Supporting Information

Enhancement of Photoluminescence and Stability of $CsPbX_3$ (X= Cl, Br, and I) Perovskite Nanocrystals with Phthalimide Passivation

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1. Sources of materials

Cesium Carbonate (Cs_2CO_3; 99.9%, Alfa Aesar), Octadecene (ODE; 90%, Alfa Aesar), Oleic acid (OA; Alfa Aesar), Oleylamine (OAm; Alfa Aesar), Lead (II) Chloride ($PbCl_2$; 98%, Aldrich), Lead (II) Bromide ($PbBr_2$; 98+%, Alfa Aesar), Lead (II) Iodide (PbI_2; 99%, Aldrich), Hexane (99%, anhydrous), n-trioctylphosphine (TOP; 90%, Aldrich), Phthalimide ($C_8H_5NO_2$; >99%, Himedia).

2. Experimental Procedures

2.1. Preparation of Cs-oleate precursor

Cs_2CO_3 (0.2 g) was taken into 15 mL capacity vial along with ODE (7.5 mL) and OA (0.88 mL), dried for 1 hour at 120 °C under open atmospheric conditions. Cs-oleate precipitates at room temperature, hence it is pre-heated upto 100 °C before use.

2.2. Synthesis and purification of $CsPbX_3$ perovskite nanocrystals

In a typical synthesis, 5 mL ODE, 0.5 mL OA, 0.5 mL OAm, and 0.188 mmol PbX_2 (52 mg $PbCl_2$ or 69 mg- $PbBr_2$ or 87 mg-PbI_2) were taken in a 20 mL vial and dried for 40 minutes at 120 °C in open atmospheric conditions. The temperature was raised to 140 °C after PbX_2 was dissolved completely. To it, 0.1 mmol of phthalimide was added to the reaction mixture. Consecutively, after the complete solvation, 0.4 mL of previously prepared Cs-oleate solution was rapid injected. The reaction was then quenched to room temperature using ice bath after 2 minutes of nucleation and subsequent growth. The crude solution was then purified via centrifugation by discarding supernatant and re-dispersing in hexane. Unlike the other synthesis reported where vacuum and nitrogen atmosphere used, here every step was carried out in open atmospheric conditions without involving any degassing steps.

3. Characterizations

3.1. Absorption and steady-state fluorescence:

Absorption and photoluminescence is recorded using Shimadzu UV-2600i and Horiba Jobin Yvon Fluorolog-3 respectively**.**

3.2. X-Ray Diffraction (XRD):

Powder X-Ray Diffraction patterns were recorded using Empyrean PANalytical X-Ray Diffractometer with Cu-Kα X-radiation (λ = 1.5406 Å) at 40 kV and 30 mA power.

3.3. Time-resolved photoluminescence:

The time resolved photoluminescence measurements were measured by a time-correlated single photon counting by TCSPC Spectrometer (Horiba Jobin Yvon IBH) with laser diode, output at 372 nm used as excitation laser source. The lamp profile was recorded by using a dilute solution of milk powder in water which act as a scatter in the sample chamber. The fluorescence decay curves were analyzed using IBH DAS6 software.

3.4. Transmission Electron Microscopy (TEM):

The samples were prepared by a droping of optimum solution of $CsPbX_3$ NCs in hexane on copper (Cu) grid coated with carbon film and analyzed using JEOL JEM-2100 High-Resolution Transmission Electron Microscope with 0.23 nm point resolution.

3.5. Photoluminescence Quantum Yield (PLQY):

Relative PLQYs were calculated by using an appropriate dye as references. For $CsPbCl_3$ NCs, 9,10-diphenylanthracene in toluene (QY= 0.93) while for $CsPbBr_3$ and $CsPbI_3$ NCs, Coumarine 153 in ethanol (QY= 0.93) and Rhodamine in ethanol (QY= 0.93) were used respectively.

3.6. X-Ray Photoelectron Spectroscopy (XPS):

XPS measurements were performed using Physical Electronics XPS/ ESCA, Model: PHI5000 Version Probe III.

