Supporting Information

Understanding the charge transfer mechanism in $CsPbBr_3$ nanocrystals and nitrogen-doped carbon quantum dots heterostructures: effect of nanocrystals' encapsulation

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Experimental section:

Characterization methods:

UV-VIS spectroscopy and photoluminescence (PL) measurements: Electronic absorption spectra were recorded using a Shimadzu UV-1900I spectrometer by taking diluted NCs solution after sonicating it. Edinburg Instrument FLS1000 was used to record the PL spectra using an excitation wavelength of λ_{ex}= 405 nm for all samples. These as synthesized NCs CPB@OA, CPB@OA@PVP NCs were diluted in toluene and CPB@SiO and CPB@SiO@PVP NCs were diluted in ethanol. Further, they were transported to a quartz cuvette for the measurements.

Powder X-ray diffraction (P-XRD): The concentrated NCs dispersed in toluene and ethanol were drop cast in a cleaned glass substrate 1 cm*1 cm. The powder X-ray Diffraction pattern of all the samples was collected on a Bruker D8 diffractometer by using Cu-K_α (λ=1.5406 Å) as incident radiation at 40 kV and 30 mA power at room temperature. PANalytical Expert's high score plus software was used to analyze the XRD data.

Transmission electron microscopy (TEM): The optimum concentration of all samples in toluene and ethanol was dropped on the carbon-coated Cu grids with 200 mesh. The TEM

images of the NCs and NCQDs were taken using a Jeol-JEM-2100 PLUS microscope operated at 200 kV to determine the shape and size of the NCs.

Fourier transform infrared spectroscopy (FTIR): FTIR spectra were recorded in thin film mode by using a Bruker Alpha-T FTIR spectrophotometer equipped with an attenuated total reflectance (ATR) module.

Time-resolved PL measurements (TRPL): The time-correlated single photon counting (TCSPC) method was implemented during the fluorescence lifetime measurements using the Edinburg Instrument FLS1000 with an output using the laser diode as an excitation source λ_{ex}= 405 nm. The NCs having the same concentration solution were placed in a quartz cuvette.

Field emission scanning electron microscope (FESEM) and energy-dispersive X-ray spectroscopy measurements: JEOL (JSM-7610F plus) instrument was used to take the FESM-EDS spectrum. The NCQDs were drop cast in glass substrate and the elemental mapping was taken to verify the presence of nitrogen in NCQDs.

X-ray photoelectron Spectroscopy (XPS): The X-ray photoelectron spectroscopy (XPS) analysis was carried out in an Omicron (series 0571) electron spectrometer.

Density functional theory (DFT): The Vienna ab initio simulation package (VASP) code based on plane wave density functional theory (DFT) was used to calculate the structural and electronic properties of carbon quantum dots adsorbed on the $CsPbBr_3$ surface.

Results and discussion:

Figure S1:

