

Instrument Details

PXRD analysis of the samples were performed with PAN analytical X-PRT PRO instrument:USA using CuK α radiation having $\lambda = 1.5406 \text{ \AA}$. The samples in powdered form (properly grinded and symmetrically distributed) were placed in the sample holder co-planarly. FT-IR studies performed with Agilent Cary 630 FTIR spectrometer;USA revealed the presence of various functional groups and different bonds formed in the doped nanocomposite. This technique does not require any specific sample preparation or reference material like traditional FT-IR where KBr utilized as reference. Surface morphology of fabricated samples were obtained using field emission gun equipped FEI-Nova Nano SEM 450 microscope (Kensington UNSW Sydney NSW 2052). Element weight percent in material was calculated using Electron dispersive spectroscopy. The powdered sample was deposited on carbon tape before being mounted on the microscope sample holder for analysis. Brunauer-Emmett-Teller (BET) analysis used for calculation of surface area (N₂ physisorption) was done by using SMART Instruments, SMART SORB 93 model after degassing at 150 °C for 3 h. The stability of the photocatalysts was determined by measuring the zeta potential using Malvern Zetasizer (Zetasizer Ver. 7.11). The band gap calculation was done by obtaining Diffuse Reflectance Spectra data using Shimadzu UV-Vis spectrometer and converting it into Tauc's plot. Infrared spectra of the synthesized nanoparticles were recorded in the range 400–4000 cm⁻¹ (Agilent ATR model). Absorbance of samples was measured with UV Spectrophotometer (Agilent Pro) and HPLC (Agilent 1260). The characteristic crystallographic features of the sample were analysed in an FEI-Tecnai G² 20 S-Twin HR-TEM microscope operated at an accelerating voltage of 200kV. XPS spectra were recorded with Al K α (1486.6eV) radiation source at the total instrumental resolution of 0.8eV for Al K α excitation source. Surface area and pore size were calculated with

Brunauer Emmett Teller (SMART SORB 93 models) curve and samples were degassed at 420 K for 4h. LC-MS Spectrometer Model Q-TOF Micro Waters model, USA was used to analysis the degradation studies.

Details of Langmuir, Freundlich, Temkin, Sip and D-R isotherms used in present study

Adsorption data through Langmuir adsorption isotherms were calculated through graph of C_e/X_e v/s C_e of the solute. Which were calculated by fitting the adsorption data into the equation:

$$\frac{C_e}{X_e} = \frac{1}{k_L X_m} + \frac{C_e}{X_m}$$

or

$$\frac{1}{X_e} = \frac{1}{C_e} \left(\frac{1}{k_L X_m} \right) + \frac{1}{X_m}$$

X_e was calculated through the equation:

$$X_e = \frac{(C_i - C_e) \times \text{Vol of solution (mL)} \times \text{Molecular weight of adsorbent}}{\text{Amount of catalyst (mg)}}$$

Freundlich Isotherm.

A typical graph of X_e v/s C_e of the solute was a straight line.

$$X_e = K_f + C_e^{1/n} \text{ and linear form is } \log X_e = \log K_f + \frac{1}{n} \log C_e$$

Where C_e is the equilibrium concentration of the pollutant solution; X_e is the amount of pollutant adsorbed per gram weight of adsorbent; K_f is the Freundlich adsorption constant (mg/g); n is adsorption intensity.

Temkin Isotherm:

$$X_e = \frac{RT}{b} \ln A + \frac{RT}{b} \ln C_e$$

Where $B=RT/b$ constant related to heat of sorption (J/mol) obtained from the Temkin plot (q_e v/s $\ln C_e$); A (slope) = Temkin isotherm equilibrium binding constant (L/g); b (intercept) =

Temkin isotherm constant; R =universal gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) T = Temperature at 298, 308 and 318 K.

As C_e values were very low, the $\ln C_e$ values were coming out to be negative. Therefore, Temkin isotherm (X_e v/s $\ln C_e$) was not plotted for present study.

Sips Isotherm

It is plotted between $1/X_e \times 10^{-2}$ (g/mg) and $(1/C_e) \times 10^{-8}$ L/mg; where (1/mg) and (mg/g) are the Sips equilibrium constant and maximum adsorption capacity values obtained from the slope and the intercept of the plot. The Sips isotherm equation is characterized by the dimensionless heterogeneity factor ‘n’ which can also be employed to describe the system’s heterogeneity when is between 0 and 1.

$$\frac{1}{X_e} = \frac{1}{X_m K_s} \left(\frac{1}{C_e} \right)^{1/n} + \frac{1}{X_m}$$

