Supporting Information

Hole transfer dynamics between $CsPbBr_3$ PNC and *p*-phenylene diisothiocyanate

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Content

Photo Luminescence Quantum Yield (PLQY) Measurement.

The PLQY of PNCs were measured using Coumarin 153 (C153) as reference standard (absolute QY 58% in ethanol). Samples for PLQY measurements were prepared by diluting the colloidal dispersion of PNCs with anhydrous toluene keeping the optical density of both the C153 and the PNCs below 0.1 at 420 nm. The absorption and PL emission spectra were measured using the instruments mentioned in the manuscript. PLQY at various excitation wavelength and concentration of PDNCS were calculated using the following equation.

$$PLQY = Q_R \times \frac{OD_R}{OD} \times \frac{I}{I_R} \times \frac{\eta^2}{\eta_R^2}$$

where PLQY, OD, I and η represents photo luminescence quantum yield, optical density, integrated intensity, and refractive index of the medium respectively. Subscript "R" refers to the reference (here C153).

Time-Resolved Photoluminescence.

PL lifetime analyses were conducted at room temperature using a HORIBA Delta Flex fluorescence lifetime measurement setup spectrometer using a 372 nm pulsed laser diode excitation. The PL decay curve of PNCs in absence and presence of PDNCS is shown in Figure 3 and were well-fitted using the following bi-exponential fitting equation.

$$I(t) = A_1 \exp\left(\frac{-t}{\tau_1}\right) + A_2 \exp\left(\frac{-t}{\tau_2}\right) + C$$

Average PL lifetime (τ_{avg}) was calculated using the following equation.

$$\tau_{avg} = \frac{\alpha_1 \tau_1^2 + \alpha_2 \tau_2^2}{\alpha_1 \tau_1 + \alpha_2 \tau_2}$$

where α, and τ are the pre-exponential factor and PL lifetime of each component respectively.

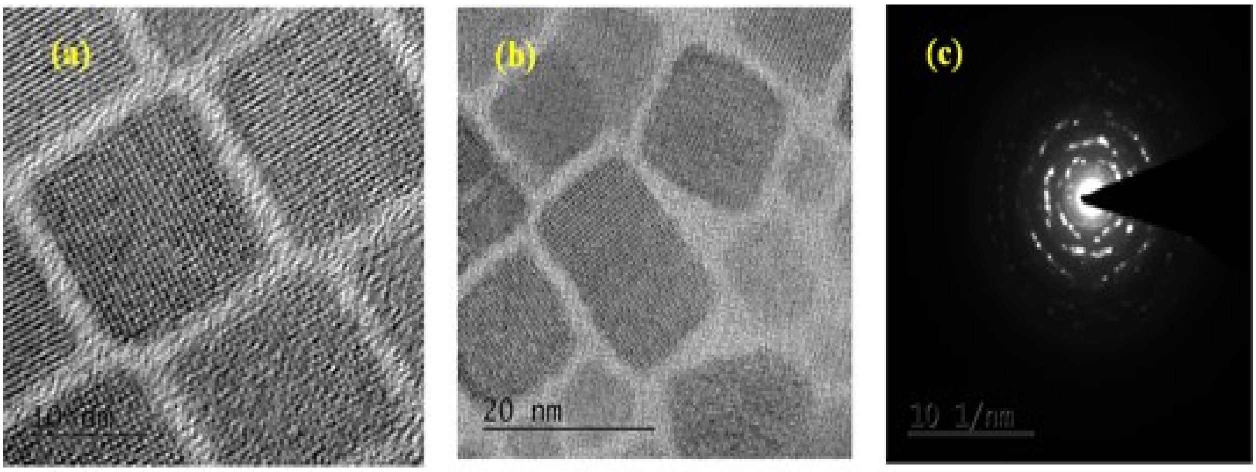

Fig S1: HRTEM images (a,b) and SAED patterns(c) of $CsPbBr_3$ NC with scale bar of 10nm (a) 20 nm (b) respectively

