

Supporting Information

Chemical Transformation Mechanism for Blue-to-Green Emitting CsPbBr₃ Nanocrystals

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Experimental Section

Chemicals

Cesium Carbonate (Cs_2CO_3 , 99.99%), Oleic acid (OA, AR), Cyclohexane (99.5%), Nitrosonium tetrafluoroborate (NOBF_4 , 95%), Oleylamine (OAm, 80%-90%), 1-Octadecene (ODE, 90%) and Hydrobromic acid (HBr, 48 wt% in H_2O) were purchased from Aladdin. Lead bromide (PbBr_2 , 98%) was purchased from Alfa. All of raw materials were used as received without further purification.

Synthesis and isolation of Cs_4PbBr_6 NCs

The synthesis details were showed in the experiment section of our previous report.¹

Synthesis of CsPbBr_3 NCs products

In this experiment, different amounts of NOBF_4 (1.0 mg, 1.5 mg, 1.8 mg, 2.5 mg and 3.5 mg) were individually added into 2 mL of cyclohexane. Subsequently, 100 μL of colloidal Cs_4PbBr_6 NCs were rapidly injected into the mixture while stirring vigorously at room temperature.

Characterization

The Photoluminescence (PL), time-resolved PL spectra, and photoluminescence quantum yield (PLQY) were recorded using an Edinburgh Instruments FS5 spectrofluorometer (UK) equipped with a built-in integrating sphere and a pulsed laser emitting at 405 nm. Absorption spectra were analyzed employing a Shimadzu UV-2600 spectrophotometer (Japan) in the UV-Vis spectral region. Powder X-ray diffraction (XRD) measurements using a Japan Rigaku X-ray diffractometer equipped with $\text{Cu K}\alpha$ radiation ($\lambda = 1.5405 \text{ \AA}$), operating at 40 kV and 40 mA. X-ray photoelectron spectroscopy (XPS) spectra were obtained using a Thermo ESCALAB 250XI X-ray photoelectron spectrometer (USA) with an $\text{Al K}\alpha$ source. For both XRD and XPS analyses, samples were prepared by depositing colloidal solutions onto glass substrates and subsequently heating them to 60 $^\circ\text{C}$, facilitating the rapid evaporation of the solvent. Transmission electron microscopy (TEM) measurements were performed with a JEM-2800 TEM (Japan) operating at an accelerating voltage of 200 kV. The dispersed nanocrystal (NCs) solution was applied onto a TEM grid and allowed to air-dry under ambient conditions. Fourier-transform infrared spectroscopy (FTIR) spectra were acquired using a Thermo Nicolet IS50 spectrometer (USA) employing the KBr pellet technique, spanning the range of 4000 to 600 cm^{-1} .

