Supplementary Information

Halide Vacancy Passivation in Cesium Lead Halide Perovskite Nanocrystals with Mixed Halide Compositions: The Impact of Prolonged Reaction Time

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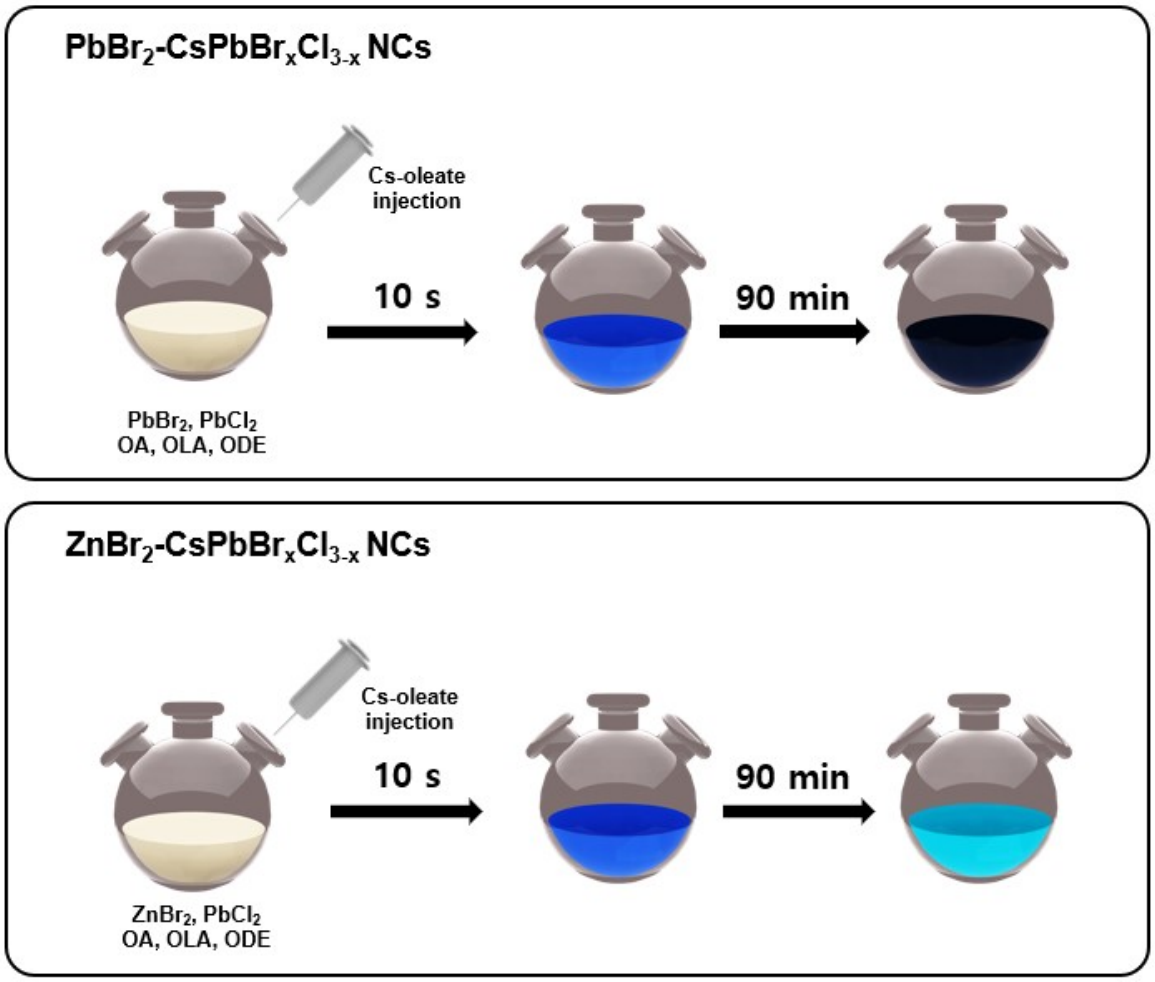


Scheme S1. Schematic illustration for the synthesis of (top) $ZnBr_2$-$CsPbBr_xCl_{3-x}$ and (bottom) $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs.

