

Electronic Supplementary Information for:
Enhance the Efficiency of CsPbX₃ (X = Cl, Br, I)
Nanocrystals via Simultaneous Surface Peeling and
Surface Passivation

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Experimental Section

Materials. Cs_2CO_3 (99.9%) was obtained from J&K Chemicals. Oleic acid (OA, 90%), octadecene (ODE, 90%) and lead (II) iodide (PbI_2 , 99.999%) were bought from Sigma-Aldrich. Lead (II) chloride (PbCl_2 , 99.999%) was purchased from Alfa Aesar. Lead (II) bromide (PbBr_2 , 99%), oleylamine (OLA, 70%), ammonium tetrafluoroborate (NH_4BF_4 , 99.995%), ammonium hexafluorophosphate (NH_4PF_6 , 99.5%), ammonium hexafluorosilicate ($(\text{NH}_4)_2\text{SiF}_6$, 98%), and ammonium hexafluorotitanate ($(\text{NH}_4)_2\text{TiF}_6$, 98%) were purchased from Aladdin. Toluene (99.5%) was obtained from Beijing Chemical Factory. All chemicals were used directly without further purification.

Preparation of cesium oleate. Cs_2CO_3 (2.50 mmol, 0.8146 g), 30 mL ODE and 2.5 mL OA were put into a 100 mL 3-neck flask, and heated to 120 °C under vacuum for 1 h. The mixture was further heated to 150 °C under N_2 and was kept for 3 h until a clear solution was obtained. Since Cs-oleate precipitates out of ODE at room-temperature, it has to be preheated to 100 °C before injection.

Synthesis of CsPbX_3 (X = Cl, Br, I) PNCs. PbX_2 (0.376 mmol, 0.1046 g PbCl_2 for CsPbCl_3 , 0.0523 g PbCl_2 and 0.0690 g PbBr_2 for $\text{CsPb}(\text{Cl}/\text{Br})_3$, 0.1380 g PbBr_2 for CsPbBr_3 , 0.0759 g PbBr_2 and 0.0780 g PbI_2 for $\text{CsPb}(\text{Br}/\text{I})_3$, 0.1733 g PbI_2 for CsPbI_3) and ODE (10 mL) were loaded into a 50 mL 3-neck flask and heated to 120 °C under vacuum for 1 h, then OLA (1 mL) and OA (1 mL) were injected into the system under the protection of N_2 . The temperature was increased to 170 °C and Cs-oleate (0.80 mL, 0.123 mmol) was quickly injected and after 5 s the solution was immediately cooled down to room temperature by immersing the flask in an ice water bath.

Purification. The CsPbX_3 PNCs were purified by centrifuging at 5000 rpm for 10 min; the supernatant containing unreacted precursors and byproducts was discarded. The precipitate was dispersed in toluene forming stable colloidal solutions for further characterization. The colloidal solutions were centrifuged at 10000 rpm for 5 min and the supernatant was discarded. Then the CsPbX_3 PNCs were dispersed in 20 mL toluene forming stable colloidal solutions.

Surface treatment of CsPbX₃ (X = Cl, Br, I) PNCs. 1 mmol treating salt (0.1048 g NH₄BF₄, 0.1630 g NH₄PF₆, 0.1781 g (NH₄)₂SiF₆ and 0.1979 g (NH₄)₂TiF₆) was added to 2 mL CsPbX₃ PNCs/toluene solutions and stirred for 3 h. Then, these mixtures were centrifuged at 10000 rpm for 1 min.

Characterizations. Absorption spectra were measured using a Shimadzu UV-2550 spectrophotometer. The PL spectra of the PNCs were collected using an Ocean Optics spectrometer. The morphology of the PNCs was characterized with a JEM-2100F transmission electron microscope (TEM). X-ray diffraction (XRD) patterns were acquired using a Bruker D8 Advance X diffractometer (Cu K α , $\lambda = 1.5406 \text{ \AA}$). X-ray photoelectron spectroscopy (XPS) was done on an ESCALAB250 spectrometer. The absolute PL QYs of the samples were obtained on a fluorescence spectrometer (FLS920P, Edinburgh Instruments) equipped with an integrating sphere. Time-resolved PL lifetime measurements were carried out using a time-correlated single-photon counting (TCSPC) lifetime spectroscopy system with a picosecond pulsed diode laser (EPL-365 nm) as the single wavelength excitation light source.