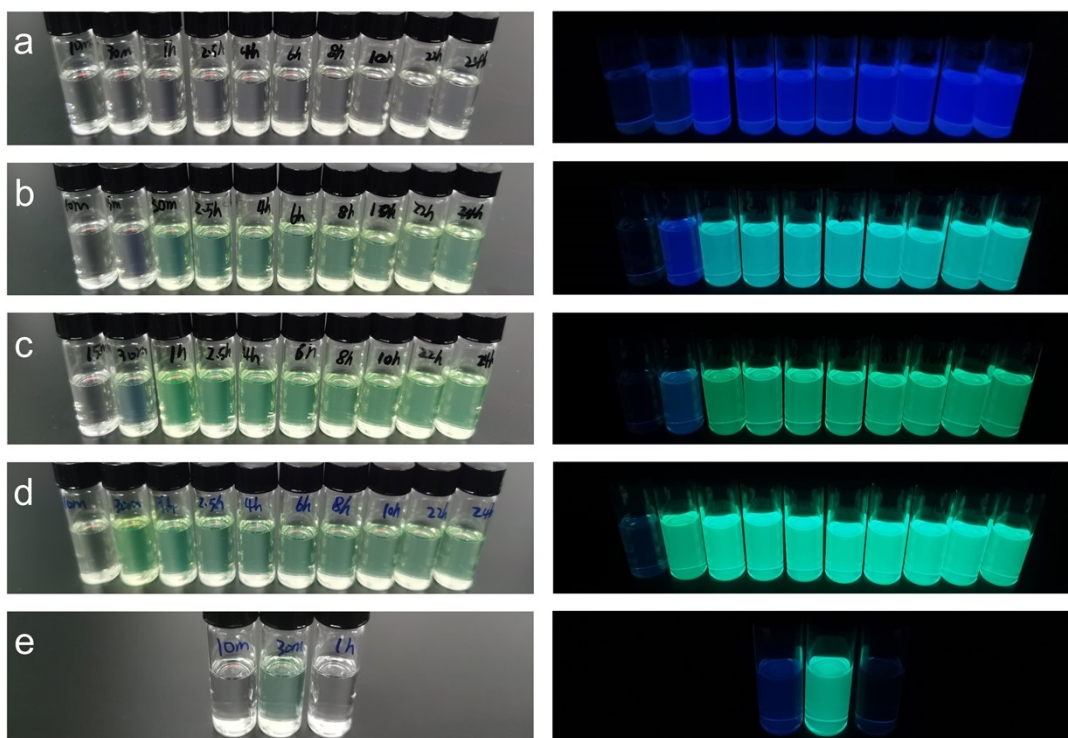


Figure S1. Photographs of the products under the ambient light (left) and 365 nm UV light irradiation (right) prepared with (a) 1.0 mg, (b) 1.5 mg, (c) 1.8 mg, (d) 2.5 mg and (e) 3.5 mg NOBF_4 at different reaction time.

