† Electronic Supplementary Information (ESI) available:

ES1- X-ray Diffraction analysis of synthesized ZnO:

Fig. (ES1) shows the Rietveld refinement of the X-ray diffraction (XRD) pattern for ZnO nanoparticles (NPs) synthesized by sol-gel method.

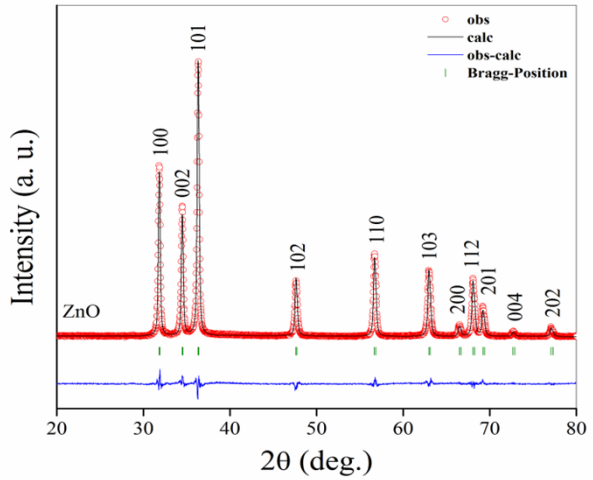

Fig ES1: XRD pattern of synthesized ZnO nanoparticles.

The well resolved peaks observed in the X-ray diffraction pattern indicate that ZnO NPs possess single phase. The red circles represent the observed data while solid line through red circles is the calculated profile. All peak positions of prepared ZnO NPs corresponding to the standard Bragg positions of hexagonal wurtzite ZnO (space group P63mc) have been shown by the vertical bars and the residue by the line respectively at the bottom of the XRD patterns and no trace of other impurities is found. The XRD pattern shows that the prepared ZnO has hexagonal wurtzite structure (with a = b =3.25 Å, c = 5.20 Å) belonging to the C46v space group (P63mc) and indexed using the standard JCPDS file for ZnO (JCPDS 36-1451). The average grain size, D, of the ZnO NPs is estimated using the Debye–Scherrer's equation

$$\frac{0.9\lambda}{\beta\, Cos\theta}$$

where, D is the particle size, λ the wavelength of radiation used (λ = 1.5406 Å), θ the Bragg angle and β is the full width at half maxima (FWHM). The average crystallite size calculated by using the Debye–Scherrer's equation is 30 nm.

ES2: TEM and SEAD images of pure ZnONPs and [PZCDT/ PZbCDT+ZnONPs]:

A typical TEM and SEAD (selected area electron diffraction) images of pure ZnONPs, complexes [PZCDT+ZnO] and [PZbCDT+ZnO] are presented in Fig. ES2. The ZnONPs are nearly spherical in shape with size between 20 and 30 nm. The average particle size obtained from TEM measurement matches well with size estimated from the XRD study. The selected area electron diffraction (SAED) pattern (Fig. ES2 (b)) shows the crystalline nature and the hexagonal-like shape of ZnONPs. Fig. ES2 (c), (d) and ES2 (e), (f) represents TEM and SAED image of complexes [PZCDT+ZnO] and [PZbCDT+ZnO] respectively. In Fig. ES2(c) and ES2(e), we observed changes in TEM images of pure ZnONPs on adsorption of PZCDT and PZbCDT. Fig. ES2 (d) and ES2(f) show SAED images of complexes [PZCDT+ZnO] and [PZbCDT+ZnO] respectively.

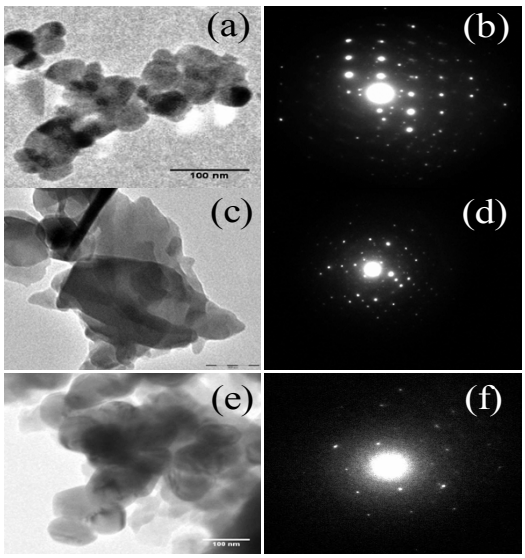

Fig.[ES2]: TEM images of (a) ZnONPs, (c) [PZCDT+ZnO], (e) [PZbCDT+ZnO], and SEAD images of (b) ZnONPs (d) [PZCDT+ZnO], (f) [PZbCDT+ZnO]

ES3: DFT calculated MEPS of PZCDT/ PZbCDT+$Ag_{n=0, 1, 2, 3, 4}$

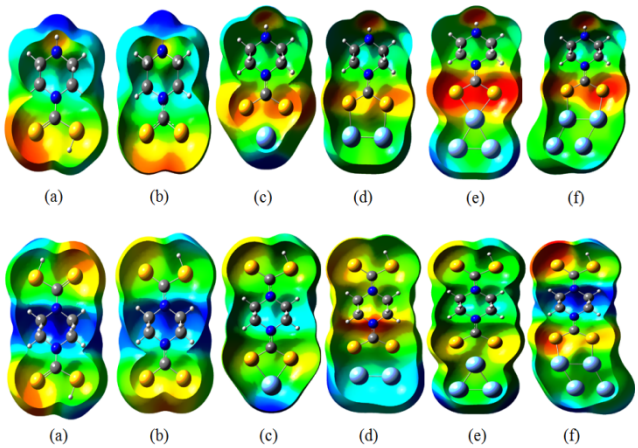

Fig ES3: Molecular electrostatic potential surfaces of optimized geometry of (a) PZCDT/PCbCDT, (b) deprotonated PZCDT/PCbCDT, (c) PZCDT/PCbCDT + Ag_1, (d) PZCDT/PCbCDT + Ag_2 (e) PZCDT/PCbCDT + Ag_3, (f) PZCDT/PCbCDT + Ag_4

ES4: DFT calculated MEPS of PZCDT/ PZbCDT+ZnO:

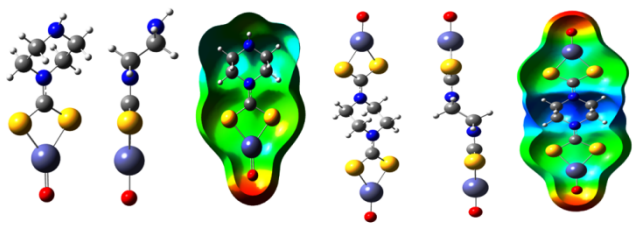

Fig ES4: Optimized structures of PZCDT +ZnO (a) front view, (b) side view, (c) MEPS of PZCDT +ZnO, and 4(ii) Optimized structures of

PZbCDT +ZnO (a) front view, (b) side view, (c) MEPS of PZbCDT +ZnO.