

## Electronic Supplementary Information

### **In-situ passivation of Pb<sup>0</sup> traps by fluoride acid-based ionic liquid enables enhanced emission and stability of CsPbBr<sub>3</sub> nanocrystals for efficient white light-emitting diodes**

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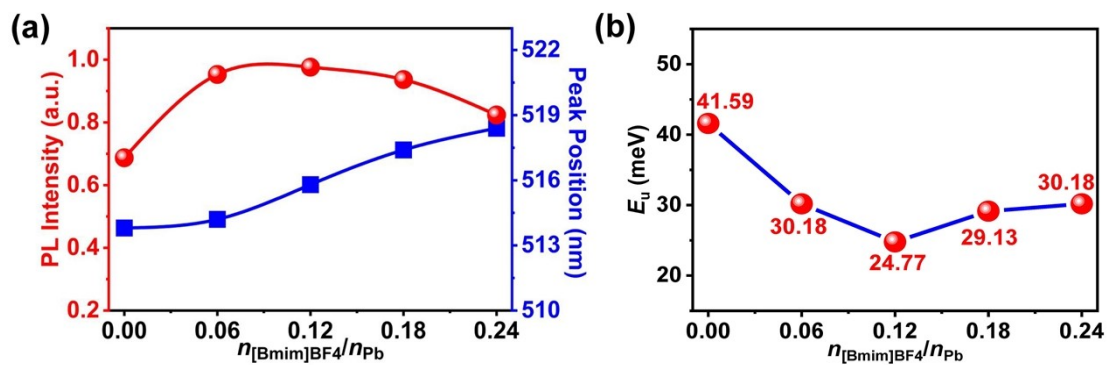


Fig. S1 (a) Evolution of PL intensity and peak positions and (b) calculated Urbach energy of CsPbBr<sub>3</sub> NCs with different  $n_{[Bmim]BF_4}/n_{Pb}$  ratios.