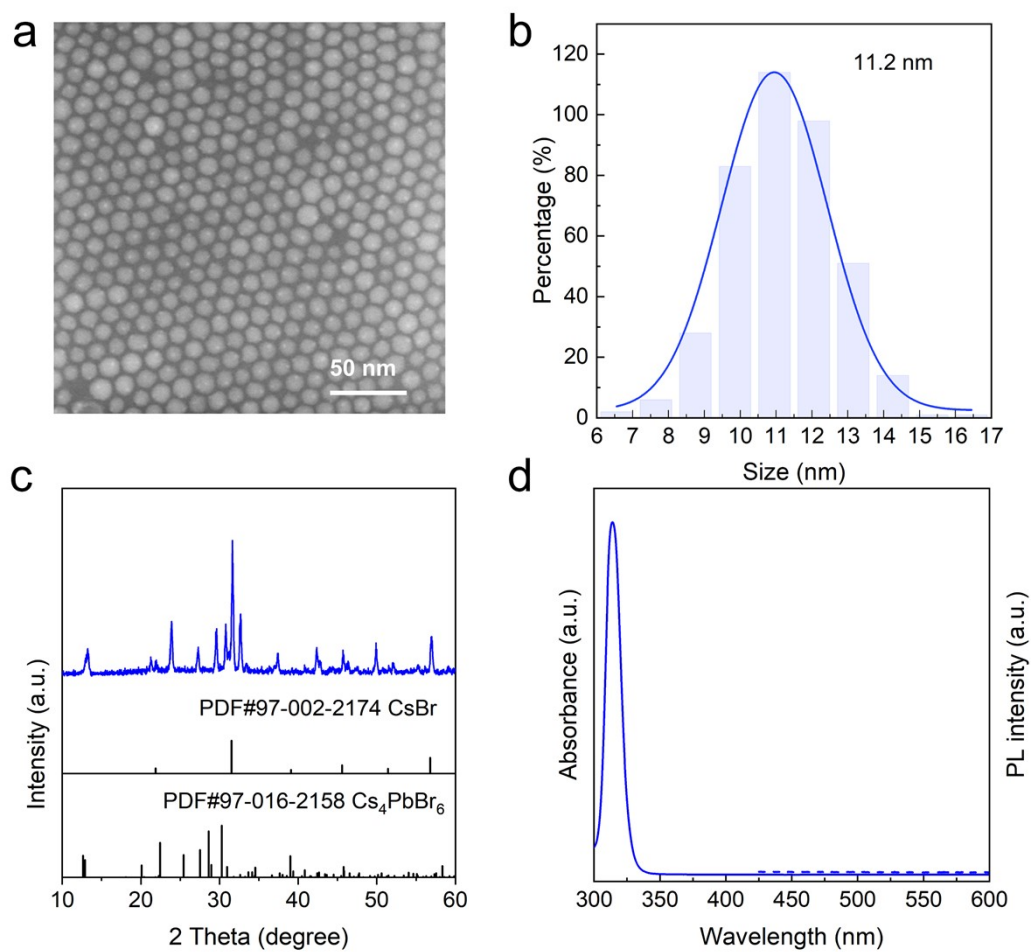


Figure S2. (a) TEM image, (b) the size distribution, (c) XRD pattern and (d) PL and Absorption spectra of Cs₄PbBr₆ NCs.

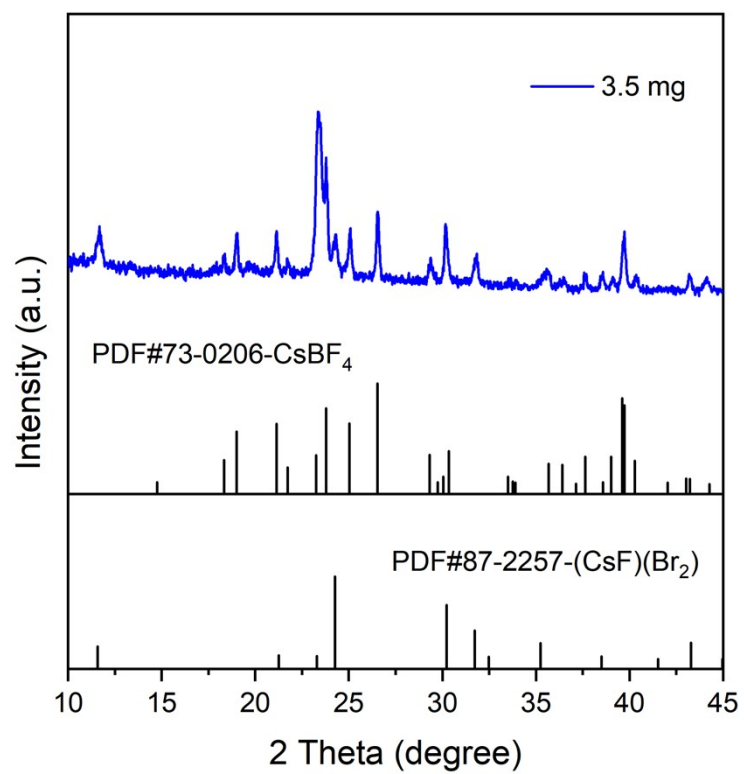


Figure S3. The XRD patterns of the nonluminescent products synthesized with 3.5 mg NOBF₄.