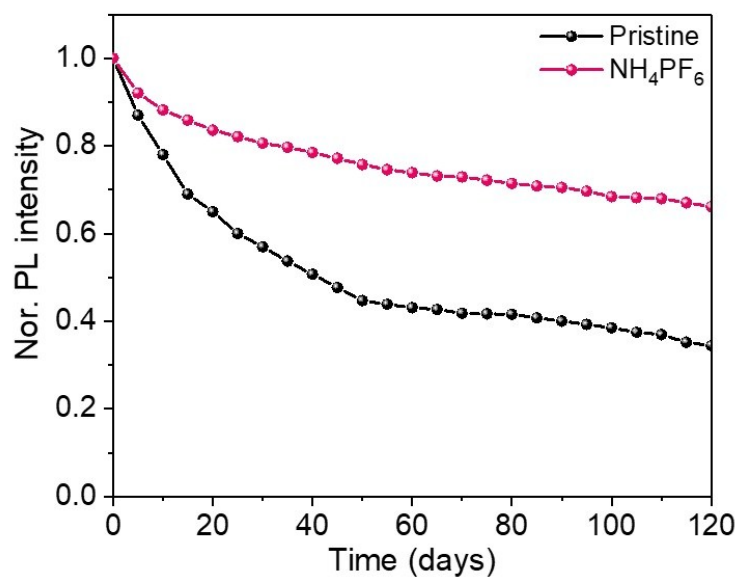


Fig. S1. Normalized PL intensity as a function of time for pristine and NH₄PF₆-treated CsPb(Cl/Br)₃ PNCs.

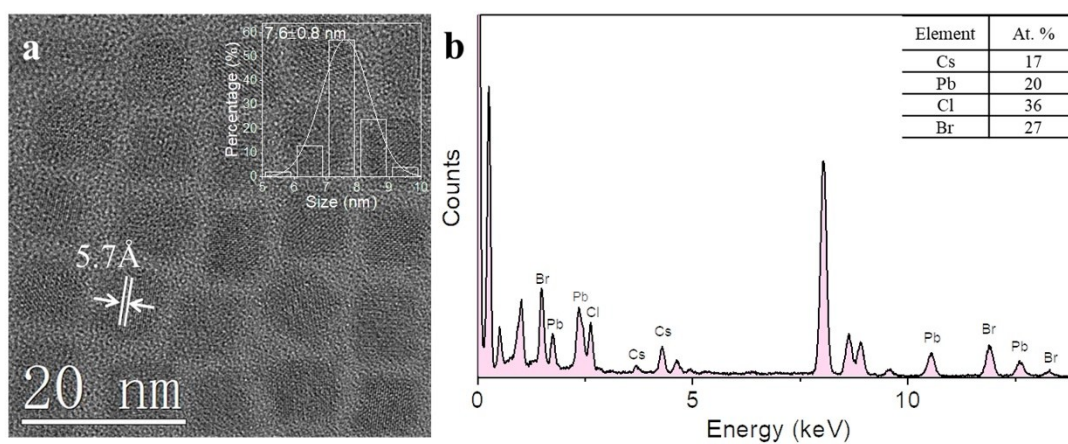


Fig. S2. (a) HRTEM image, particle size histogram and (b) EDS spectrum of CsPb(Cl/Br)₃ PNCs treated by (NH₄)₂TiF₆ for 3 h.

