

†Electronic Supporting Information (ESI)

Postsynthesis Mn-Doping in CsPbI₃ Nanocrystals to Stabilize the Black Perovskite Phase

Wasim J. Mir,^a Abhishek Swarnkar,^{a,b} Angshuman Nag^{a,b,*}

^aDepartment of Chemistry, and ^bCentre for Energy Science, Indian Institute of Science Education and Research (IISER), Pune, 411008, India.

*Corresponding author's e-mails: AN: angshuman@iiserpune.ac.in

Chemicals: Lead bromide (PbBr₂, 99.999%), lead iodide (PbI₂, 99.999%), manganese (II) bromide (MnBr₂, 98%), manganese (II) iodide (MnI₂, 99.9%), cesium carbonate (Cs₂CO₃, 99.9%), oleic acid (OA, 90%), 1-octadecene (ODE, 90%), oleylamine (OLA, 98%), hexane (anhydrous, 95%) and methyl acetate (MeOAc, 99.5%) are purchased from Aldrich, and are used without further purification. Acetone (99.0%, SDFCL), hexane (99.99%, Rankem) and toluene (99.5%, Rankem) are purchased from a local vendor.

Supporting Figures:

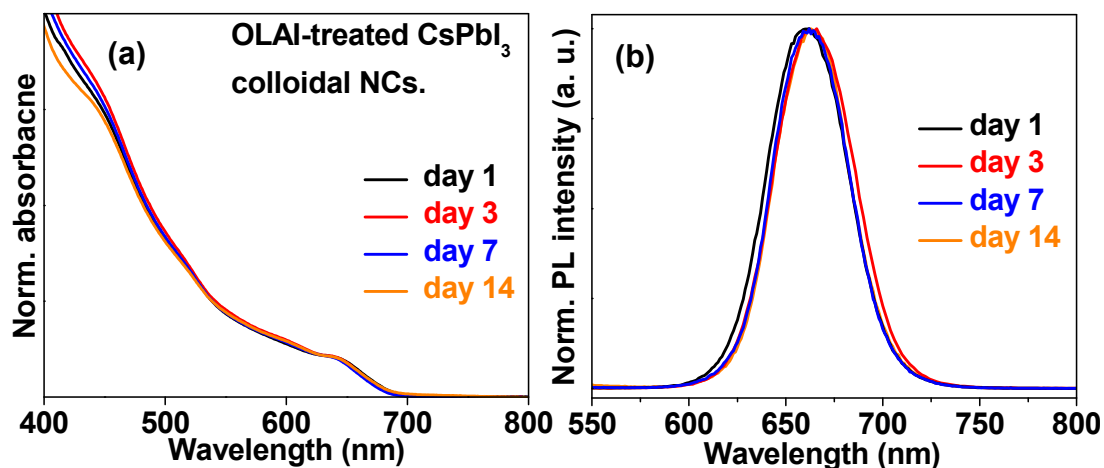


Figure S1. (a) UV-visible absorption and (b) normalized PL spectra of OLAI-treated colloidal CsPbI₃ NCs from day 1 to day 14 .

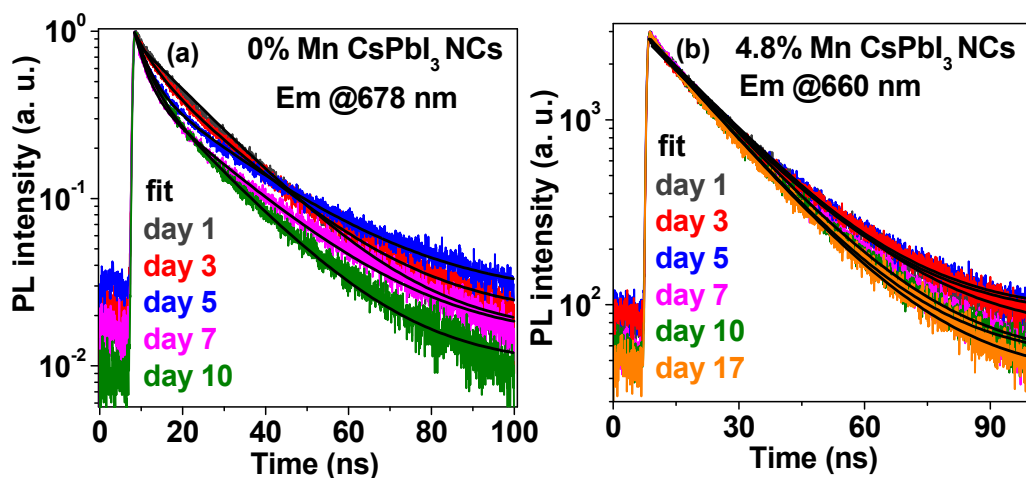


Figure S2. PL decay dynamics recorded at corresponding emission peak maximum of (a) undoped CsPbI₃ NCs, and (b) 4.8% Mn-doped CsPbI₃ NCs for PL data given in Figure 4 of main manuscript. The PL decay is recorded after excitation with 405 nm picosecond pulsed diode laser.

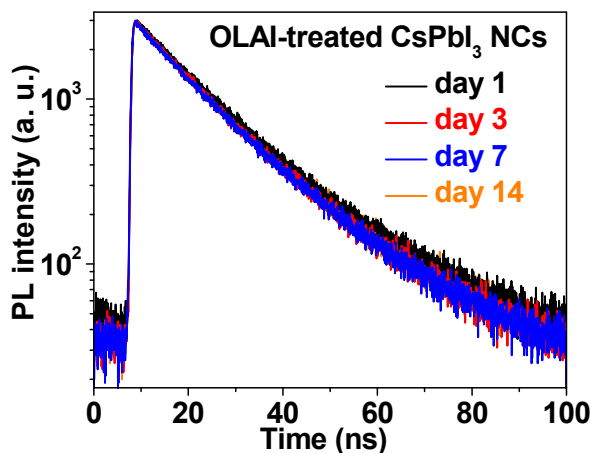


Figure S3. PL decay dynamics at emission peak maximum for OLAI treated undoped CsPbI₃ NCs corresponding to PL spectra given in Figure S1b. The PL decay is recorded after excitation with 405 nm picosecond pulsed diode laser.