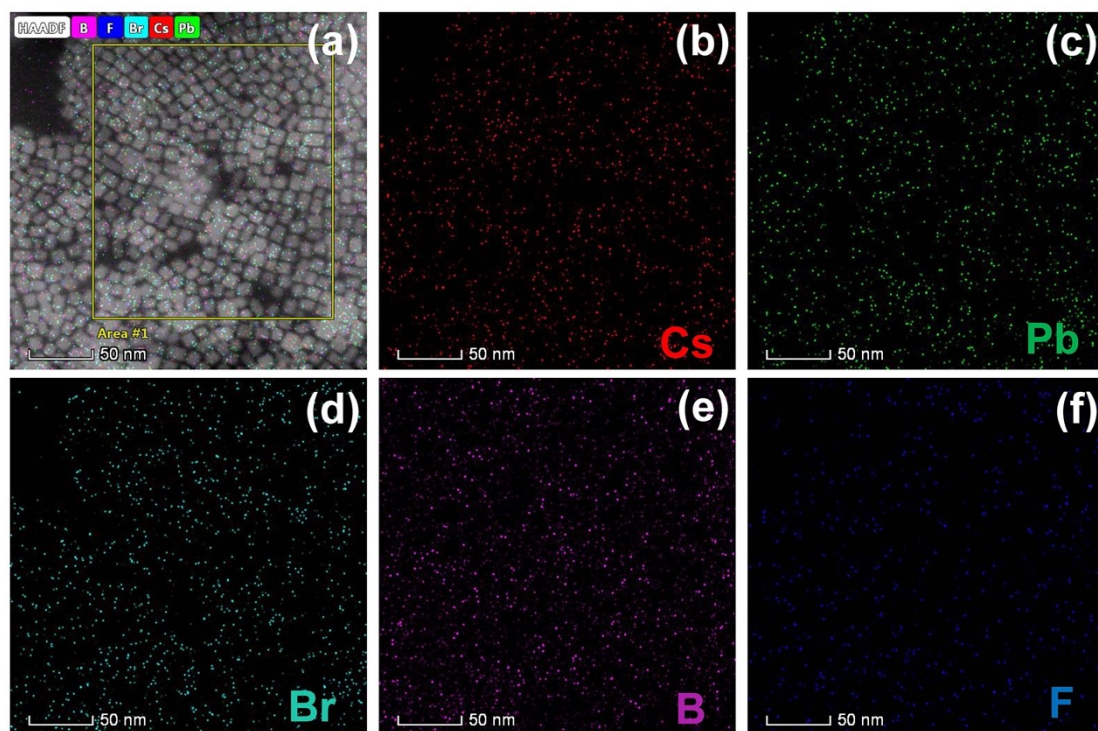
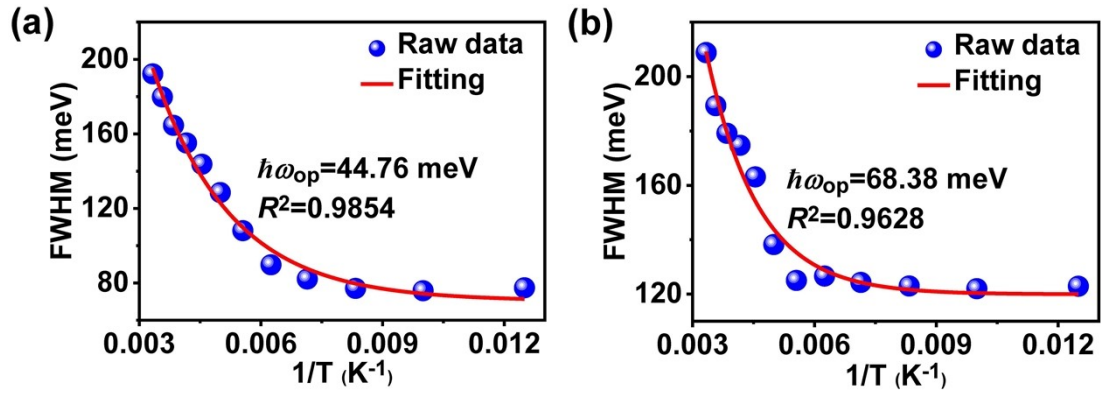
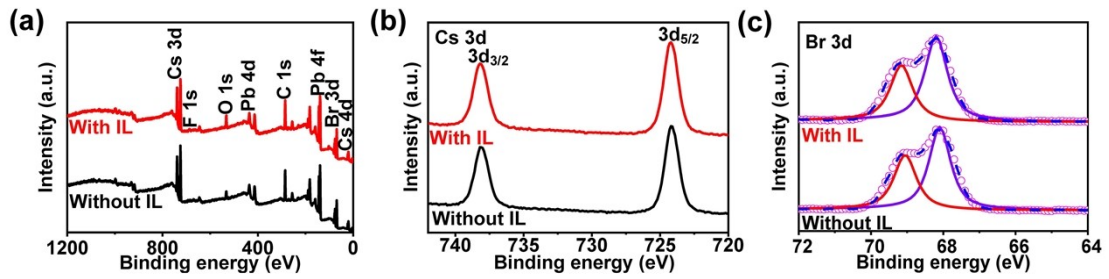


Fig. S2 (a) HAADF-STEM image, (b) Cs, (c) Pb, (d) Br, (e) B, and (f) F elemental maps of CsPbBr<sub>3</sub> NCs prepared with  $n_{[Bmim]BF_4}/n_{Pb}=0.12$ .



**Fig. S3** Plot of the FWHM of CsPbBr<sub>3</sub> NCs prepared (a) without and (b) with the assistance of [Bmim]BF<sub>4</sub> as a function of 1/T.



**Fig. S4** XPS (a) survey spectra, and (b) Cs 3d core-level, and (c) Br 3d core-level spectra of CsPbBr<sub>3</sub> NCs prepared with and without the assistance of [Bmim]BF<sub>4</sub>.