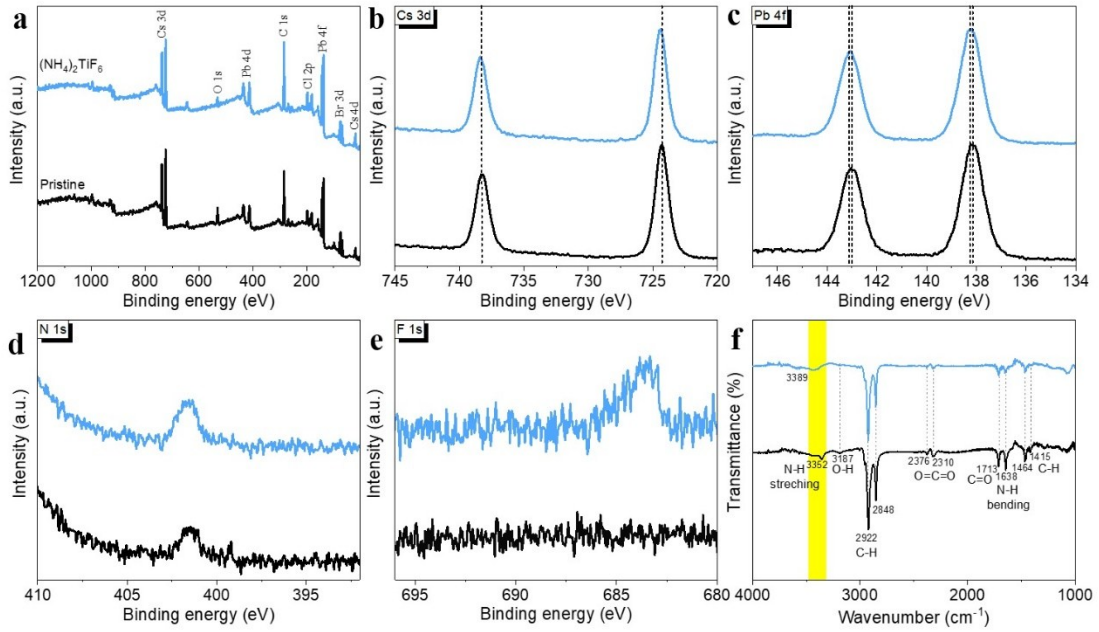


Fig. S3. (a) XPS spectra, (b-e) high-resolution XPS spectra of Cs ($3d_{3/2}$, $3d_{5/2}$), Pb ($4f_{5/2}$, $4f_{7/2}$), N 1s and F 1s, (f) FTIR spectra of of pristine (black lines) and $(\text{NH}_4)_2\text{TiF}_6$ -treated (blue lines) $\text{CsPb}(\text{Cl}/\text{Br})_3$ PNCs.

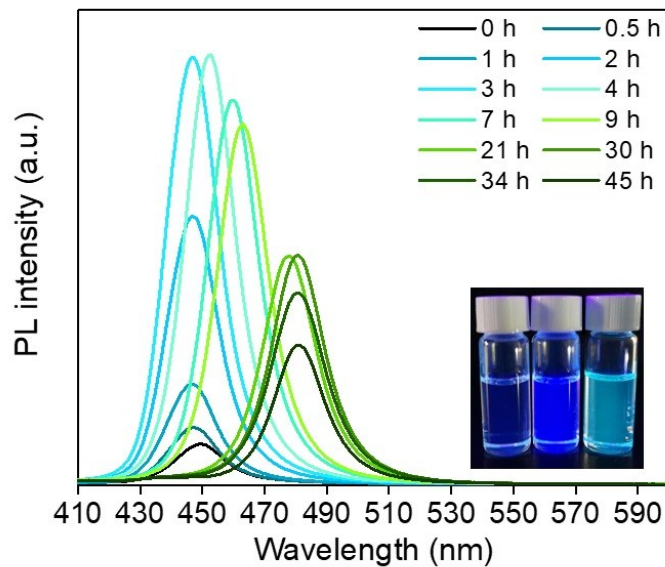


Fig. S4. PL spectra with photograph of the NH_4PF_6 treated PNCs under 365 nm UV-light.