4. Results and Discussion

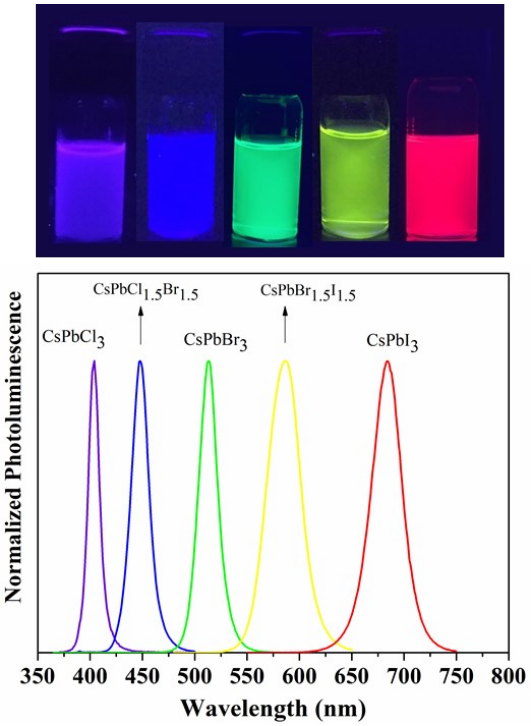

Figure-S1: Photoluminescence spectra of $CsPbX_3$ NCs with phthalimide passivation of different halide composition covering most of the entire visible range.

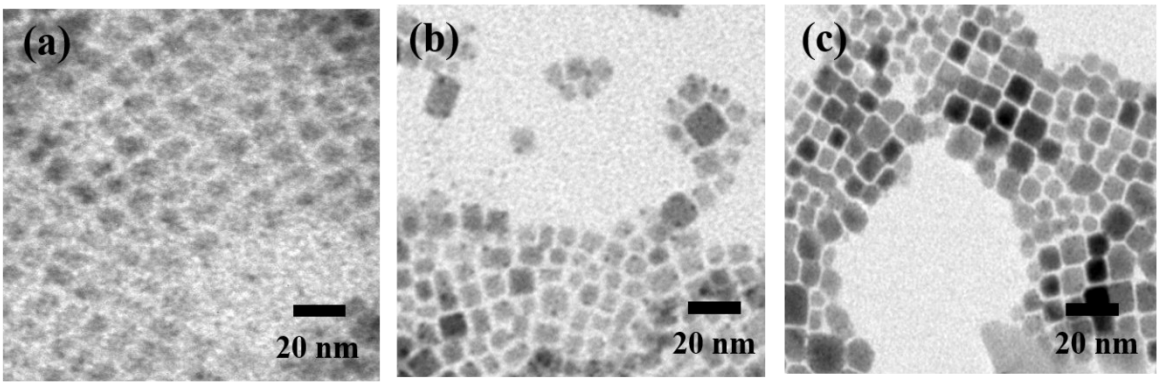

Figure-S2: Transmission Electron Microscope images of as-synthesized (a) $CsPbCl_3$, (b) $CsPbBr_3$, and (c) $CsPbI_3$ NCs without phthalimide.

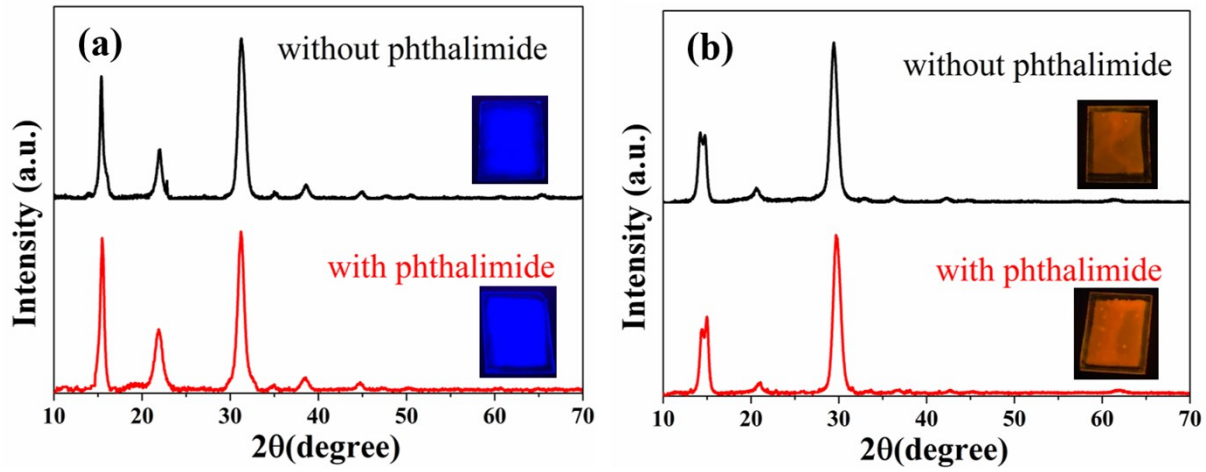

Figure-S3: XRD patterns of $CsPbCl_{1.5}Br_{1.5}$ and $CsPbBr_{1.5}I_{1.5}$ perovskite NCs with and without phthalimide and inset is their respective photograph taken under UV light illumination of wavelength 365 nm.