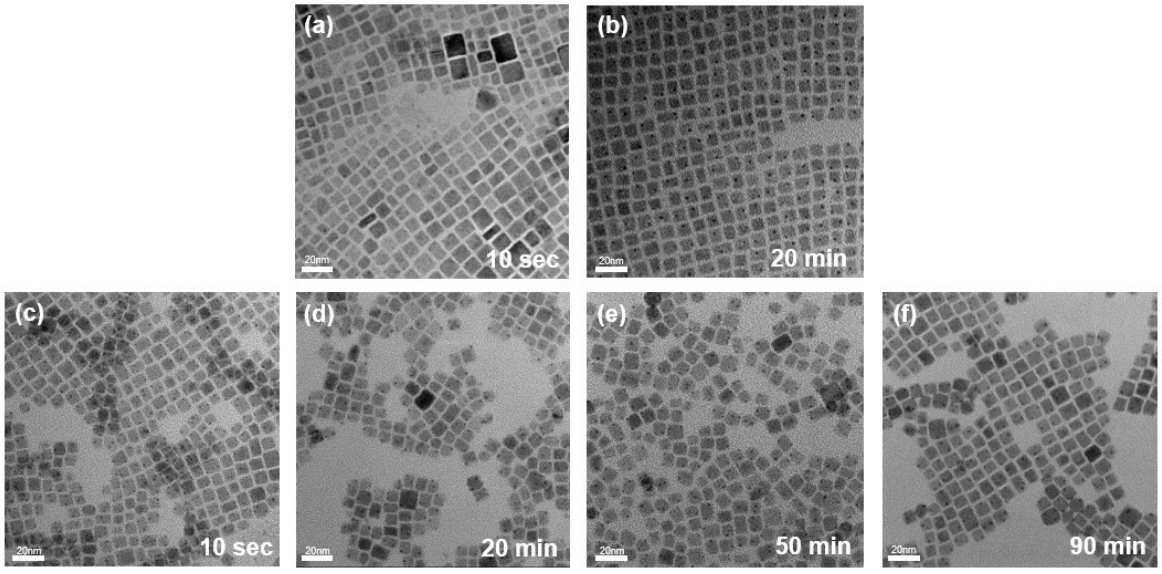


Fig. S1. TEM images of (a)-(b) $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs and (c)-(f) $ZnBr_2$-$CsPbBr_xCl_{3-x}$ NCs with different reaction time.

Table S1. Size analysis data of perovskite NCs with different reaction times. The sizes were measured based on TEM images

Perovskite NCs	Size
$PbBr_2$-$CsPbBr_xCl_{3-x}$ 10 sec	10.5 ± 1.0
$PbBr_2$-$CsPbBr_xCl_{3-x}$ 20 min	10.5 ± 1.8
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 10 sec	10.5 ± 2.0
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 20 min	10.5 ± 1.4
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 50 min	10.5 ± 2.1
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 90 min	10.4 ± 2.0

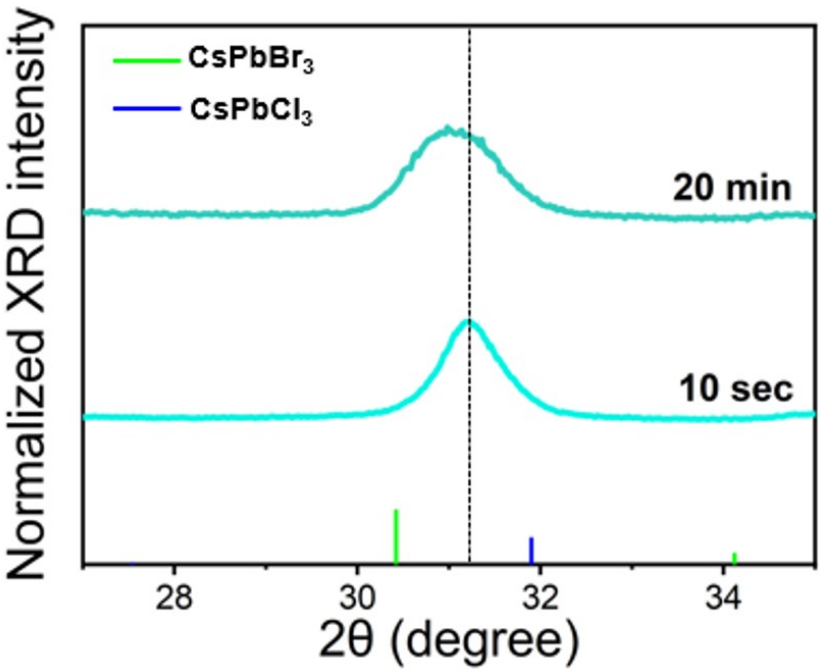


Fig. S2. XRD patterns of $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs with the reaction time of (bottom) 10 sec and (top) 20 min, respectively.

