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Effect of solvents on the structural and optical properties of ZnO nanoparticles and ZnO-CNT nanohybrids

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Introduction

- In this work, we studied the structural, morphological and optical properties of ZnO nanoparticles (NP) synthesized using aqueous and non-aqueous ethanol with anhydrous and dihydrate acetate precursors, and ZnO-CNT nanohybrids (NH).
- Table.1 provides the list of samples synthesized in this study with hydrated and dehydrated precursors along with the solvents .
- By changing the solvent medium and zinc precursor ZnO NP of different shapes and sizes were obtained.
- A ~5 fold enhancement in the near band emission (NBE) and suppression in the defect level emission (DLE) were observed from ZnO-CNT nanohybrids, indicating passivation of surface states.

Various defects in ZnO NP

Depending on the synthesis conditions (temperature, time, solvent and precursor) ZnO NP contain various emitting surface or volume defects (Fig. 1).

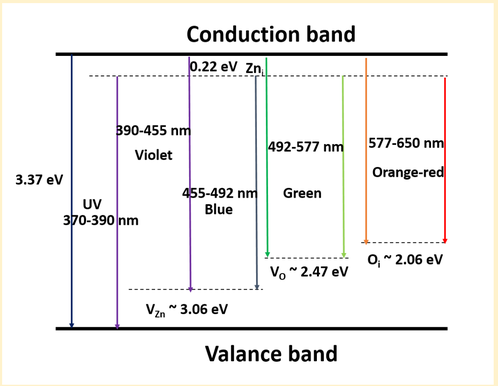

Figure 1. Defects in the structure of ZnO NP.

Sample Name	Solvent	Zinc Precursor	Ratio
A	Pure ethanol	Zinc acetate anhydrous	1:2
B	Pure ethanol	Zinc acetate dihydrate	1:2
C	70% ethanol	Zinc acetate dihydrate	1:2
D	70% ethanol	Zinc acetate dihydrate	1:1.5
E	70% ethanol	Zinc acetate dihydrate	1:3
D-CNT	70%ethanol	Zinc acetate dihydrate	1:1.5
E-CNT	70% ethanol	Zinc acetate dihydrate	1:3

Table 1. List of samples, ratios correspond to quantities of zinc precursors to NaOH.

XRD and FTIR results

- Figure 2 shows the XRD patterns of ZnO NP. The peaks (100), (002), (101), (102), and (110) correspond to hexagonal Wurtzite structure (a = 3.25 Å and c = 5.20 Å) of ZnO. The calculated particle sizes of samples A, B, and C are ~4.8 nm, ~9.2 nm, and ~48 nm, respectively, from Scherrer's equation.
- Figure 3 consists of FTIR spectra of ZnO NP prepared using two solvents and two precursors. The hydroxyl, organic and metal-oxygen bands obtained from the spectra are indicated.

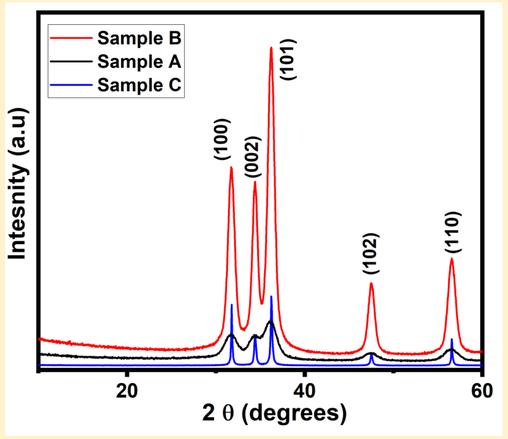

Figure 2. XRD patterns of samples B, A and C.

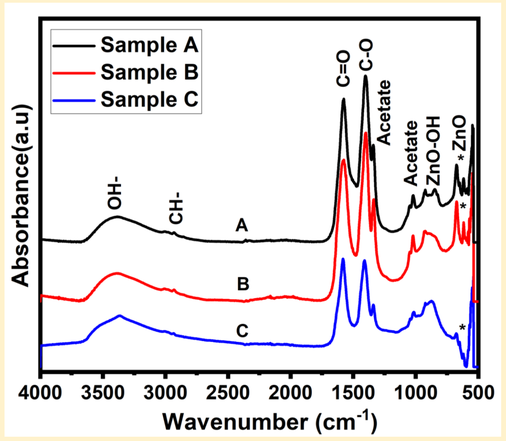

Figure 3. FTIR spectra of samples A, B and C

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Conclusions

- Using aqueous ethanol route in the synthesis produces ZnO NP with a variety of sizes and shapes.
- The hydrolytic route that uses dihydrate acetate precursor with non-aqueous ethanol is capable of producing spherical ZnO NP of more uniform sizes .
- XRD patterns highlight that no secondary phases is formed during the synthesis.
- Presence of water during the synthesis creates a well-oxygenated ZnO with almost negligible point and extended defects.
- ZnO synthesized with pure ethanol harbors both volume and surface related defects.
- Combining ZnO with CNT is effective in passivating surface defects and increasing the UV emission due to suppression of these trap states.

TEM results

TEM study shows that samples A and B have spherically shaped ZnO NP with the average particle sizes of ~5 nm, smallest among the three samples. Needle and hexagonal shaped NP are present in sample C, whose particle size is the highest. These results corroborate with the XRD results.