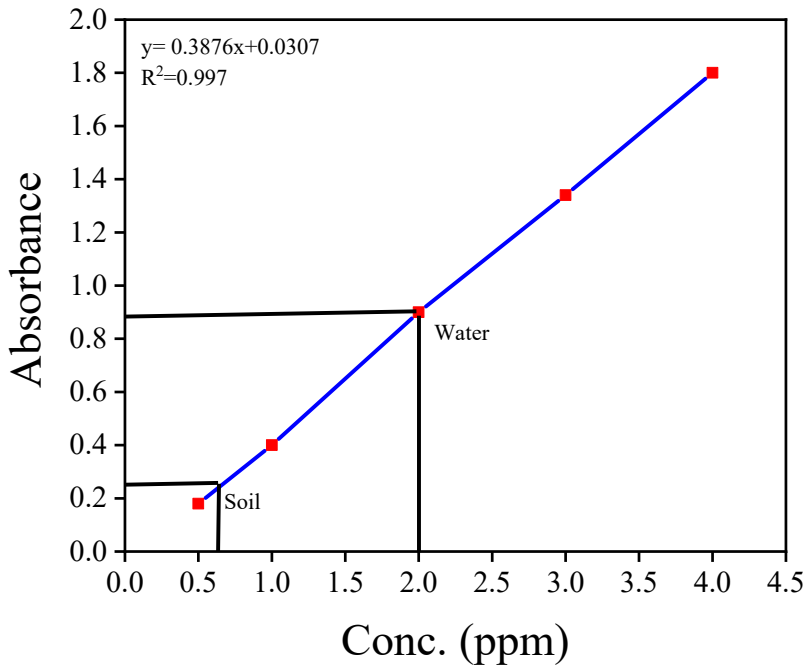


Figure 1S: Calibration curve for spiked tobacco solution in water and soil

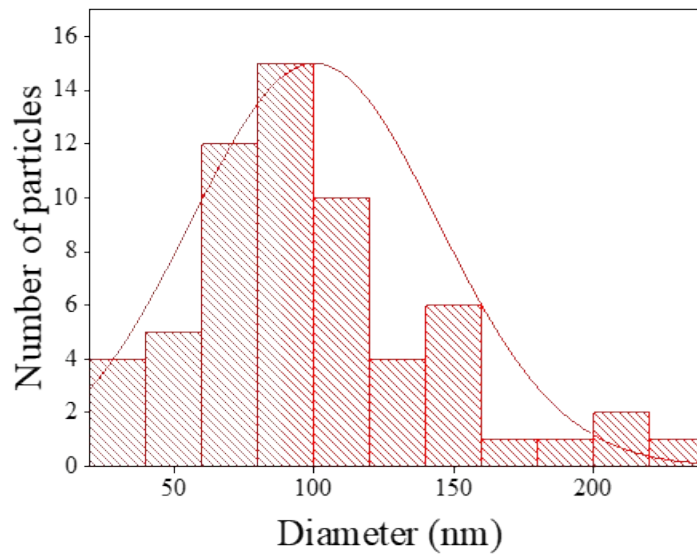


Figure 2S: Estimated size distribution of nanocomposite (ZnO@ZnHCC)