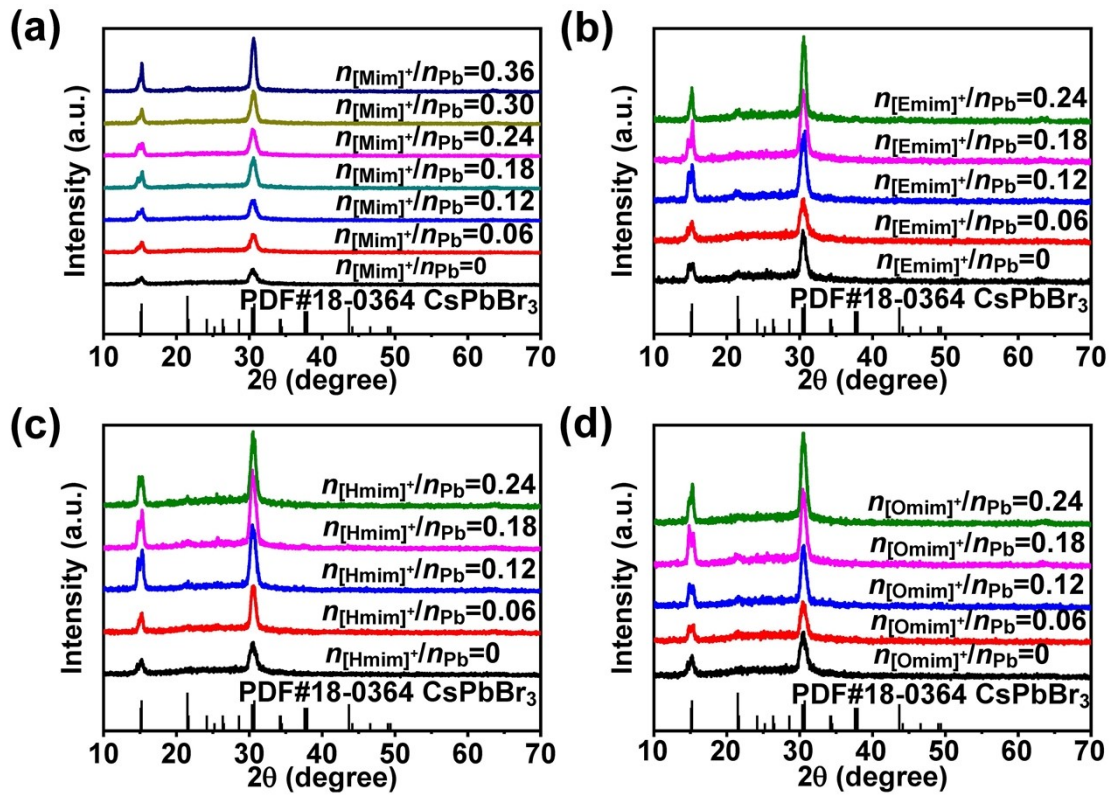
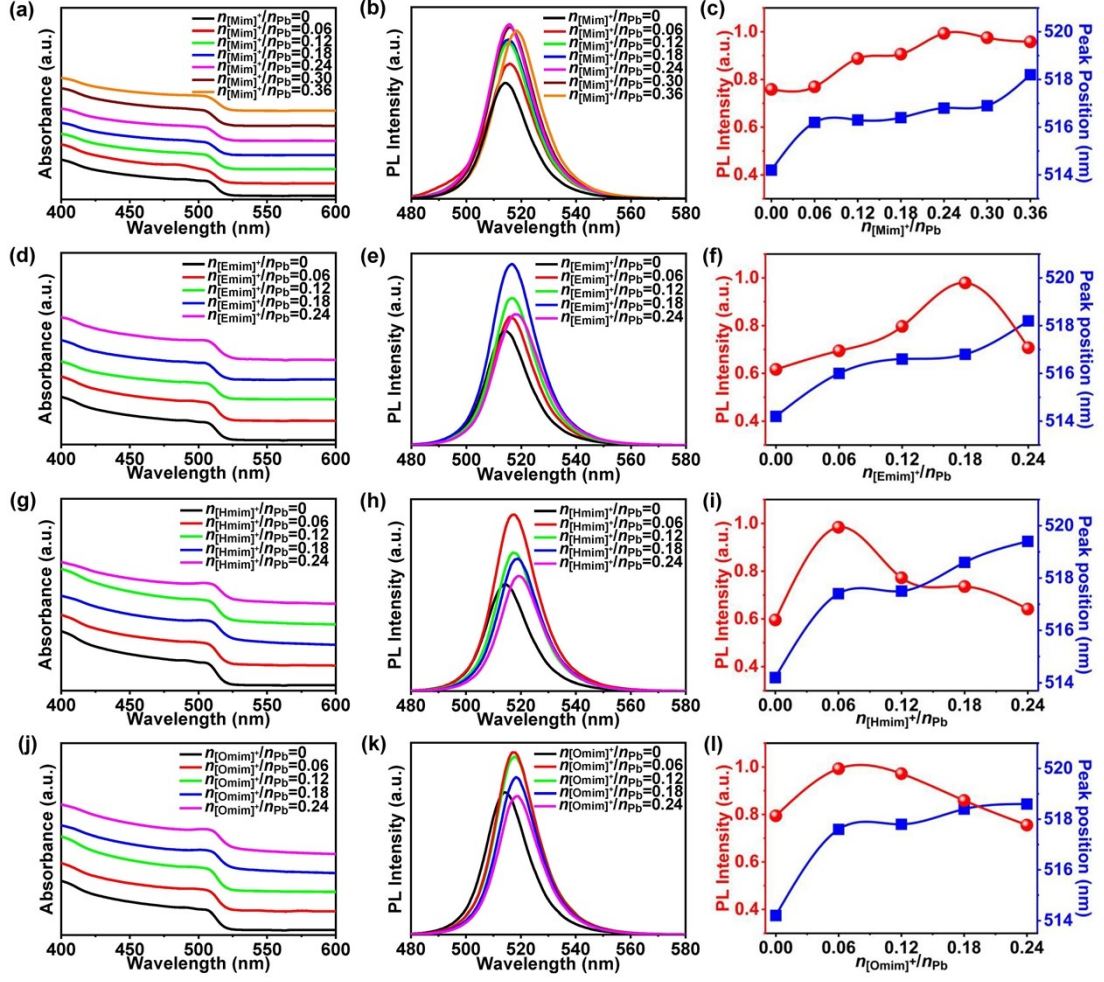


