Electronic Supplementary Material (ESI) for Dalton Transactions.

Enhancing the Stability of $CsPbX_3$ (X = Br, I) Through Combination with Y-zeolites for WLED Application

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Computation methods

Spin-polarized GGA calculations have been performed based on density functional theory (DFT), as implemented in the Vienna ab initio Simulation Package (VASP). The electrons of Cs($5s^25p^66s^1$), Pb($5p^{10}6s^26p^2$), Zn($3d^{10}4s^2$), Br($4p^54s^2$), I($5p^55s^2$), and Cl($3s^23p^5$) were treated as valence electrons. The geometry optimizations were performed until the total energies and the forces on the atoms converged to 10^{-4} eV and 0.02 eV $Å^{-1}$, respectively. A 2 × 2 × 2 k (Cs_4PbCl_6), 11 × 11 × 11 k (CsCl), 11 × 11 × 11 k ($CsPbBr_3$), 11 × 11 × 11 k ($CsPbI_3$), 2 × 2 × 2 k ($ZnBr_2$), 6 × 6 × 6 k ($ZnCl_2$), 2 × 2 × 2 k (ZnI_2), -point grid was used, and the cutoff energy for the plane wave basis was set to 400 eV. Effects of spin-orbit coupling were included throughout the calculations.

The Perdew-Burke-Ernzerhof (PBE) function within the generalized gradient approximation was used for the exchange-correlation energy. The formation energy of the reaction process is expressed as,

$$E_f = 2E(Cs_4PbCl_6) - 2E(CsPbBr_3) - 6E(CsCl) - 3E(ZnCl_2) + 3E(ZnBr_2) \quad (1)$$

$$E_f = 2E(Cs_4PbCl_6) - 2E(CsPbI_3) - 6E(CsCl) - 3E(ZnCl_2) + 3E(ZnI_2) \quad (2)$$

where, $E(Cs_4PbCl_6)$, $E(CsPbBr_3)$, $E(CsPbI_3)$, $E(CsCl)$, $E(ZnCl_2)$, $E(ZnBr_2)$ and $E(ZnI_2)$ *are the*, energy of pristine Cs_4PbCl_6, $CsPbBr_3$, $CsPbI_3$, $CsCl$, $ZnCl_2$, $ZnBr_2$, and ZnI_2.

Table 1| Formation energy of Cs_4PbCl_6, $CsPbBr_3$, $CsPbI_3$, $CsCl$, $ZnCl_2$, $ZnBr_2$, and ZnI_2

Structures	E_f (eV)	PBE (eV)	Number of units
Cs_4PbCl_6	-37.66562	-225.99372	6
CsCl	-6.5438814	-6.5438814	1
$CsPbBr_3$	-15.898891	-15.898891	1
$CsPbI_3$	-14.065143	-14.065143	1
$ZnBr_2$	-7.1238653	-227.96369	32
$ZnCl_2$	-8.2212935	-32.885174	4
ZnI_2	-5.9942619	-191.81638	32