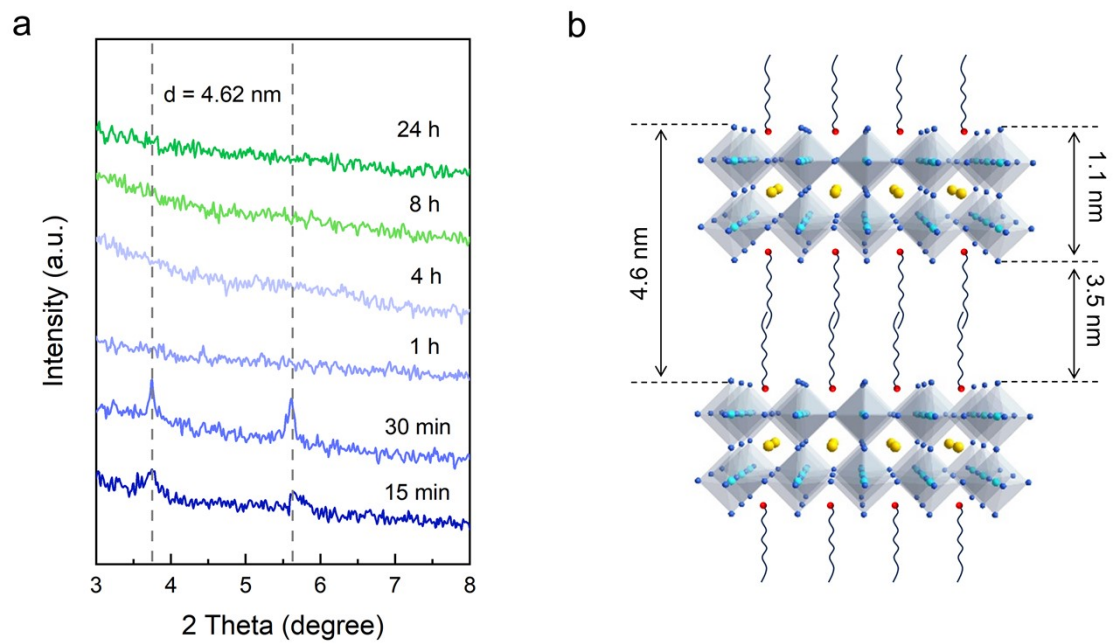


Figure S4. (a) Small angle XRD pattern of the products obtained with 1.8 mg NOBF₄ at different times. (b) Schematic diagram of the assembled CsPbBr₃ NPLs.