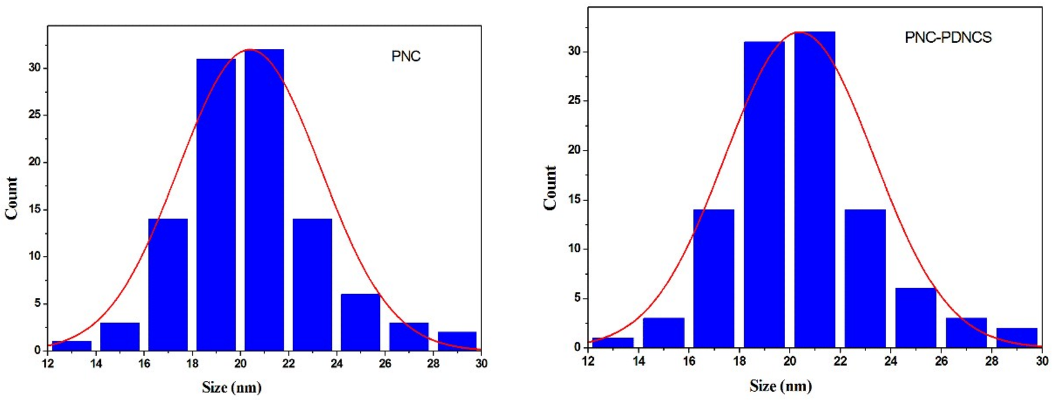

Fig S2: Bar diagram of the average size distribution of $CsPbBr_3$ nano crystals obtained in the TEM study.

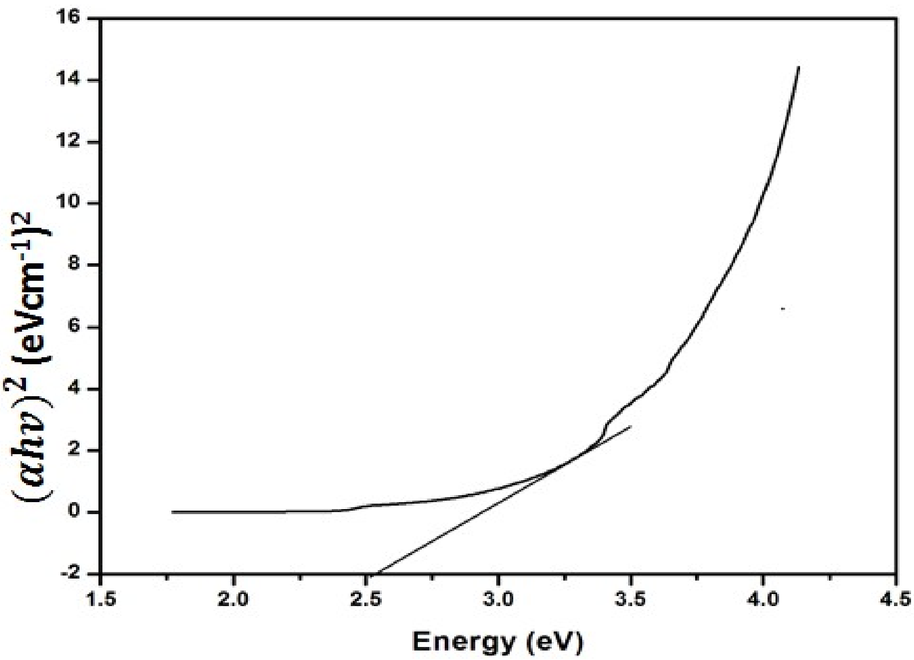

Fig S3: Tauc plot to calculate the band gap of the $CsPbBr_3$ PNC.

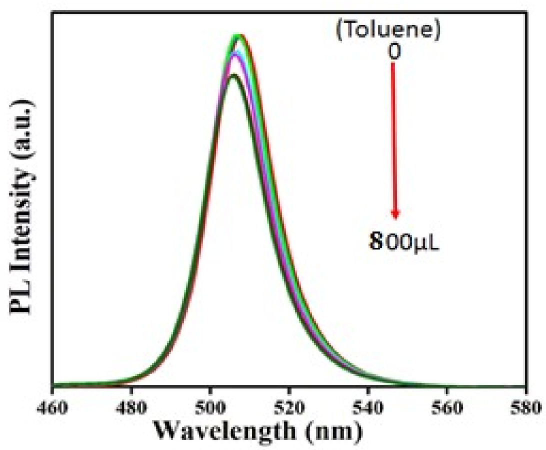

Fig S4: Photo luminescence spectra of $CsPbBr_3$ nanocrystals solution in toluene with addition of excess amount of solvent (toluene) corresponding up to the maximum volume of PDNCS added during the present study.

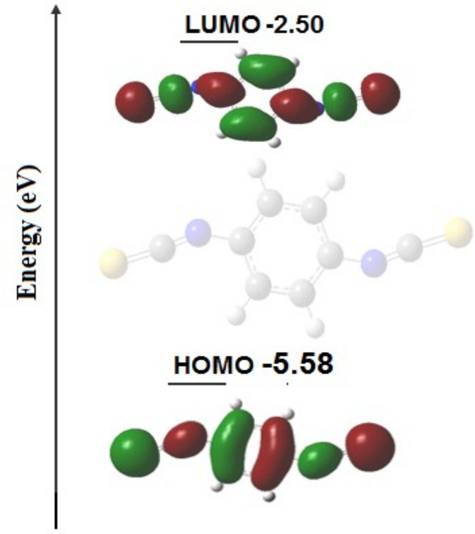

Fig S5: DFT optimized geometry and HOMO-LUMO gap of PDNCS using TPSSTPSS/CCPVDZ level of theory.