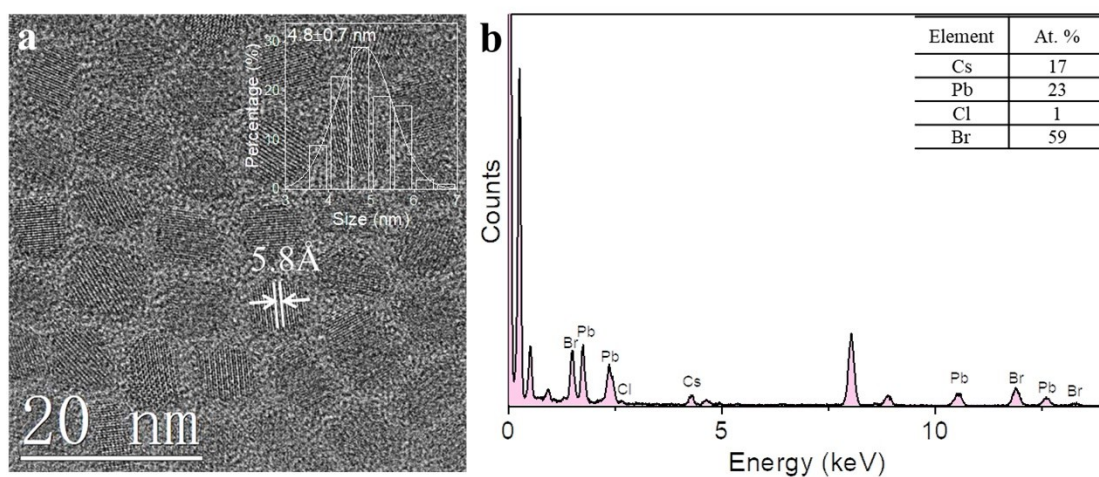


Fig. S5. (a) HRTEM image, particle size histogram and (b) EDS spectrum of NH_4PF_6 -treated $\text{CsPb}(\text{Cl}/\text{Br})_3$ PNCs at 30 h.

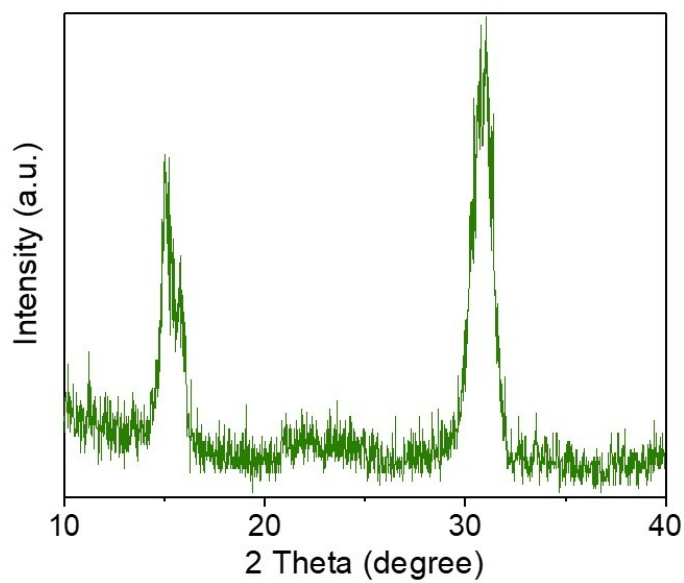


Fig. S6. XRD pattern of NH_4PF_6 -treated $\text{CsPb}(\text{Cl}/\text{Br})_3$ PNCs at 30 h.

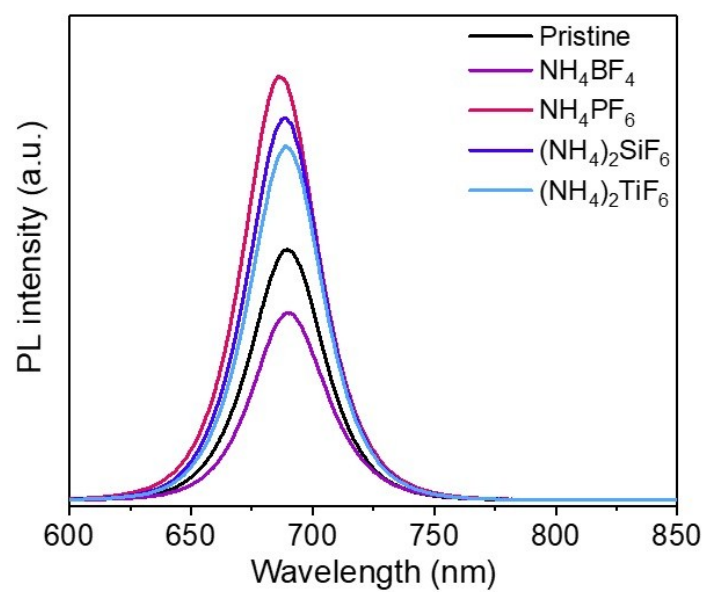


Fig. S7. PL spectra of pristine and (NH₄BF₄, NH₄PF₆, (NH₄)₂SiF₆ and (NH₄)₂TiF₆) treated CsPbI₃ PNCs.