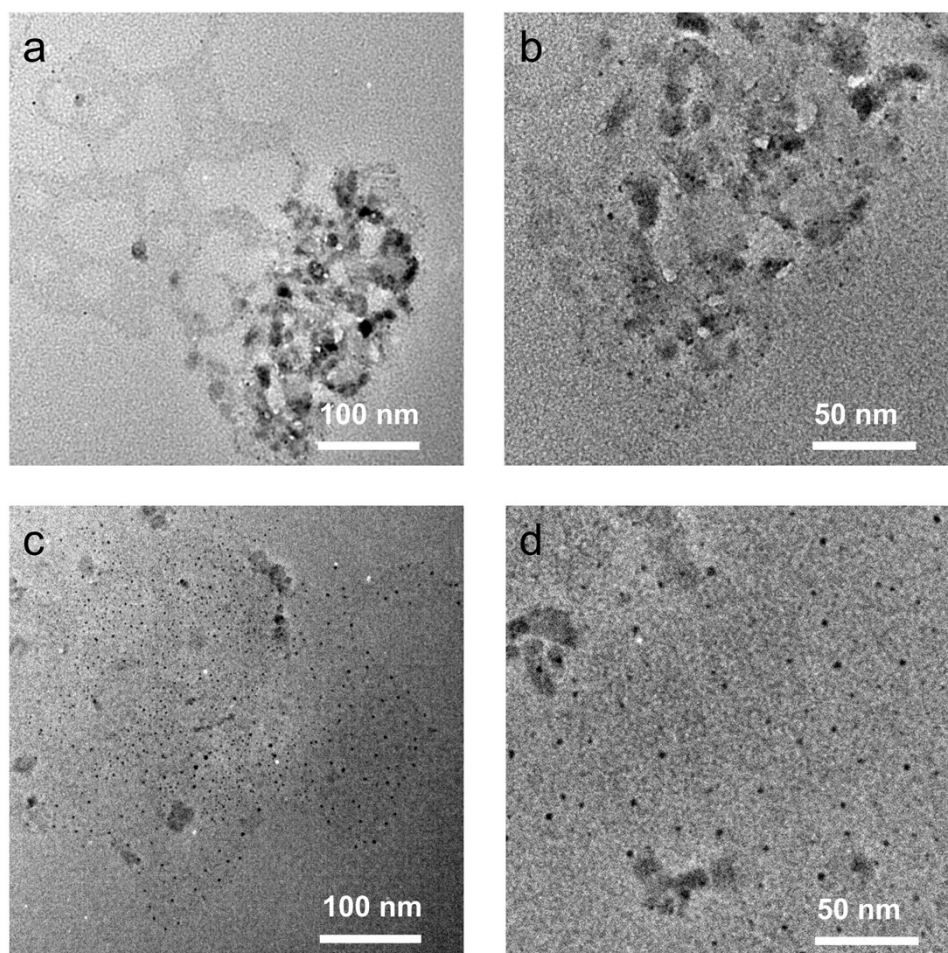


Figure S5. The TEM images of the luminescent products obtained with 1.8 mg NOBF_4 at (a, b) 15 min, (c, d) 30 min.