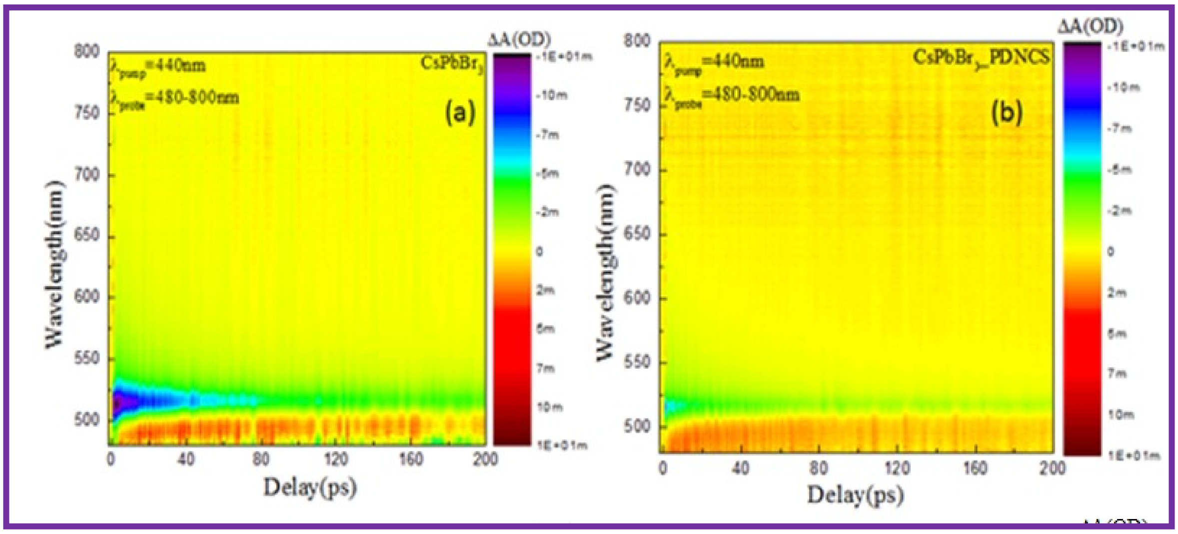

Fig S6: 2D pseudo-colour TA plot of (a) $CsPbBr_3$ PNCs and (b) CsPbBr3-PDNCS system at 440 nm pump excitation

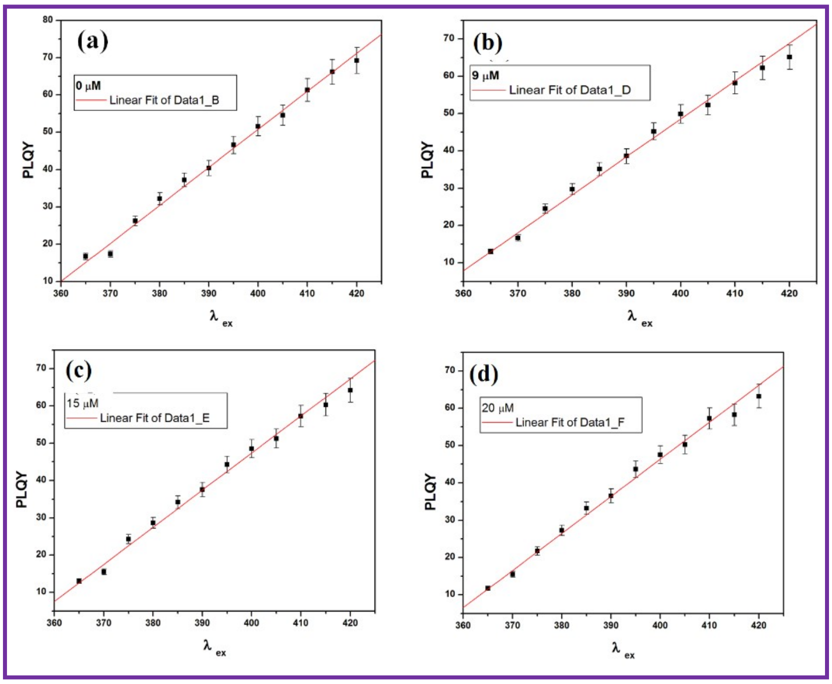

Fig S7: Plots of PLQY vs λ_{ex} (nm) for a given concentration (a) 0mM, (b) $5mM$, (c) 9 mM, (d) 15mM, (e) 20 mM, (f) 25mM