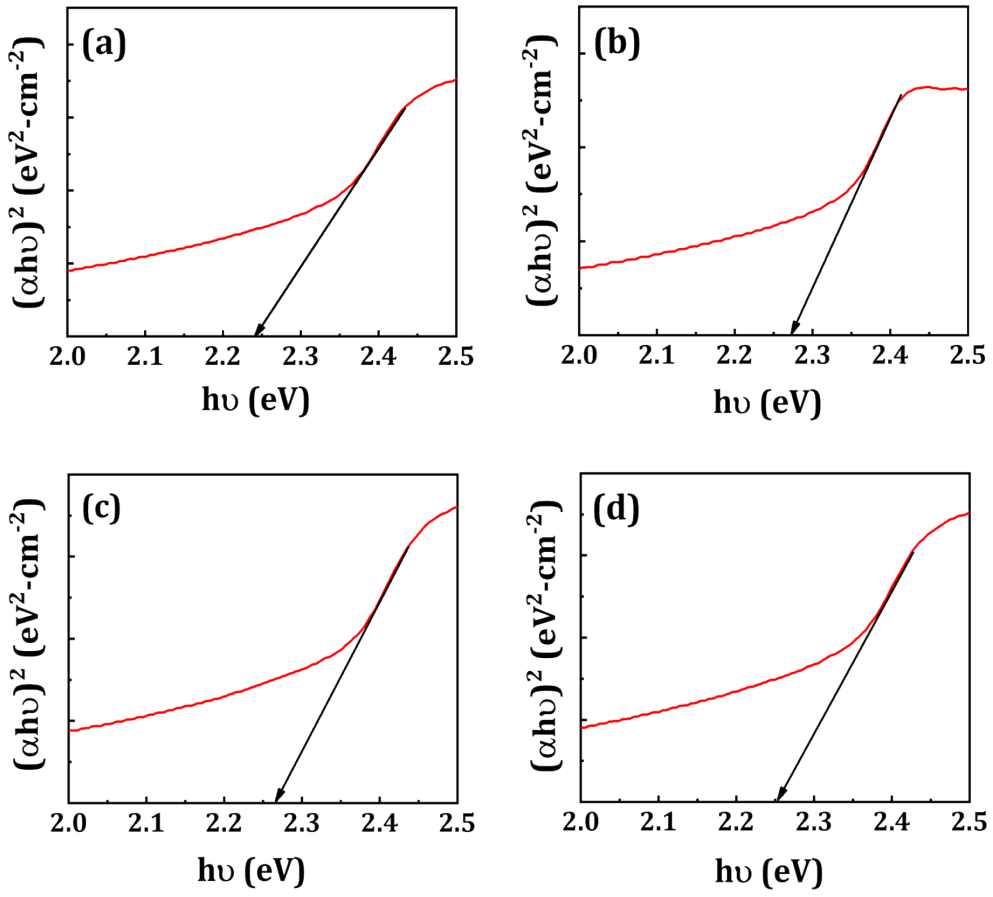


Figure S1: Tauc plots of (a) CPB@OA, (b) CPB@OA@PVP, (c) CPB@SiO, and (d) CPB@SiO@PVP NCs.

Figure S2:

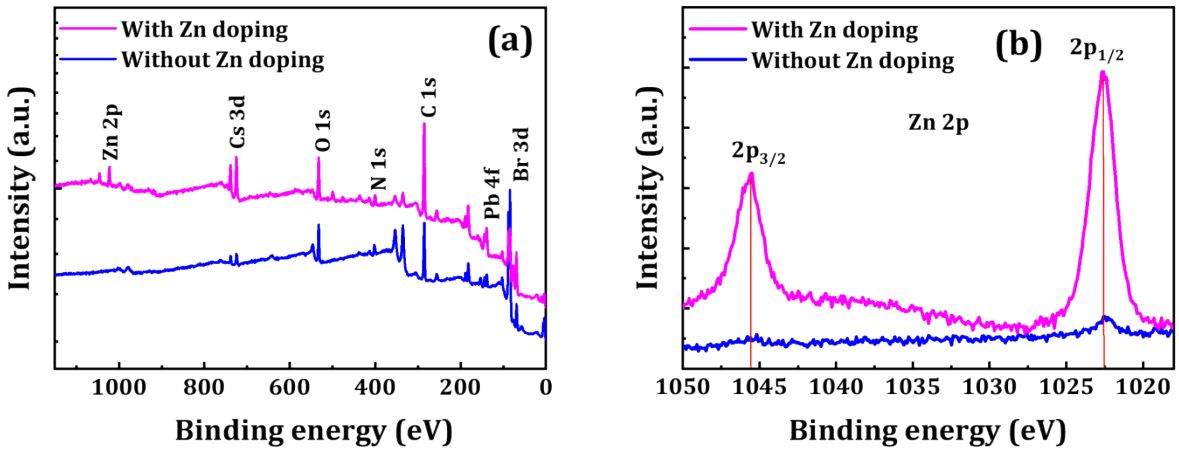


Figure S2: (a) Core XPS pattern of $CsPbBr_3$ NCs without Zn and with Zn-doping, and (b) high-resolution XPS patterns of Zn 2p chemical state, as shown in legends.