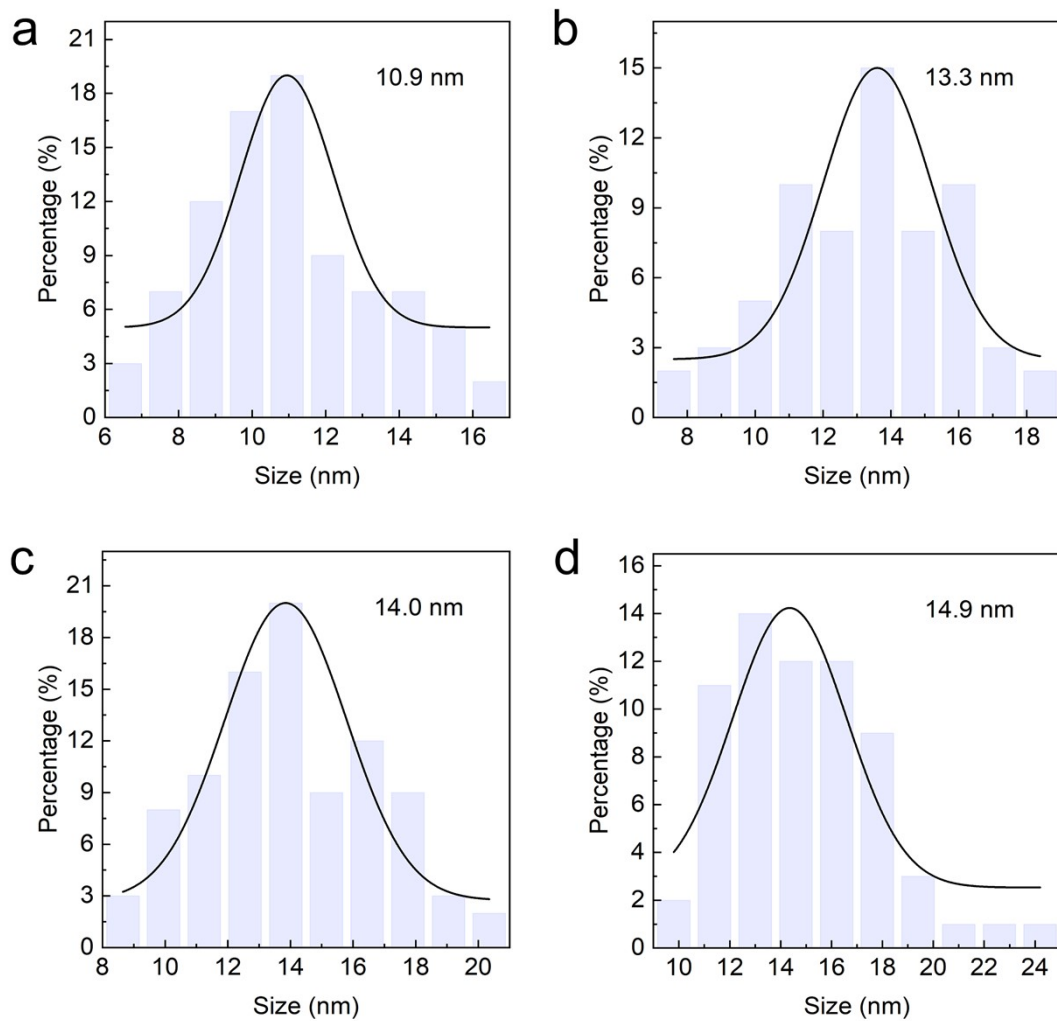


Figure S6. Size distribution of the newly formed CsPbBr₃ NCs obtained with 1.8 mg NOBF₄ at (a) 1h, (b) 4h, (c) 8h and (d) 24h.

