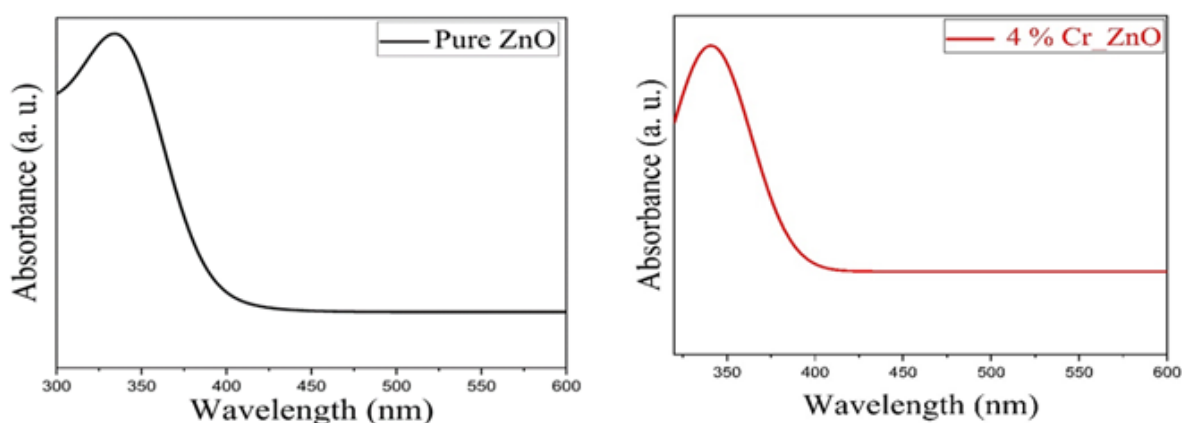


Figure 4: UV-Visible absorption spectra of Undoped ZnO and 4% Cr doped ZnO.

With incorporation of Chromium in the ZnO host lattice, the morphology changes from spherical shapes to elongated, highly anisotropic columnar grains. This structural transformation suggests that chromium ions preferentially adsorb onto specific crystallographic growth planes of ZnO during co-precipitation. By altering the surface free energy, the presence of chromium suppresses isotropic growth and promotes unidirectional assembly, producing distinct columnar features.

3.4 UV-Visible

The UV-Vis spectra at room temperature for both undoped and Cr-doped ZnO samples are presented in Figure 4. A maximum absorption was observed for all samples, indicating a red shift compared to the bulk ZnO samples. This observed red shift in the absorption edge can be attributed to the reduced particle size. The band gap was determined by plotting the absorption data (E) against $(\alpha h\nu)^2$. The band gaps of the chromium-doped ZnO samples ranged from

3.495 to 3.472 eV. Figure 5. shows that the α -absorption shifts slightly towards lower energy levels as the chromium content increases. Furthermore, the band gap decreased with increasing Cr concentration.

The findings are summarized in Table 2. The reduction in the band gap (E_g) with increasing Cr content is ascribed to the interactions between the s-d and p states, as well as the smaller average grain size.

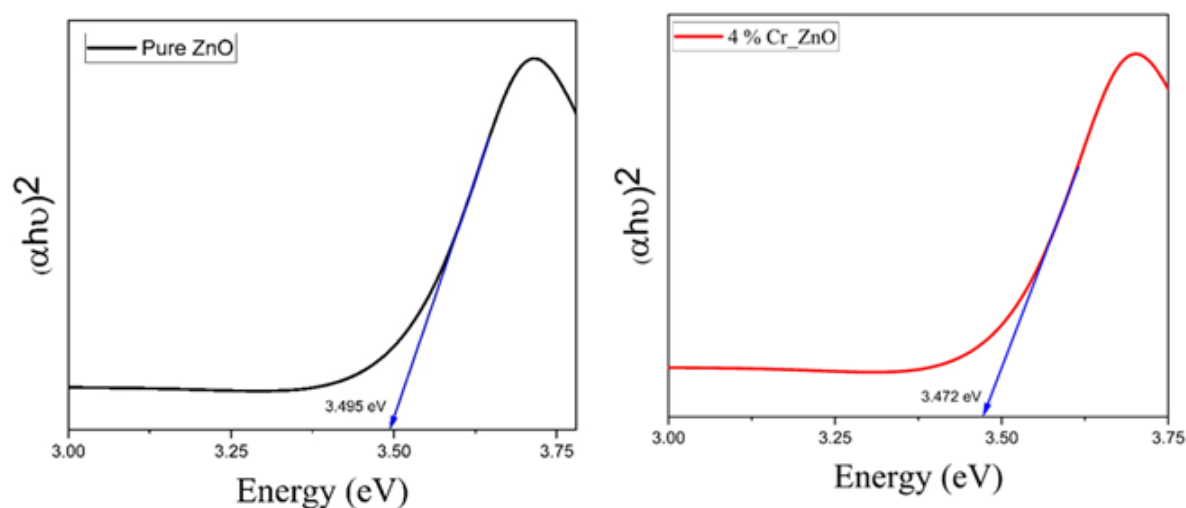


Figure 5: Tauc plots of: Undoped ZnO and 4% Cr doped ZnO.

Table 2: Band gaps of undoped and Cr-doped ZnO samples

Sl. No.	Sample Id	Energy band gap (eV)
1.	Undoped ZnO	3.495
2.	4% Cr doped ZnO	3.472

The primary cause of bandgap reduction is the strong spin-exchange interaction between the localized band states s-like conduction band states and p-like valence band states of the host ZnO matrix and the localized 3d electron orbitals of the replacing Cr ions. The s-d exchange interaction shifts the conduction band edge downward, while the p-d exchange interaction pushes the valence band edge upward, thus narrowing the fundamental band gap.

The structural analysis confirms a simultaneous increase in the average crystallite size. This growth slightly reduces quantum confinement configurations across the boundary interfaces, allowing the absorption edges to shift toward lower energies.

4 Conclusion

Single-phase chromium-doped zinc oxide nanostructures have been successfully synthesized via a chemical co-precipitation route at ambient temperature. Structural validation via X-ray diffraction confirmed the formation of a pure hexagonal wurtzite matrix without any secondary chromium oxide or metallic cluster impurities, proving that Cr ions substitute cleanly into the Zn^{2+} sites.

The lattice metrics a and c expand with doping of Chromium, while the mean crystallite size ranges between 12 and 13 nm. FESEM analysis revealed a striking morphological transition from uniform spherical nanoparticles to elongated columnar grains due to doping of chromium. FTIR

analysis verified the presence of the characteristic tetrahedral Zn-O framework stretching vibrations.

Finally, UV-Vis spectrophotometry demonstrated a systematic reduction in the direct optical band gap due to chromium doping. This red-shift behaviour is attributed to strong sp-d spin-exchange interactions between the host band states and the localized 3d orbitals of the chromium dopants. These combined structural, morphological, and optoelectronic modifications confirm that chemically synthesized $\text{Zn}_{1-x}\text{Cr}_x\text{O}$ nanostructures are highly promising materials for advanced optoelectronic assemblies and spintronic devices.

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Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

Data Availability Statement

All the data used are included in the manuscript and they can be made available separately on rea-

sonable request.

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