Electronic Supplementary Information

Chemically derived defects in ZnO synthesized in different organic solvents and their photocatalytic activities

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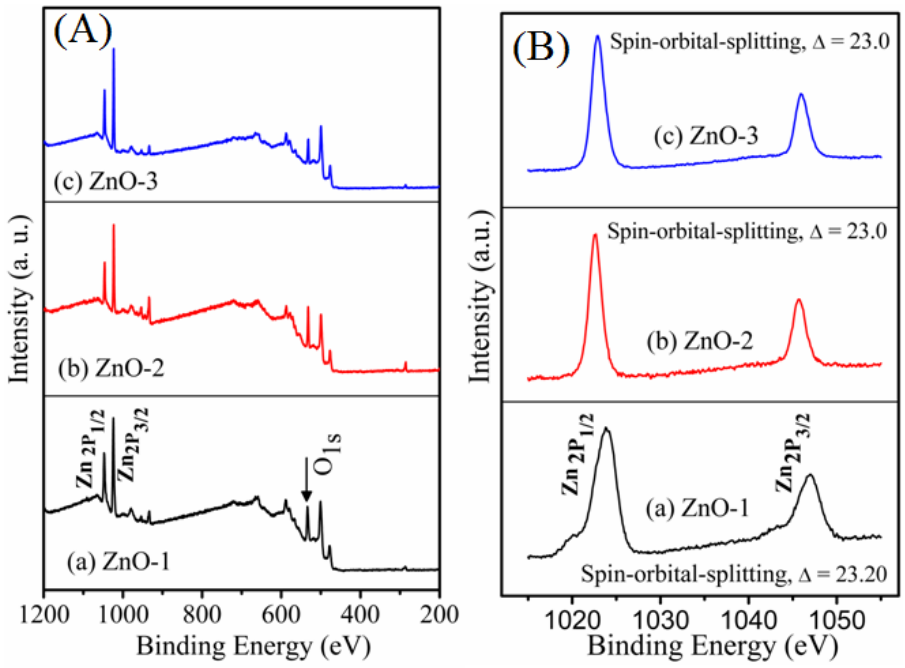

Figure S1. (A) X-ray photoelectron survey spectrum of the different ZnO NCs where main photoelectron peaks can be assigned to Zn2p and O1s derived bands. (B) Zn2p doublet spectral lines of ZnO-1, ZnO-2 and ZnO-3.

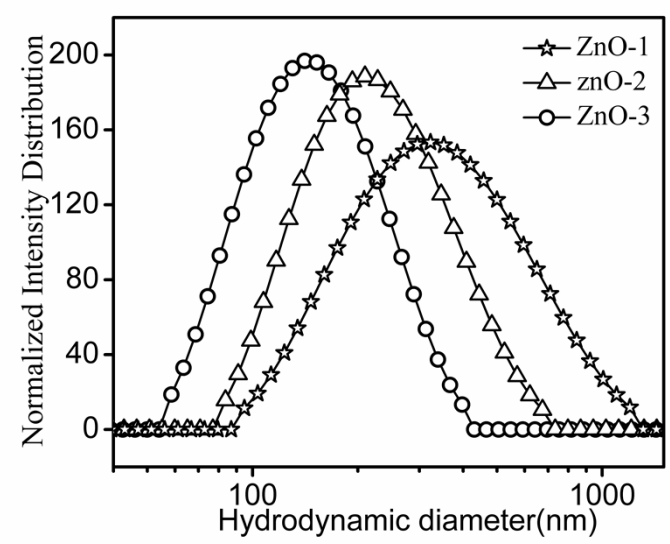

Figure S2. Hydrodynamic diameter (nm) of ZnO-1, ZnO-2 and ZnO-3 NCs.

The hydrodynamic diameter (H_D) of ZnO NCs are exhibited in Figure S2. The H_D of ZnO-1, ZnO-2 and ZnO-3 are 350, 200 and 100 nm respectively and follow the same order as exhibited in their respective TEM microstructures.

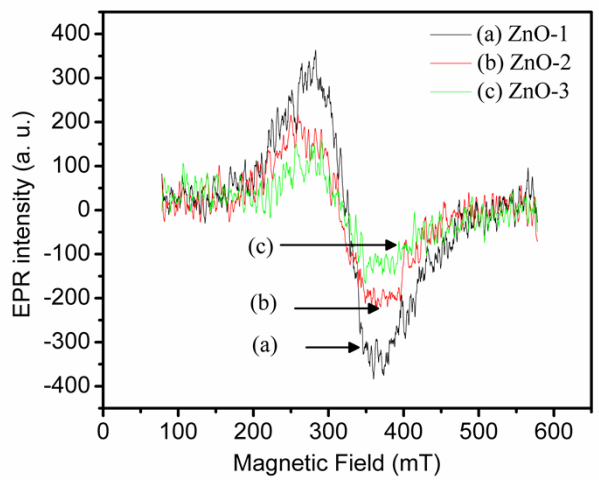

Figure S3. EPR spectra of (a) ZnO-1, (b) ZnO-2 and (c) ZnO-3 NCs.

To confirm our hypothesis of ZnO-1 having highest SDs as discussed in PL spectra (Figure 9), Electron Paramagnetic Resonance (EPR) spectra of samples have been recorded and investigated. The EPR is widely accepted as a very sensitive local probe to detect paramagnetic defects/centers in pristine ZnO. For comparison, the measurements were done at same parameters having equal weight of samples. Figures S3 depict the EPR spectra of ZnO-1, ZnO-2 and ZnO-3 measured at the X band (8.75-9.65 GHz). A strong EPR signal at ~ 338.7 mT appears in all ZnO samples (Figure S3). This suggests that these NCs possess the same types of paramagnetic defects due to singly charged oxygen vacancies with unpaired electrons (V_{oS}^{+}) available at the surface of ZnO [1, 2]. It has been observed that g values of all ZnO NCs are same whereas the intensity of the signal at g ~ 1.9929 in ZnO-1 is considerably suppressed as compared to ZnO-3. Here, the intensity of EPR signals of ZnO NCs at g ~ 1.9929 follows almost the same trend as that of visible emission in the PL spectra (Figure 9).

References

1. A. Prakash, S. K. Misra and D. Bahadur, *Nanotechnology*, 2013, 24, 095705.
2. B. Panigrahy, M. Aslam, D. S. Misra, M. Ghosh and D. Bahadur, *Adv. Funct. Mater.*, 2010, 20, 1161-1165.