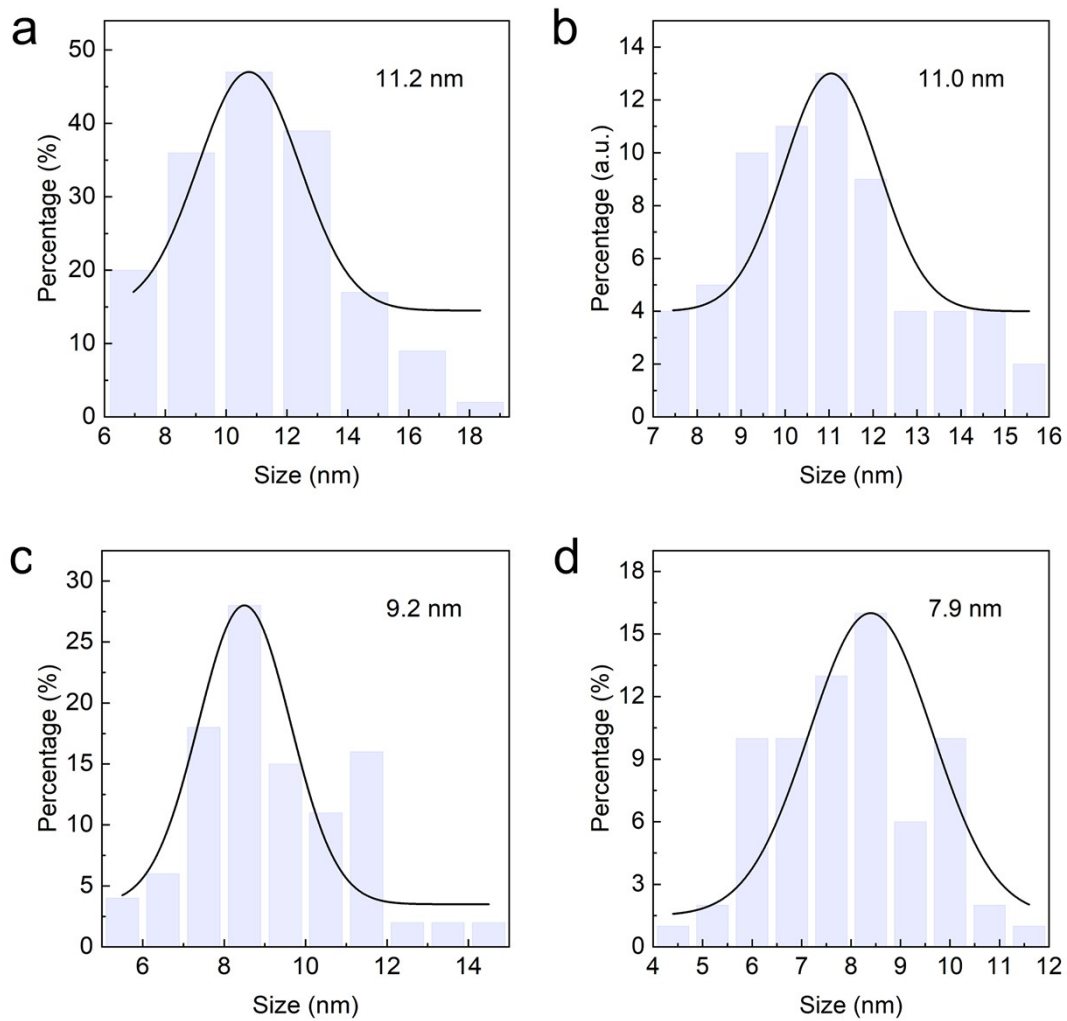


Figure S7. Size distribution of pristine Cs_4PbBr_6 NCs obtained at (a) 1h, (b) 4h, (c) 8h and (d) 24h.

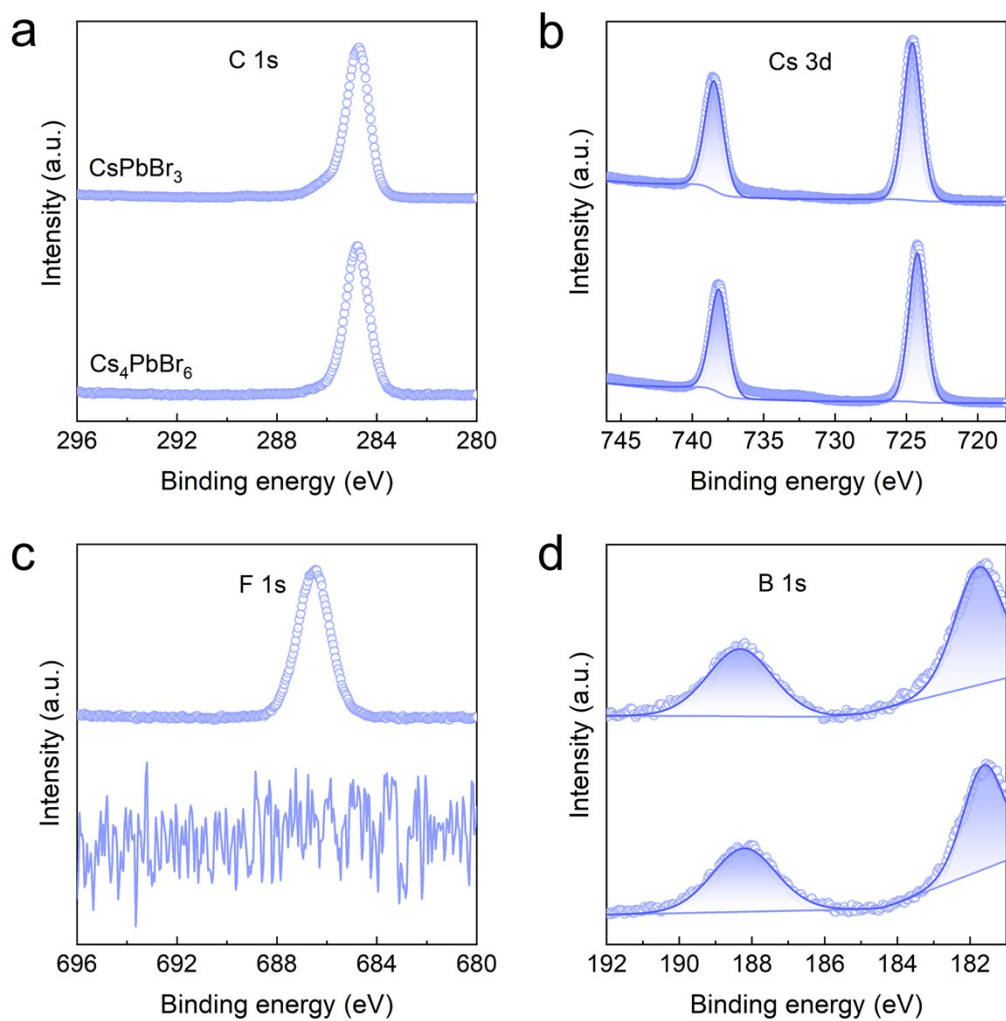


Figure S8. High-resolution XPS spectra for (a) C-1s, (b) Cs-3d, (c) F-1s, (d) B-1s.