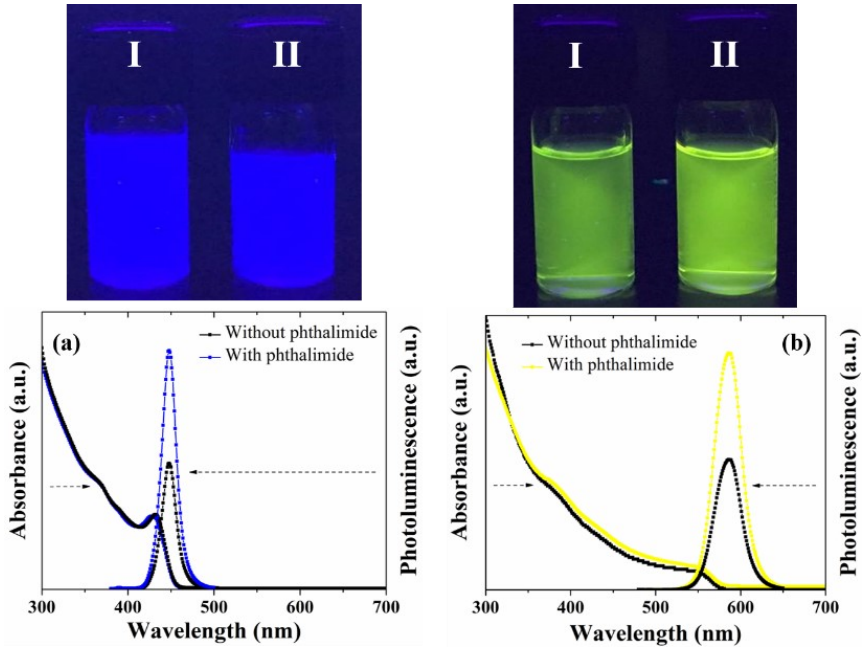

Figure-S4: (a) The photographs of (a) $CsPbCl_{1.5}Br_{1.5}$ NCs and (b) $CsPbBr_{1.5}I_{1.5}$ NCs labelled (I) without and (II) with phthalimide under UV light (365 nm, 8 W/cm^2) and their respective UV-Vis absorbance and photoluminescence spectra.

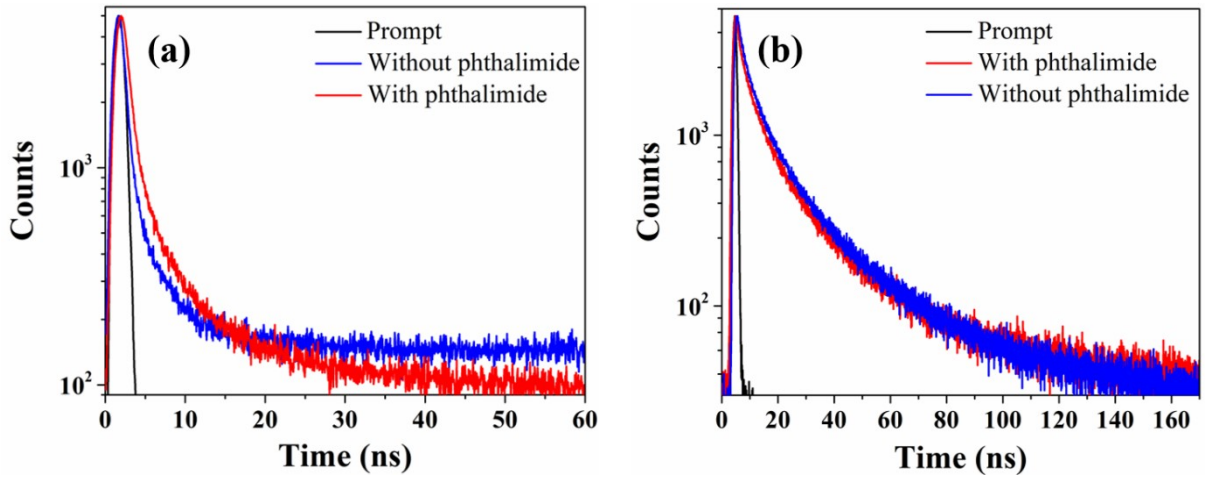

Figure-S5: PL decay profiles of (a) CsPbCl1.5Br1.5 NCs and (b) CsPbBr1.5I1.5 NCs without phthalimide (blue line) and with phthalimide (red line).