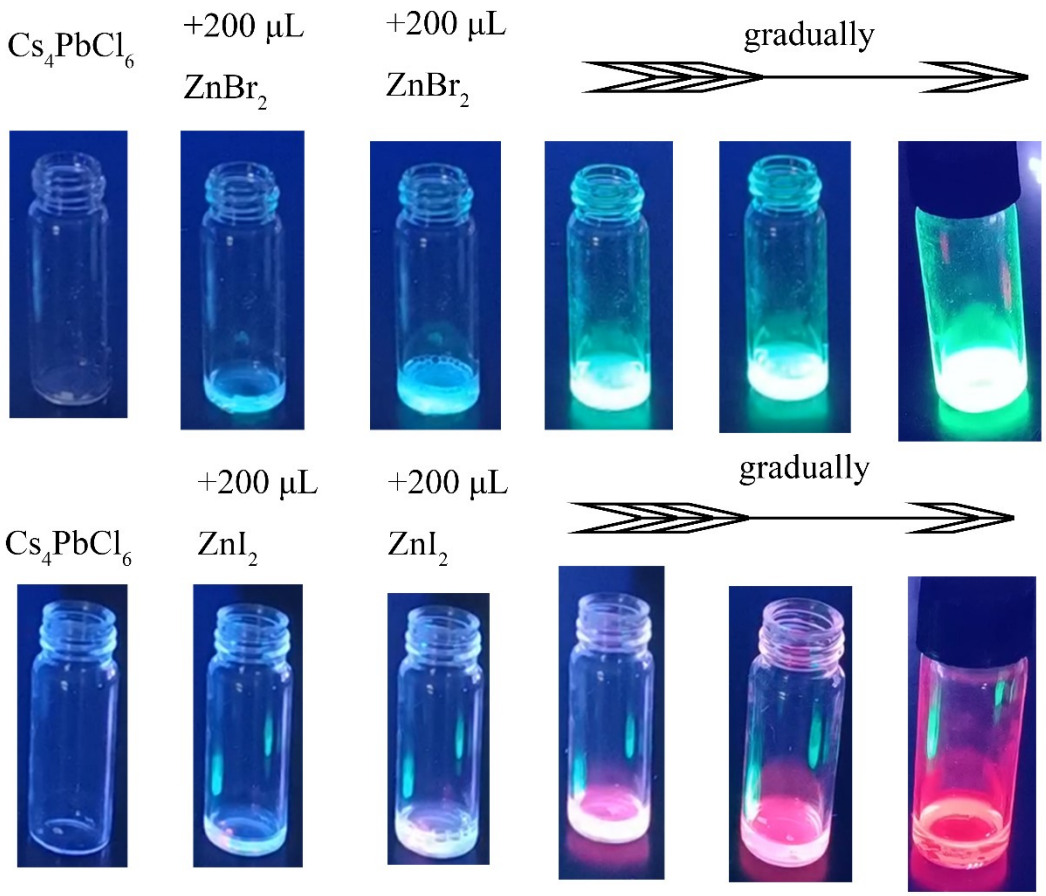

Figure S1. Photographs showing the transformation process of Cs_4PbCl_6 NCs to $CsPbBr_3$ and $CsPbI_3$ NCs.