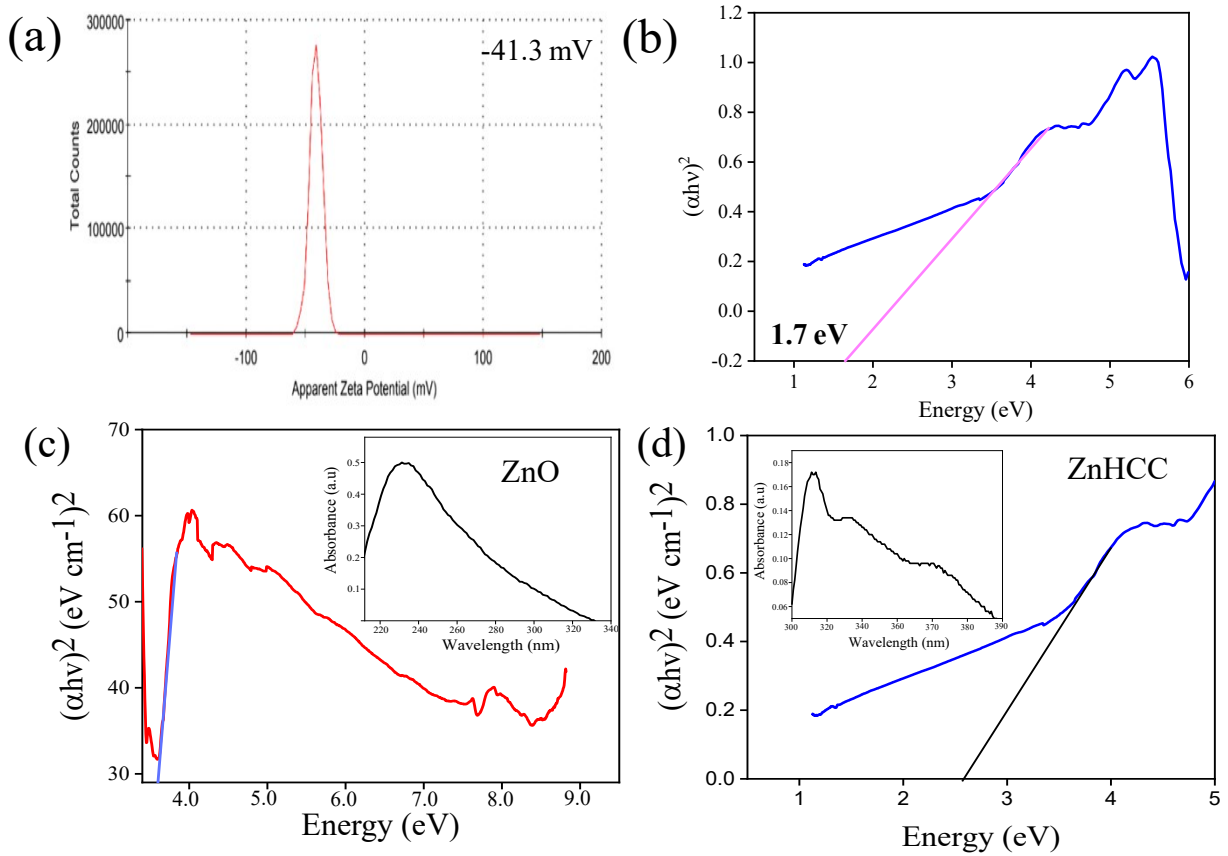


Figure 3S: Zeta potential and band gap of synthesized nanocomposite

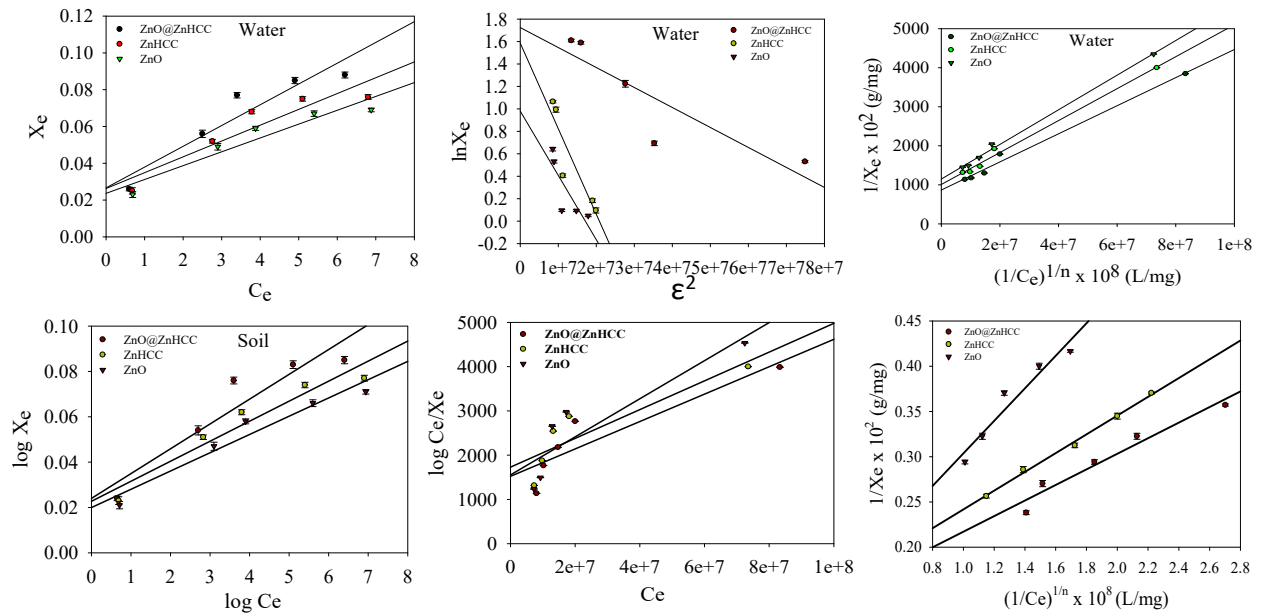


Figure 4S. Freundlich, Temkin, DR model and Sips model for hexavalent Chromium. Triplicate experiments (n=3) were evaluated for estimation of error bar.