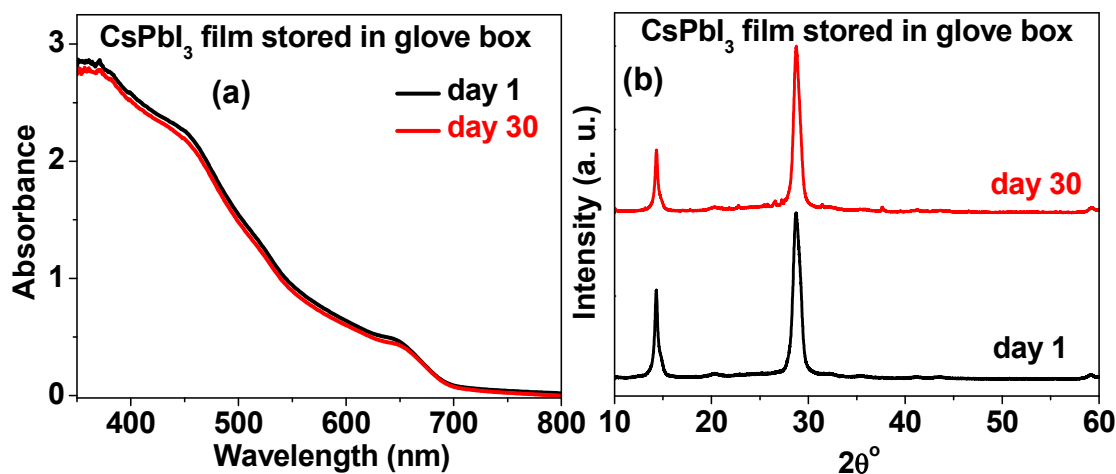


Figure S4. (a) Absorption spectra and (b) XRD patterns of undoped CsPbI₃ NCs on day 1 and day 30 after storing the film inside a N₂ filled glove box. No noticeable phase transition is observed in the black phase of undoped CsPbI₃ NCs film.

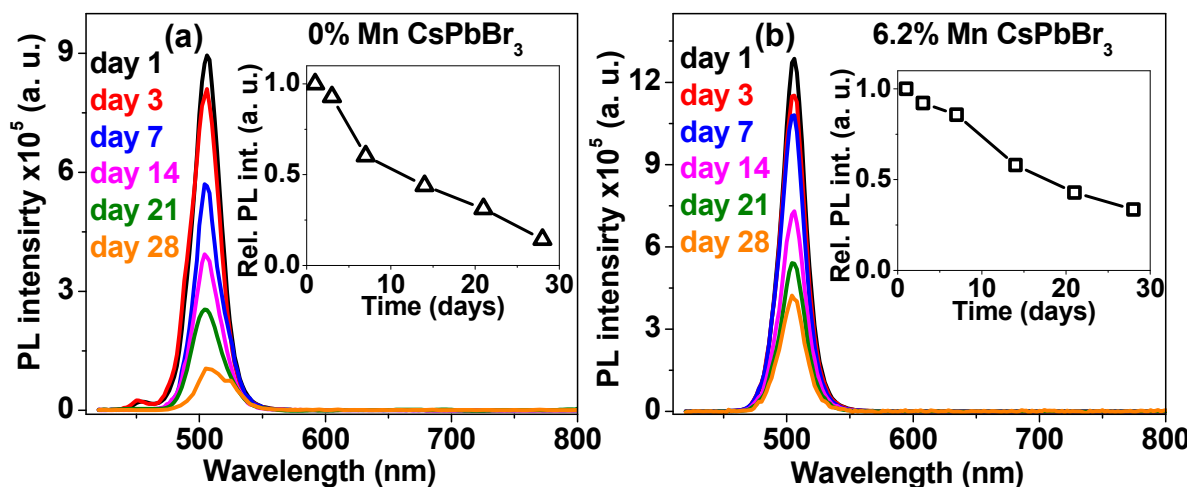


Figure S5. PL spectra from day 1 to day 28 for (a) undoped CsPbBr₃ NCs film and (b) 6.2% Mn-doped CsPbBr₃ NCs film under ambient conditions. Inset of (a) and (b) shows their corresponding normalized PL intensity variation with time, symbols denote experimental data and solid line shows trend.

Table S1. Best fit parameters of PL decay dynamics for undoped and 4.8% Mn-doped CsPbI₃ NCs dispersed in toluene corresponding to the data given in Figure S2.

0% Mn CsPbI ₃ nanocrystals	$y = a_1 * \exp\left(-\frac{t}{\tau_1}\right) + a_2 * \exp\left(-\frac{t}{\tau_2}\right) + y_o$			
	a ₁ (%)	τ ₁ (ns)	a ₂ (%)	τ ₂ (ns)
day 1		17.1	-	-
day 3	30	19.2	70	4.5
day 5	10	22.5	90	3.4
day 7	5	19.9	95	2.8
day 10	20	16.5	80	7.0
4.8% Mn CsPbI ₃ nanocrystals	$y = a * \exp\left(-\frac{x}{\tau}\right) + y_o$			
	τ (ns)			
day 1	18.0			
day 3	17.4			
day 5	18.2			
day 7	18.2			
day 10	16.7			
day 17	16.7			