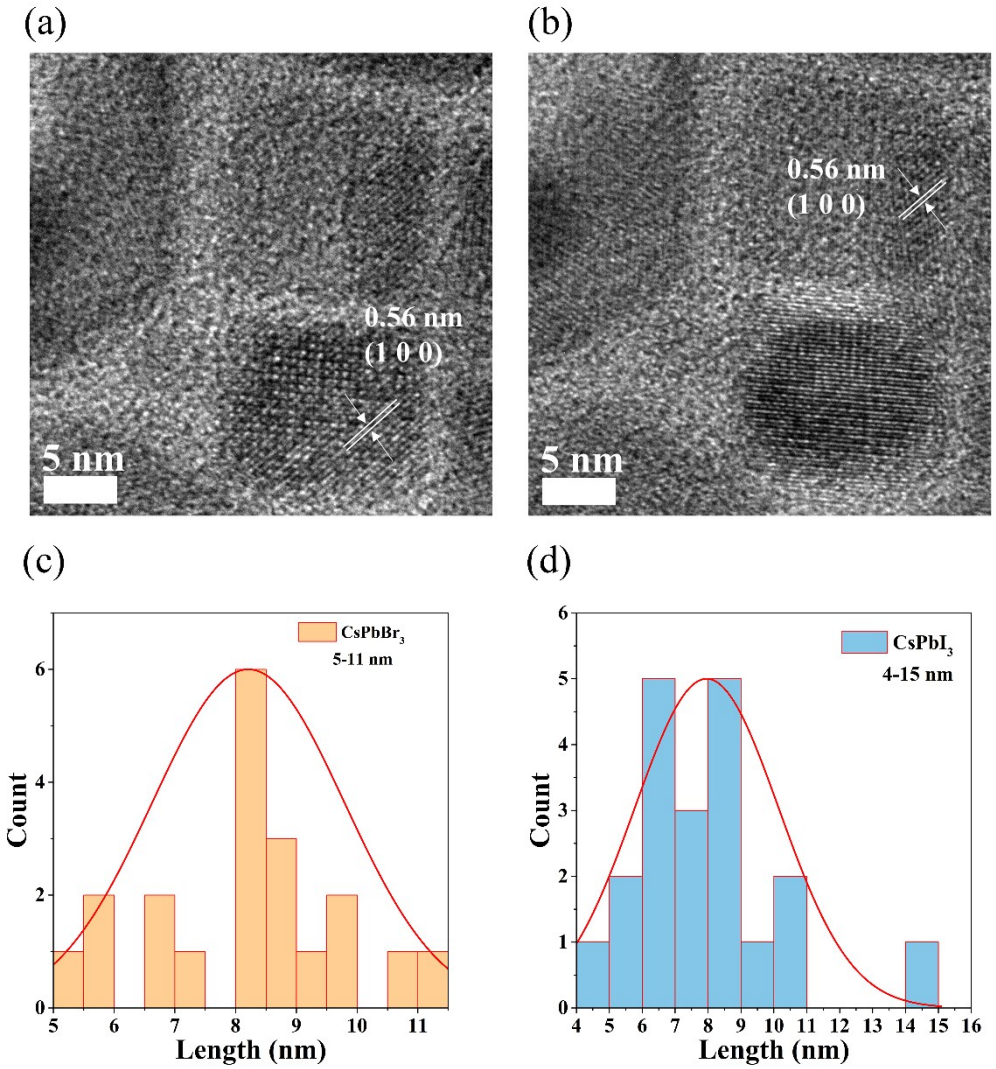

Figure S2. (a-b) HRTEM of a single $CsPbBr_3$ and $CsPbI_3$ NCs. (c-d) Size distribution histogram of $CsPbBr_3$ and $CsPbI_3$ NCs.

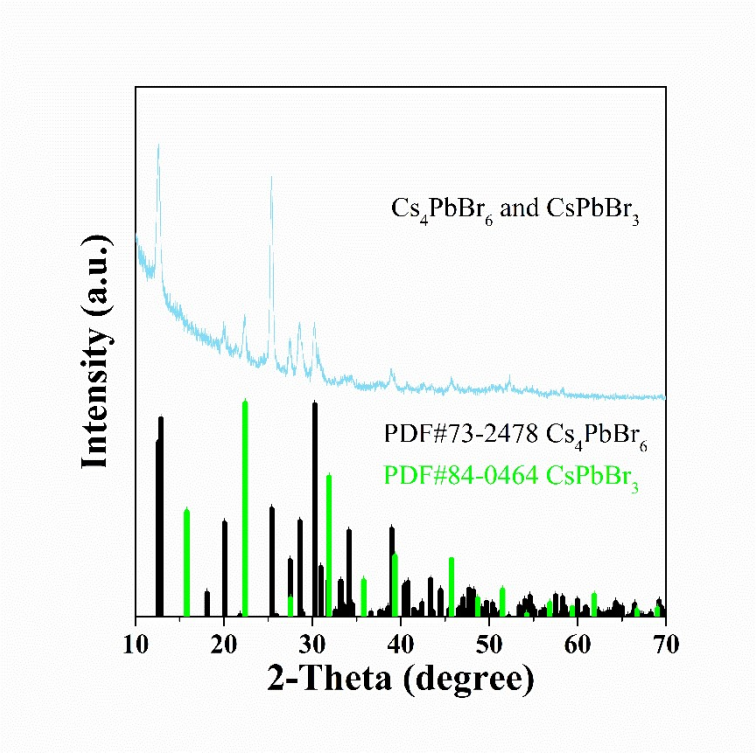

Figure S3. XRD pattern of prepared NCs with $ZnBr_2$ solution in excess.