Table S1: PLQY (%) $CsPbBr_3$ PNC in presence various concentration of PDNCS ($\lambda_{ex} = 420nm\ and\ \lambda_{em}$ = 509 nm)

PDNCS (mM)	**Quenching Efficiency (%)**
0.14	15.80
0.28	21.95
0.42	35.18
0.56	50.18
0.70	59.94
0.84	69.62
0.98	75.09
1.11	81.81
1.24	85.80
1.34	89.06

Table S2: Stern-Volmer quenching constant (K_{sv}), average PL lifetime (τ_{avs}), PL quenching constant (K_q) and hole transfer constant (K_{ht}) of $CsPbBr_3$ PNC in presence of quencher, PDNCS.

Sample	K_{sv}(mM^{-1})	τ_{avs}(ns)	K_q ($M^{-1}ns^{-1}$)	Hole transfer constant (K_{ht}) (s^{-1})
$CsPbBr_3$	2.84	6.67	425.78	31.5×10^7

Table S3: Calculated PLQY as a function of λ_{ex} and [PDNCS] for $CsPbBr_3$ PNC.

.(a)

[PDNCS] mM	λ_{ex} (nm)	PLQY
0	365	16.675
	370	17.39
	375	26.269
	380	32.2
	385	37.256
	390	40.45
	395	46.562
	400	51.587
	405	54.562
	410	61.325
	415	66.211
	420	69.232

(b)

[PDNCS] mM	λ_{ex} (nm)	PLQY
5	365	14.301
	370	17.02
	375	25.133
	380	31.365
	385	35.265
	390	39.48
	395	45.521
	400	50.205
	405	53.265
	410	60.25
	415	65.002
	420	68.786

(c)

[PDNCS] mM	λ_{ex} (nm)	PLQY
9	365	13.071
	370	16.652
	375	24.547
	380	29.773
	385	35.2
	390	38.569
	395	45.2
	400	49.865
	405	52.25
	410	62.211
	415	58.202
	420	65.106

(d) **(e)** **(f)**

[PDNCS] mM	λ_{ex} (nm)	PLQY
(d)	365	13.04
	370	15.523
	375	24.307
	380	28.665
	385	34.23
15	390	37.547
	395	44.265
	400	48.56
	405	51.23
	410	57.266
	415	60.315
	420	64.222

[PDNCS] mM	λ_{ex} (nm)	PLQY
	365	11.728
	370	15.5
	375	21.771
	380	27.3
	385	33.265
20	390	36.524
	395	43.65
	400	47.554
	405	50.258
	410	57.254
	415	58.214
	420	63.225

[PDNCS] mM	λ_{ex} (nm)	PLQY
	365	9.851
	370	15.26
	375	19.725
	380	26.658
	385	32.25
25	390	35.302
	395	42.15
	400	46.522
	405	48.44
	410	55.1
	415	57.395
	420	61.428

Table S4: PLQY without PDNCS and with PDNCS (29mM)

λ_{ex} (nm)	PLQY (0 mM)	PLQY (29mM)	Percentage decrease of PLQY in presence of PDNCS
365	16.6	8.3	50
370	17.3	13.9	20
375	26.2	17.3	33.7
380	32.2	25.5	20.6
385	37.2	31.1	16.3
390	40.4	35	13.3
395	46.5	41.5	10.8
400	51.5	45.5	11.6
405	54.5	47.9	12
410	61.3	52.1	14.9
415	66.2	55.2	16.5
420	69.2	58.3	15.6

References.

(1) Mandal, S., Mukherjee, S., De, C. K., Roy, D., Ghosh, S., & Mandal, P. K. (2020). Extent of shallow/deep trap states beyond the conduction band minimum in defect-tolerant $CsPbBr_3$ perovskite quantum dot: control over the degree of charge carrier recombination. *The Journal of Physical Chemistry Letters*, *11*(5), 1702-1707.

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(3) Venkateswarlu, D., Swetha, T., Akhil, S., Palabathuni, M., Mishra, N., & Singh, S. P. (2023). Surface engineering of $CsPbBr_3$ perovskite nanocrystals: hole transfer dynamics and enhanced photocurrent response using a novel organic molecule. *Materials Advances*, *4*(8), 1935-1940.

(4) Dhanabalan, B., Castelli, A., Palei, M., Spirito, D., Manna, L., Krahne, R., & Arciniegas, M. (2019). Simple fabrication of layered halide perovskite platelets and enhanced photoluminescence from mechanically exfoliated flakes. *Nanoscale*, *11*(17), 8334-8342.