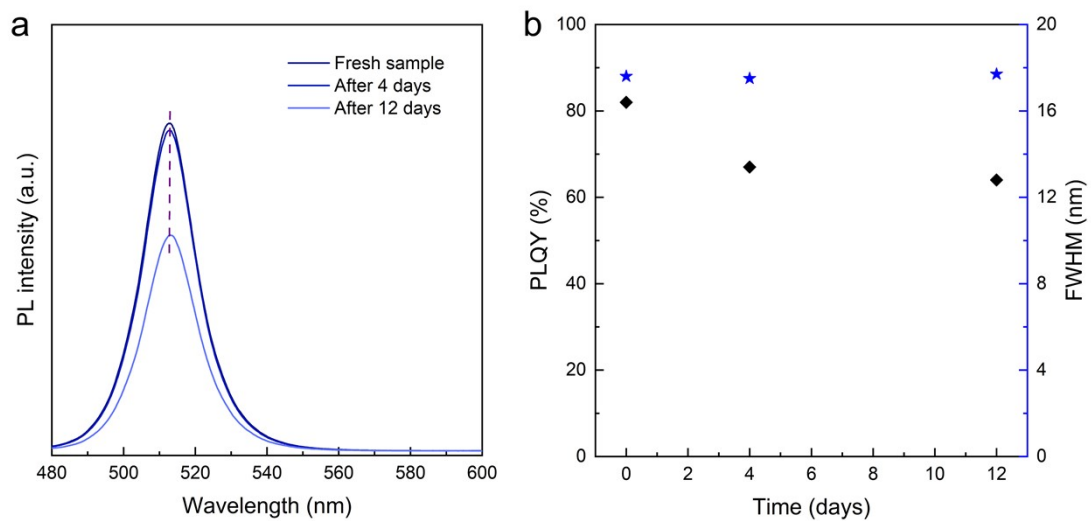


Figure S9. (a) The PL spectra, (b) FWHM and PLQY of the luminescent products stored in the cyclohexane.

Table S1. Fitting data for PL decay of luminescent products synthesized with 1.8 mg NOBF₄ at different reaction time.

Reaction time (h)	2.5	4	6	8	10	22	24
A ₁ (%)	0.08	0.77	0.87	0.26	0.69	0.39	0.49
T ₁ (%)	1.62	4.13	4.38	2.86	3.88	0.58	3.55
A ₂ (%)	0.83	0.19	0.06	0.71	0.32	0.87	0.48
T ₂ (%)	4.97	7.42	11.58	5.41	6.53	4.78	5.86
T _{ave} (%)	4.90	5.20	5.50	5.00	5.00	4.80	5.00

Table S2. Fitting data for PL decay of luminescent products synthesized with 2.5 mg NOBF₄ at different reaction time.

Reaction time (h)	1	2.5	4	6	8	10	22	24
A ₁ (%)	0.04	0.03	0.05	0.04	0.79	0.05	0.05	0.05
T ₁ (%)	0.76	0.68	1.14	0.87	3.87	1.15	0.76	0.67
A ₂ (%)	0.84	0.83	0.83	0.86	0.05	0.82	0.84	0.86
T ₂ (%)	4.38	4.20	4.26	4.25	10.08	4.26	4.22	4.17
T _{ave} (%)	4.40	4.20	4.20	4.20	4.70	4.20	4.20	4.10

Reference

1 R. Yun, H. Yang, Y. Li, Y. Liu, Y. Chu, S. Wu, X. Liu, X. Zhang, L. Zhang and X. Li, Inorganic Ligand Triggered Transformation from Cs₄PbBr₆ Nanocrystals to Blue-Emitting CsPbBr₃ Nanoplatelets, *Chem. Mater.*, 2023, **35**, 424-431.