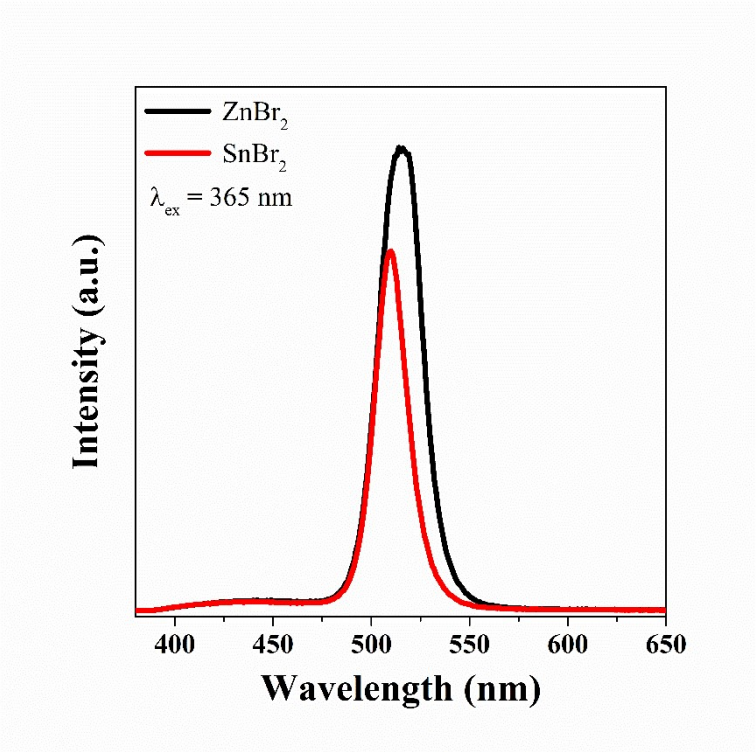

Figure S4. PL emission spectra of $CsPbBr_3$ NCs through $ZnBr_2$ and $SnBr_2$ solution triggered transformed.

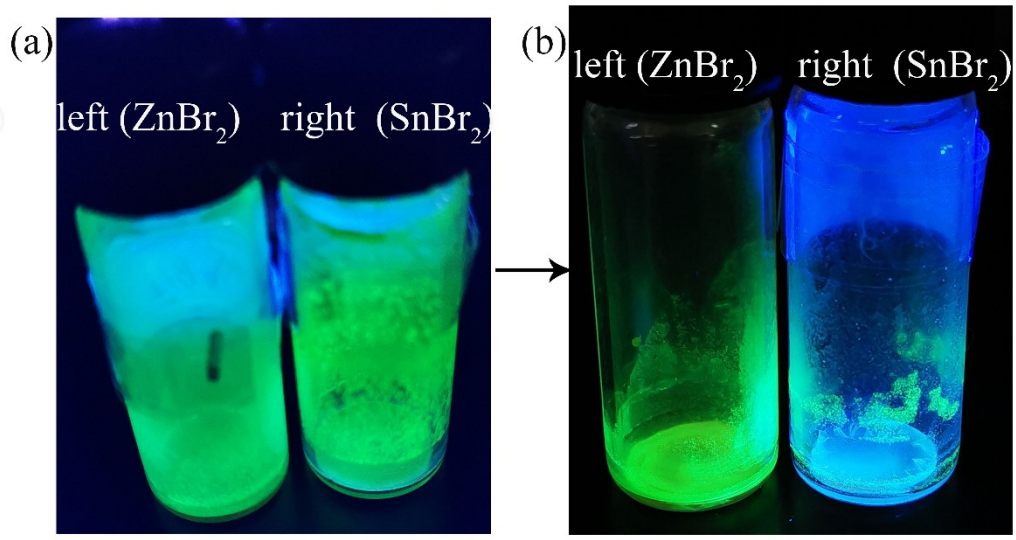

Figure S5. Photographs showing the stability of $CsPbBr_3$ NCs obtained through (a) 100 µL and (b) 1500 µL $ZnBr_2$ and $SnBr_2$ solution triggered transformed.