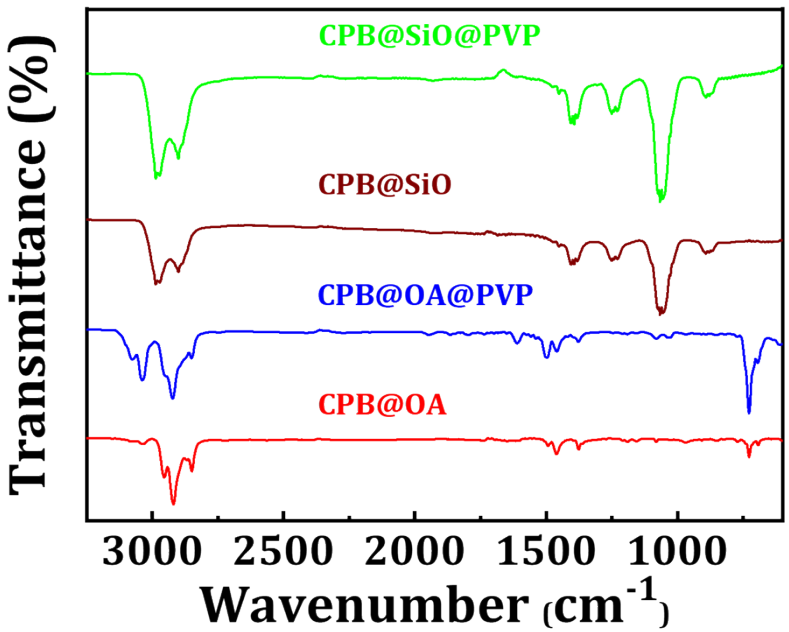
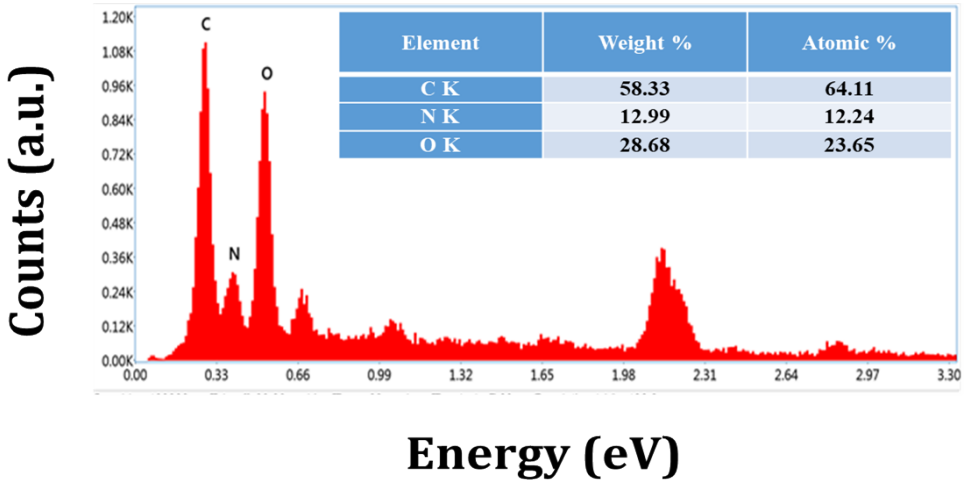


Figure S3: FTIR spectra of CPB@OA, CPB@OA@PVP, CPB@SiO, and (d) CPB@SiO@PVP NCs.

Figure S3:

Figure S4:



Element	Weight %	Atomic %
C K	58.33	64.11
N K	12.99	12.24
O K	28.68	23.65

Figure S4: EDS spectrum of NCQDs film showing all the elements present on the surface. Inset: EDS data obtained from FESEM image showing both the weight and atomic percentage of different elements.

Figure S5:

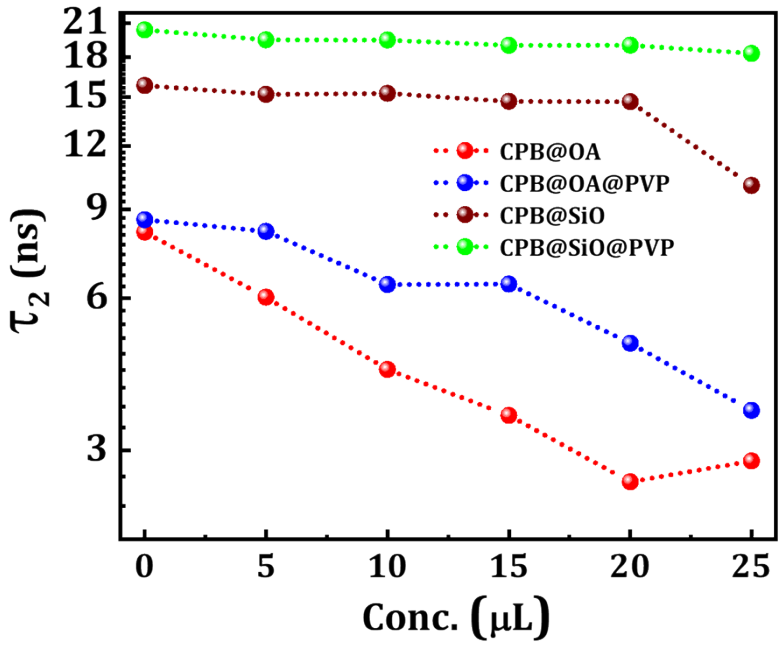


Figure S5: Decay component (τ_2) of NCs over addition of different volumes of NCQDs as shown in legend.