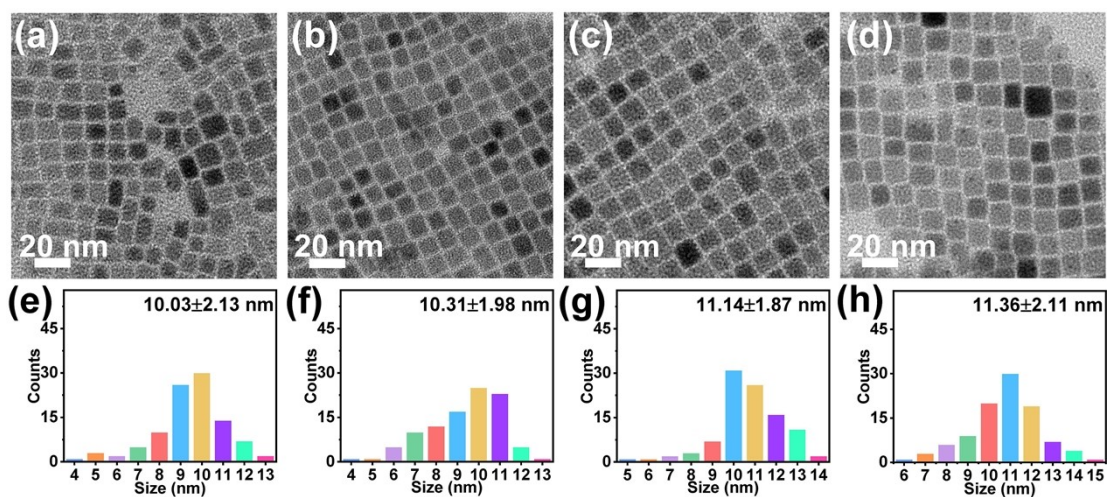
Fig. S5 XRD patterns of CsPbBr<sub>3</sub> NCs prepared with different chain length of ionic liquid: (a)

[Mim]BF<sub>4</sub>, (b) [Emim]BF<sub>4</sub>, (c) [Hmim]BF<sub>4</sub>, and (d) [Omim]BF<sub>4</sub>.

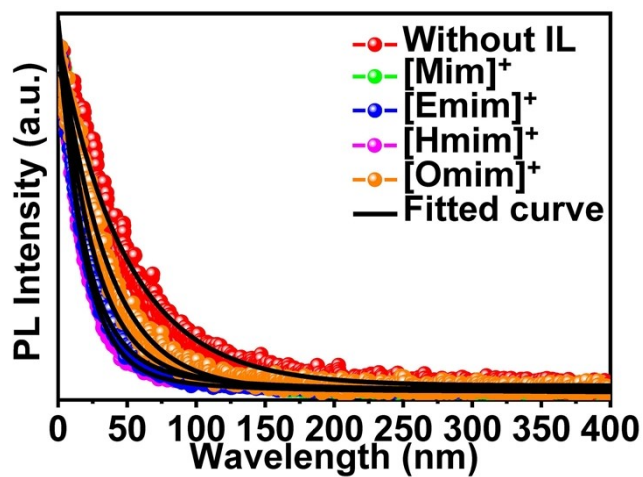


**Fig. S6** Absorption spectra, PL spectra, and evolution of PL intensity and peak positions in dependence with the values of the molar ratios of (a-c)  $n_{[Mim]}^+/n_{Pb}$ , (d-f)  $n_{[Emim]}^+/n_{Pb}$ , (g-i)  $n_{[Hmim]}^+/n_{Pb}$ , (j-l)  $n_{[Omim]}^+/n_{Pb}$ .