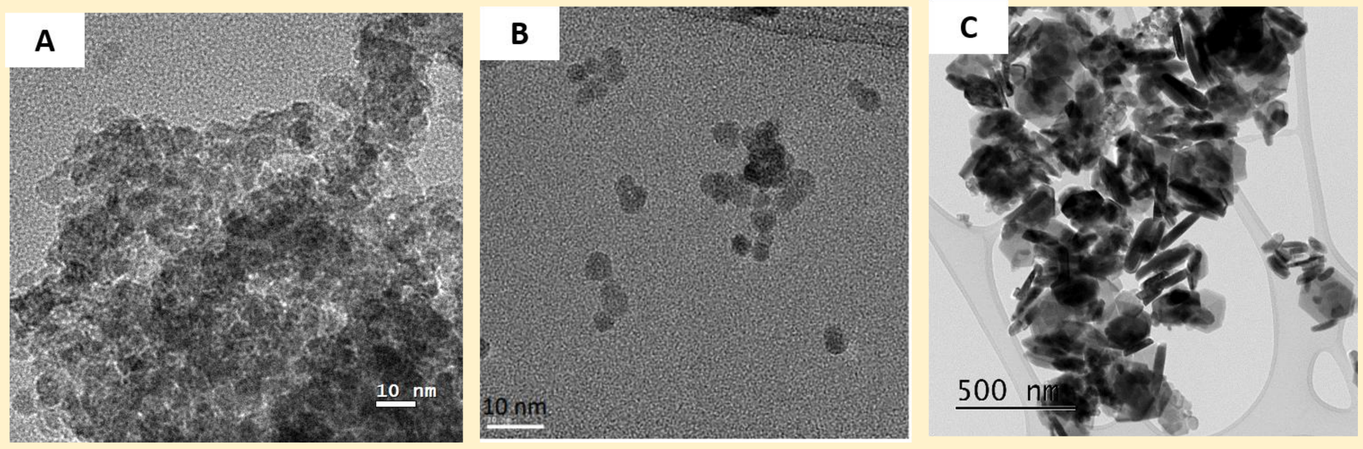

Figure 4. TEM images of ZnO NP for (a) Sample A, (b) Sample B, and (c) Sample C.

PL spectroscopy results

- In figure 5, the quantum yield of sample C is the lowest as compared to samples A and B. This suggests non-radiative defect states are present in sample C.
- In samples A and B, the DLE region is dominated by green components at ~2.5 and ~2.2 eV which correspond to volume (V_O^+) and surface (V_O^{++}) oxygen vacancies, respectively.
- Volume and surface related oxygen vacancies are negligible in sample C, synthesized in the presence of water.

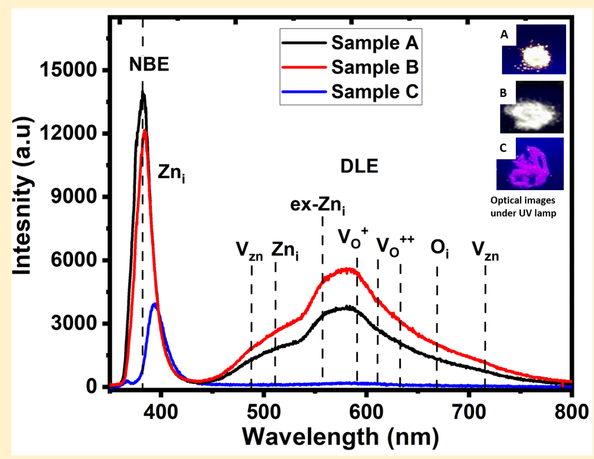

Figure 5. PL emission spectra of samples A, B and C. The inset shows their respective optical images under a UV lamp of 365 nm wavelength.

For the ZnO-CNT samples

- The DLE is suppressed and the NBE is amplified and blue-shifted.
- A ~5-fold enhancement in the UV emission from ZnO-CNT nanohybrids was obtained.
- PL emission from surface oxygen vacancies (V_O^{++}) at ~2.2 eV was suppressed by adding CNT as it blocks the adsorption of O_2^- and OH^- on the surface of ZnO NP.

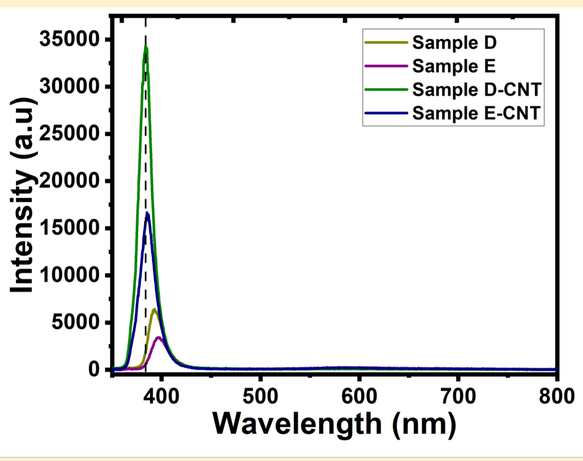

Figure 6. PL emission spectra of samples D, E, D-CNT and E-CNT.

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