Figure S6:

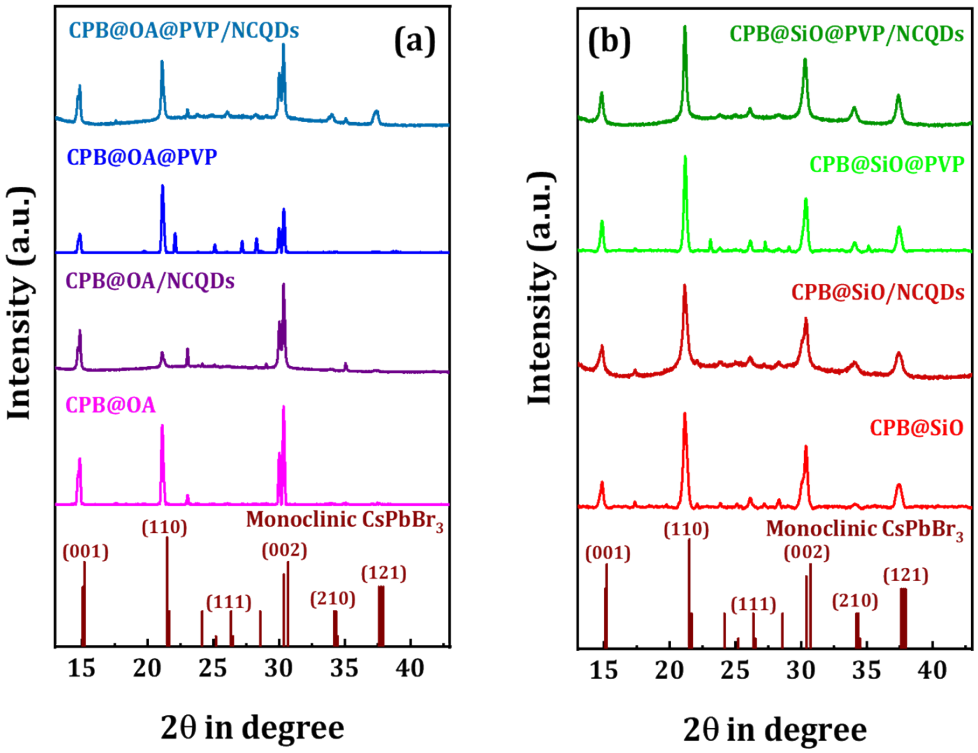


Figure S6: XRD Diffraction patterns of (a) CPB@OA and CPB@OA@PVP, (b) CPB@SiO and CPB@SiO@PVP NCs with and without NCQDs as marked in the Figure.

Figure S7:

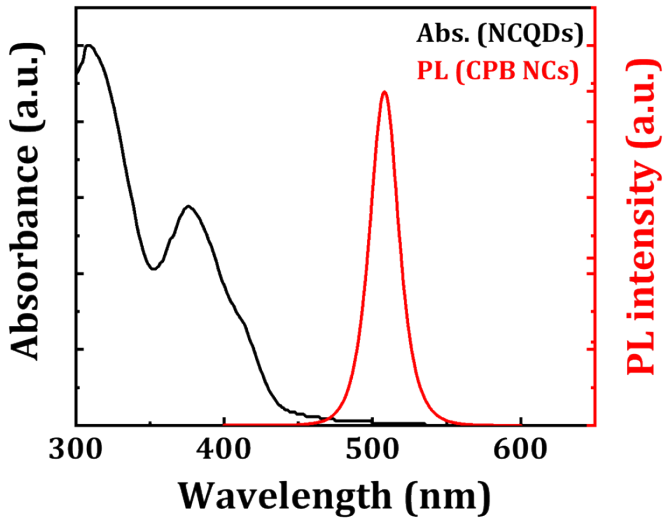


Figure S7: Absorption and PL spectra of the acceptor (NCQDs) and donor ($CsPbBr_3$ NCs) respectively as shown in legends.