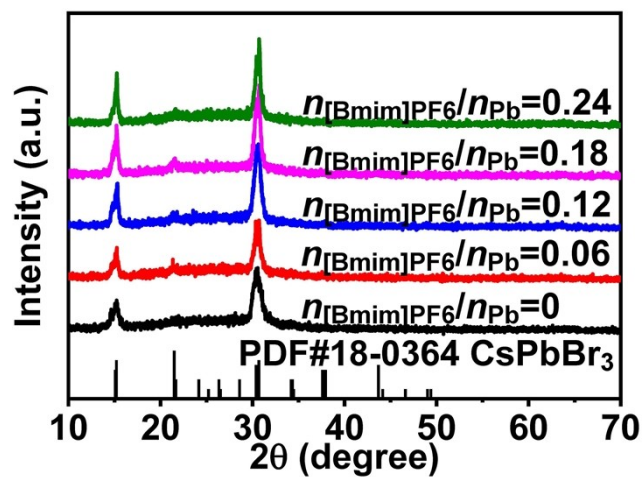




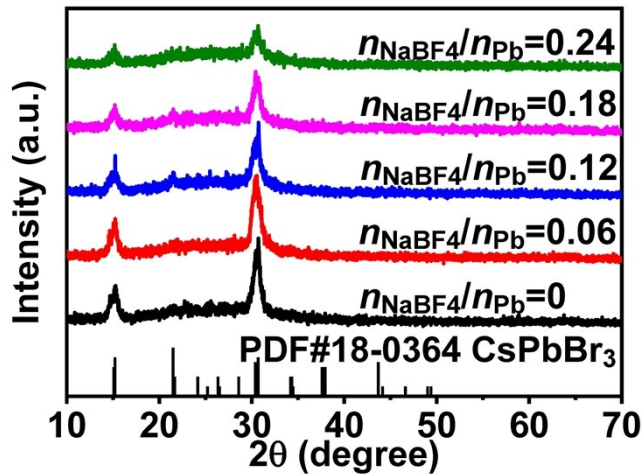
**Fig. S7** TEM images and size distribution histograms of CsPbBr<sub>3</sub> NCs prepared by using ionic liquid with different chain length: (a, e) [Mim]BF<sub>4</sub>, (b, f) [Emim]BF<sub>4</sub>, (c, g) [Hmim]BF<sub>4</sub>, and (d, h) [Omim]BF<sub>4</sub>.



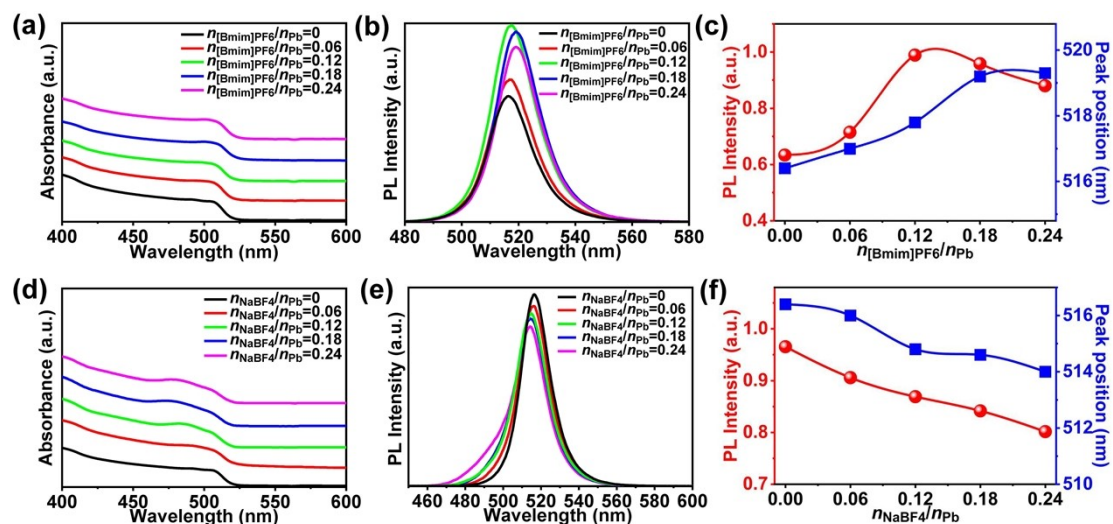
**Fig. S8** Decay curves of CsPbBr<sub>3</sub> NCs prepared by using ionic liquid with different chain length.