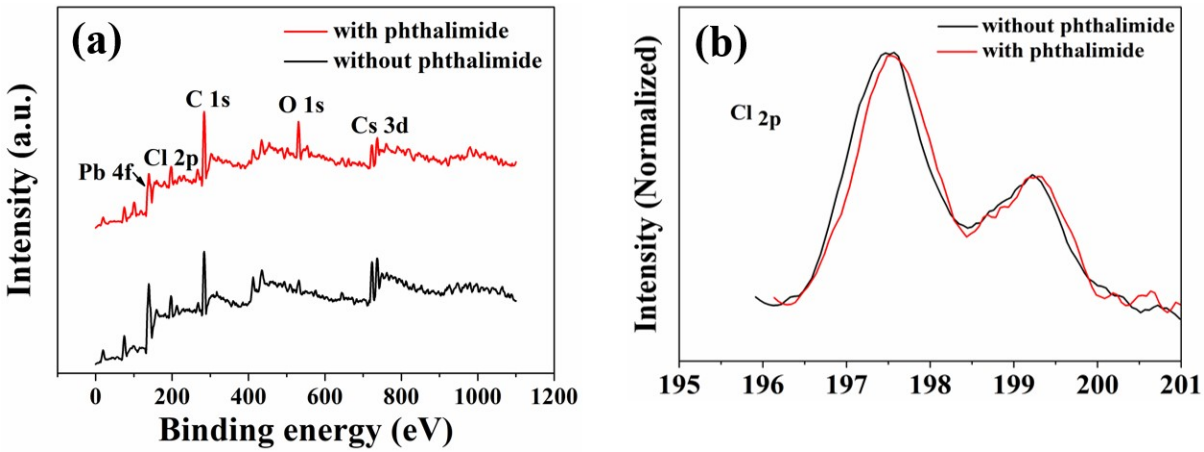

Figure-S6: XPS full survey spectra of $CsPbCl_3$ NCs (b) Core-level XPS spectra of chloride of $CsPbCl_3$ NCs without phthalimide (black line) and with phthalimide (red line) passivation.

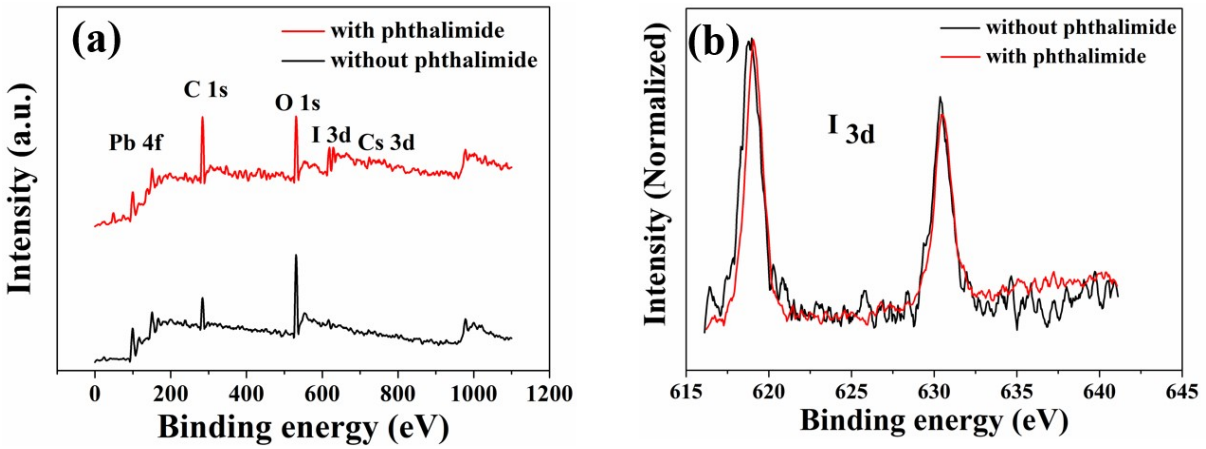

Figure-S7: XPS full survey spectra of $CsPbI_3$ NCs (b) Core-level XPS spectra of iodide of $CsPbI_3$ NCs without phthalimide (black line) and with phthalimide (red line) passivation.