Figure S8:

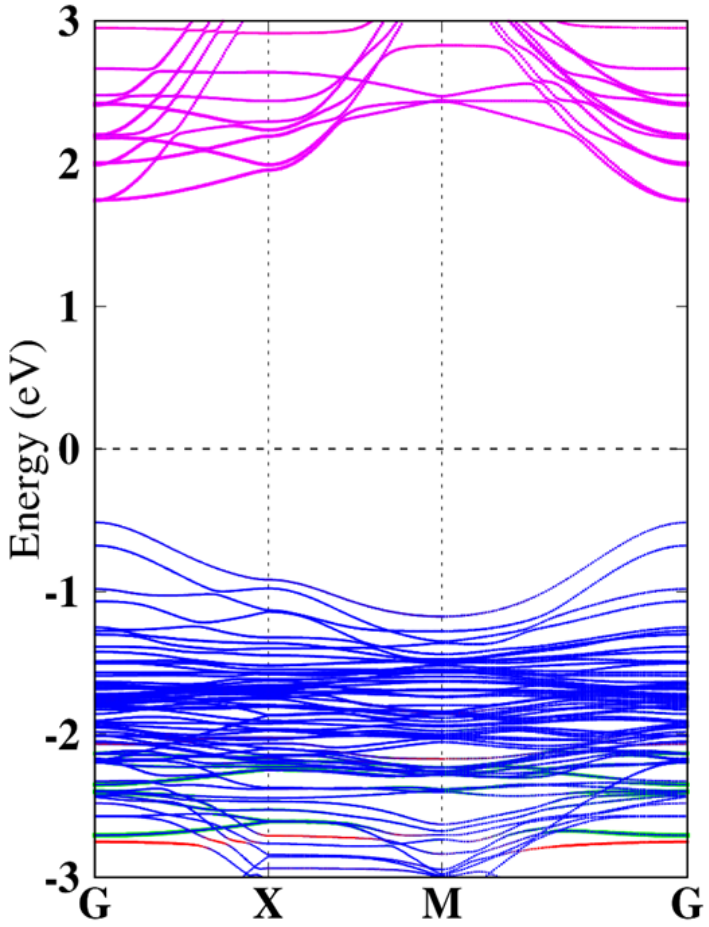


Figure S8: Projected band structures of $CsPbBr_3$ slab with NH_3 molecule.

Table S1: PL decay lifetime of CPB@OA NCs.

Volume of NCQDs (μL)	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{avg} (ns)
0	0.86	0.91	0.30	8.11	6.21
5	0.82	0.92	0.29	6.03	4.48
10	0.78	0.81	0.28	4.34	3.73
15	0.77	0.74	0.26	3.52	2.47
20	0.74	0.66	0.24	2.6	1.83
25	0.72	0.63	0.23	2.86	1.33

Table S2: PL decay lifetime of CPB@OA@PVP NCs.

Volume of NCQDs (μL)	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{avg} (ns)
0	0.56	1.22	0.47	8.58	7.51
5	0.53	1.87	0.40	8.14	6.69
10	0.68	1.73	0.40	6.39	4.93
15	0.69	1.74	0.39	6.4	4.10
20	0.64	1.16	0.35	4.89	3.77
25	0.68	0.66	0.27	3.6	2.69

Table S3: PL decay lifetime of CPB@SiO NCs.

Volume of NCQDs (µL)	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{avg} (ns)
0	0.52	3.18	0.42	15.82	13.29
5	0.54	2.55	0.42	15.19	12.92
10	0.54	3.34	0.37	15.26	12.39
15	0.52	3.09	0.42	14.71	12.01
20	0.68	2.71	0.30	14.69	11.19
25	0.56	1.89	0.37	10.03	9.82

Table S4: PL decay lifetime of CPB@SiO@PVP NCs.

Volume of NCQDs (µL)	A_1	τ_1 (ns)	A_2	τ_2 (ns)	τ_{avg} (ns)
0	0.62	3.78	0.34	20.37	16.17
5	0.58	3.12	0.34	19.47	16.01
10	0.57	3.22	0.33	19.46	15.85
15	0.6	2.96	0.36	18.99	15.70
20	0.59	3.51	0.36	19.00	15.42
25	0.61	2.96	0.37	18.31	15.09