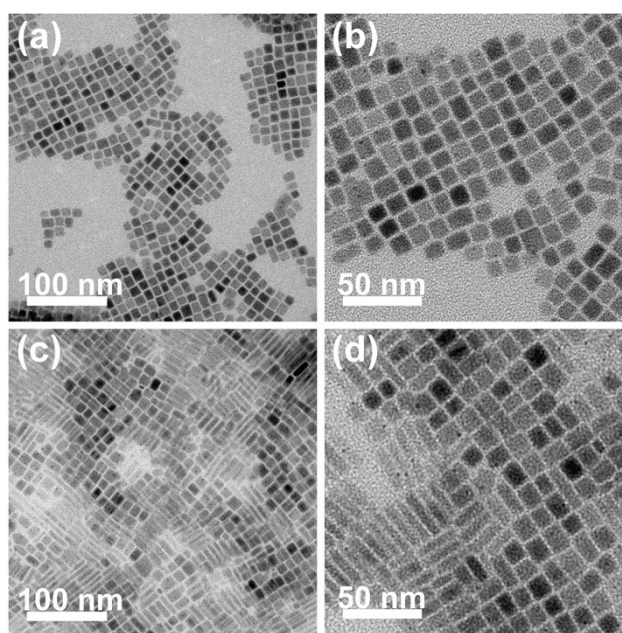
**Fig. S9** XRD patterns of CsPbBr<sub>3</sub> NCs prepared with different  $n_{[\text{Bmim}]\text{PF}_6}/n_{\text{Pb}}$  ratios of 0, 0.06, 0.12, 0.18, and 0.24.



**Fig. S10** XRD patterns of CsPbBr<sub>3</sub> NCs prepared with different  $n_{\text{NaBF}_4}/n_{\text{Pb}}$  ratios of 0, 0.06, 0.12, 0.18, and 0.24.

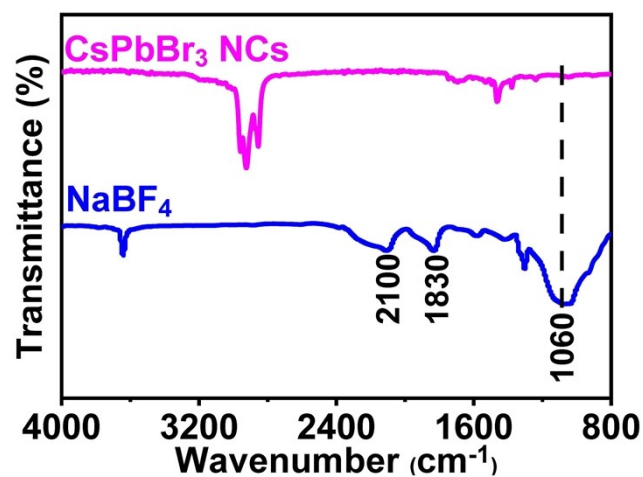


**Fig. S11** Absorption spectra, PL spectra, and evolution of PL intensity and peak positions in dependence with the values of the molar ratios of (a-c)  $n_{[\text{Bmim}]\text{PF}_6}/n_{\text{Pb}}$ , (d-f)  $n_{\text{NaBF}_4}/n_{\text{Pb}}$ .