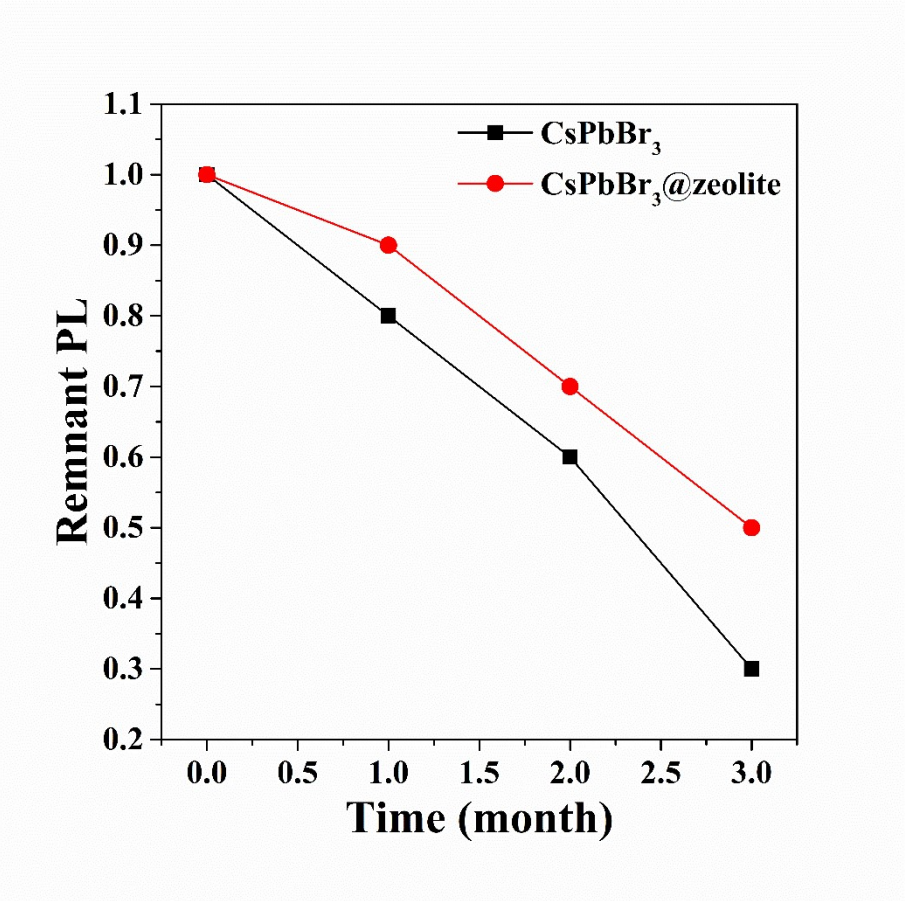

Figure S6. Remnant PL of $CsPbBr_3$ NCs and $CsPbBr_3$@zeolite in different time.

Table S2. Comparison of specific surface area and pore size of mesoporous silicon before and after loading samples.

sample	BET surface (m^2/g)	Pore volume (cm^3/g)	Pore size (nm)
Zeolite-Y	768.8	1.3	5.6
$CsPbBr_3$@zeolite	456.7	0.9	5.8

Table S3. Summary of emitting materials and PeLED Performances.

Emitting materials	PLQY (%)	FWHM (nm)	Luminous efficiency (lm/W)
$CsPbBr_3$	92	19	147.82
$CsPbBr_3$@zeolite	83	20	107.17
$CsPbI_3$	50	36	130.56
$CsPbI_3$@zeolite	46	37	103.24

Video S1. More intuitive transformation process.