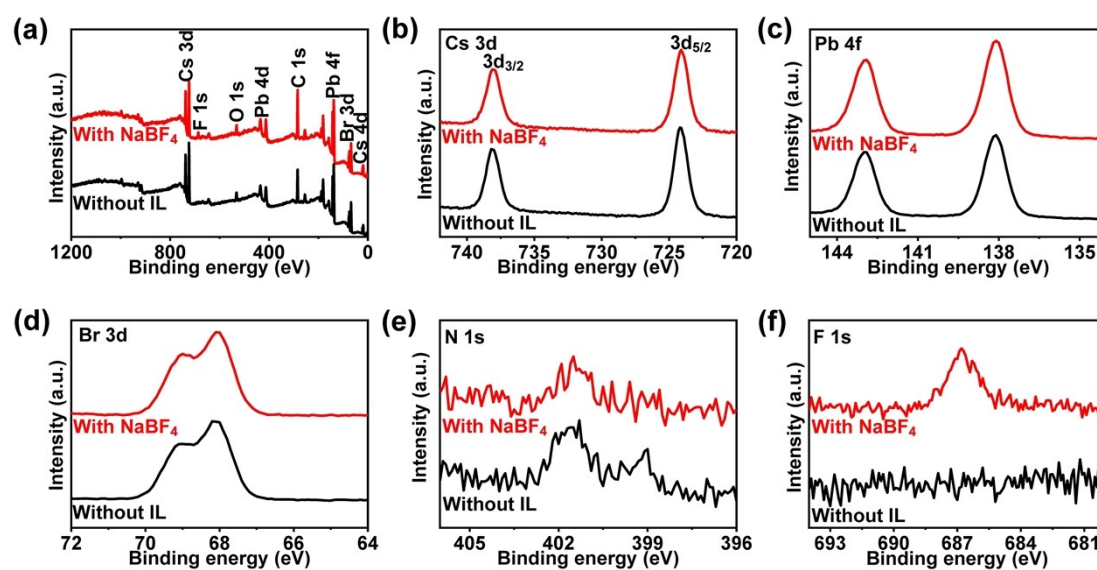


**Fig. S12** TEM images of CsPbBr<sub>3</sub> NCs prepared using (a, b) [Bmim]PF<sub>6</sub>, and (c, d) NaBF<sub>4</sub> as additives.





**Fig. S13** FT-IR spectra of  $\text{NaBF}_4$  and  $\text{CsPbBr}_3$  NCs prepared with the assistance of  $\text{NaBF}_4$ .



**Fig. S14** XPS (a) survey spectra, and (b) Cs 3d core-level, (c) Pb 4f core-level, (d) Br 3d core-level, (e) N 1s core-level, and (f) F 1s core-level spectra of  $\text{CsPbBr}_3$  NCs prepared with and without the assistance of  $\text{NaBF}_4$ .

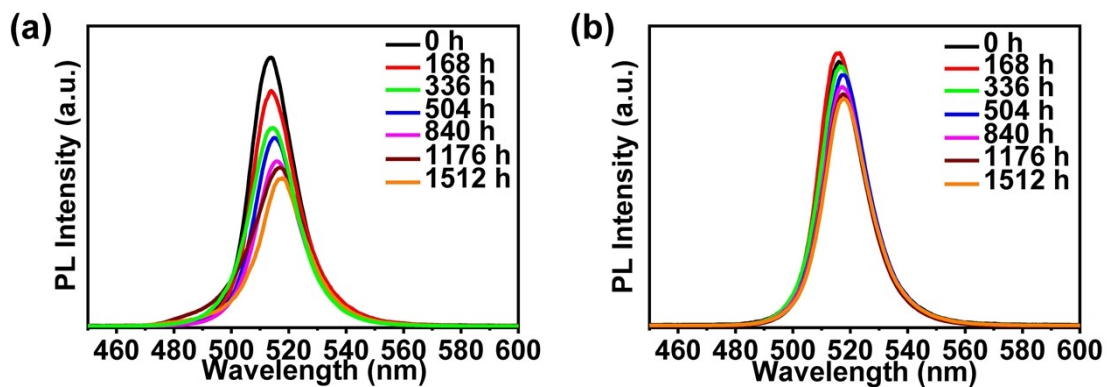


Fig. S15 PL spectra of CsPbBr<sub>3</sub> NCs prepared (a) without and (b) with the assistance of [Bmim]BF<sub>4</sub> in dependence with the storage time.

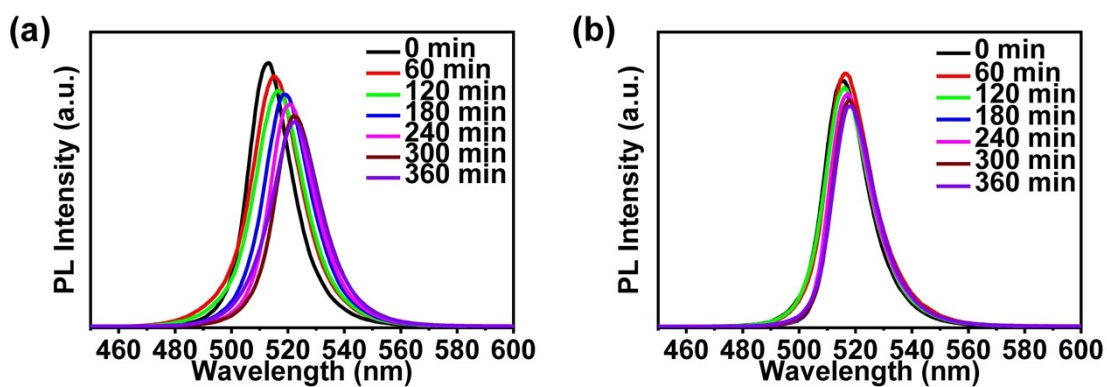


Fig. S16 PL spectra of CsPbBr<sub>3</sub> NCs prepared (a) without and (b) with the assistance of [Bmim]BF<sub>4</sub> in dependence with the irradiation time of UV light.

**Table S1** FWHM data and calculated average size of CsPbBr<sub>3</sub> NCs prepared with different  $n_{[\text{Bmim}]\text{BF}_4}/n_{\text{Pb}}$  ratios.

$n_{[\text{Bmim}]\text{BF}_4}/n_{\text{Pb}}$	Plane	FWHM/ $^\circ$	Calculated Size <sup>a</sup> /nm	Intensity
0	(200)	0.806	10.11	119
0.06	(200)	0.788	10.34	135
0.12	(200)	0.727	11.21	208
0.18	(200)	0.695	11.72	243
0.24	(200)	0.580	14.05	414

<sup>a</sup> Calculated size is obtained from Scherrer equation:  $D=K\lambda/B\cos\theta$ , where D represents the particle size of NCs, B represents the FWHM of (200) plane, and  $\theta$  represents the diffraction angle. K is equal to 0.89.

**Table S2** Fitting parameters of PL decay curves and calculated  $k_r$  and  $k_{nr}$  of CsPbBr<sub>3</sub> NCs with different  $n_{[\text{Bmim}]\text{BF}_4}/n_{\text{Pb}}$  ratios.

$n_{[\text{Bmim}]\text{BF}_4}/n_{\text{Pb}}$	$\tau_1/\text{ns}$	$B_1/\%$	$\tau_2/\text{ns}$	$B_2/\%$	$\chi^2$	$\tau_{av}/\text{ns}$	$k_r/\text{s}^{-1}$	$k_{nr}/\text{s}^{-1}$
0	12.88	80.12	120.87	19.88	0.9965	88.43	$7.22\times 10^6$	$4.09\times 10^6$
0.06	10.67	92.13	60.73	7.87	0.9845	27.05	$3.46\times 10^7$	$2.38\times 10^5$
0.12	10.13	95.32	65.70	4.68	0.9850	23.55	$4.01\times 10^7$	$2.32\times 10^5$
0.18	14.65	88.61	78.27	11.39	0.9946	40.55	$2.23\times 10^7$	$2.39\times 10^5$

**Table S3** Fitting parameters of PL decay curves of CsPbBr<sub>3</sub> NCs prepared by using ionic liquid with different chain length.

Sample	$\tau_1/\text{ns}$	$B_1/\%$	$\tau_2/\text{ns}$	$B_2/\%$	$\chi^2$	$\tau_{av}/\text{ns}$
Without IL	12.88	80.12	120.87	19.88	0.9965	88.43
[Mim]BF <sub>4</sub>	12.73	89.15	80.01	10.85	0.9952	41.89
[Emim]BF <sub>4</sub>	12.55	92.41	85.73	7.59	0.9968	38.85
[Hmim]BF <sub>4</sub>	11.69	94.49	75.72	5.51	0.9962	29.24
[Omim]BF <sub>4</sub>	34.47	85.37	87.33	14.63	0.9840	50.47

**Table S4** Storage, UV light, and water stability of perovskite NCs.

Materials	Storage	UV light	Water	Ref
CsPbBr <sub>3</sub> @SiO <sub>2</sub> Janus NCs	The NC film presents bright emission after storage in air for 4 days	The NC film shows slight drop (~2%) of PL intensity	Maintaining 80% of PL intensity after being treated water for 7 days	[66]
Quasi-2D CsPbBr <sub>3</sub> NCs	–	Keeping more than 85% of PL intensity after 120 min UV light irradiation	Remaining 87% of PL intensity after 168 h water treatment	[67]
CsPbBr <sub>3</sub> /Pb-MA composite	–	Maintaining 43% of initial PL intensity after 36 h UV light irradiation	Holding 83% of PL intensity after being immersed in water for 192 h	[68]
4-Bromo-butyric acid passivated CsPbBr <sub>3</sub> NCs	–	–	Maintaining 79% of PL intensity after 72 h in aqueous solution	[69]
[Bmim]BF <sub>4</sub> passivated CsPbBr <sub>3</sub> NCs	Holding 85% of initial PL intensity after storage 1512 h	Retaining ~90% of initial intensity after continuous irradiation under a UV light for 360 min	Reserving 67.5% of initial emission intensity after 21 days water treatment	This work