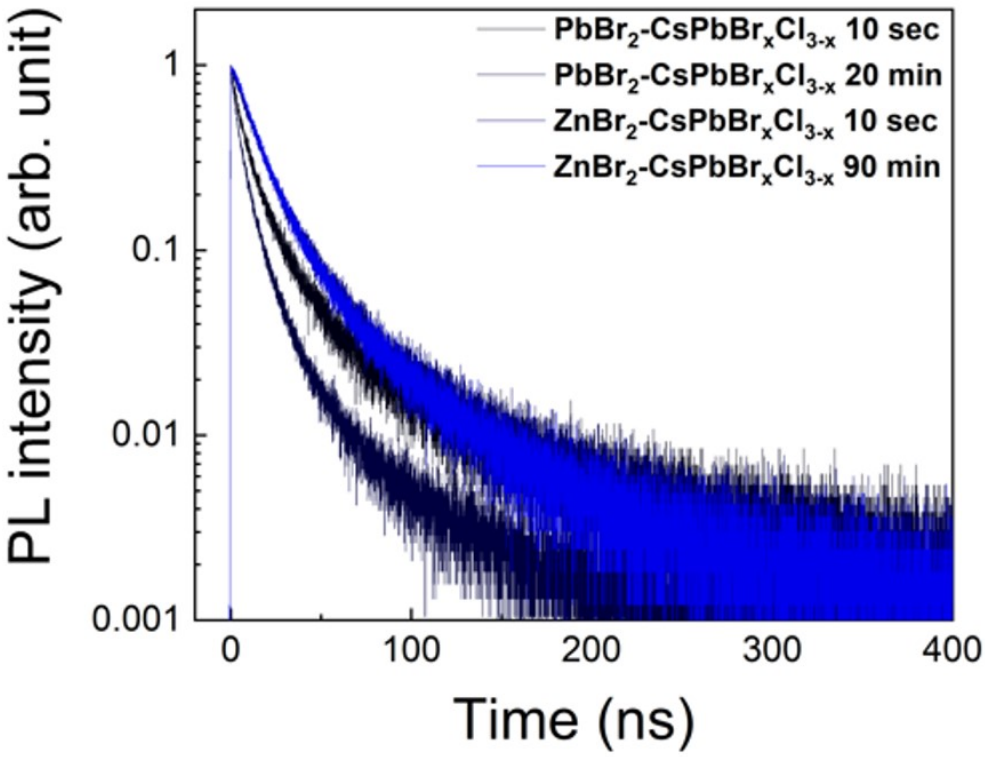


Fig. S3. TRPL decay curves of $ZnBr_2$-$CsPbBr_xCl_{3-x}$ NCs and $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs with different reaction time.

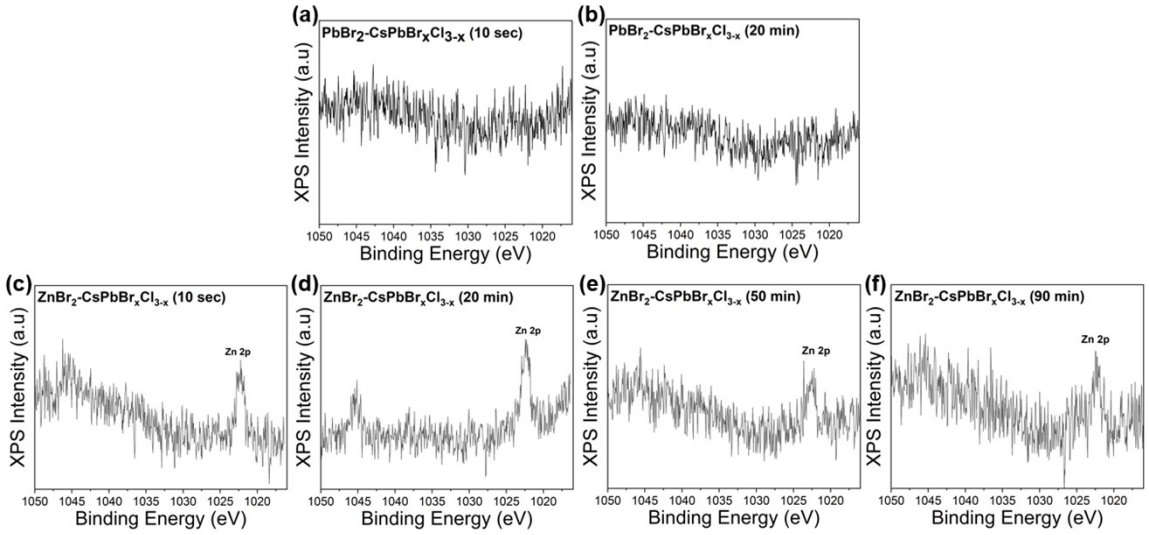


Fig. S4. XPS Zn 2p spectrum of (a)-(b) $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs and (c)-(f) $ZnBr_2$-$CsPbBr_xCl_{3-x}$ NCs with different reaction time.

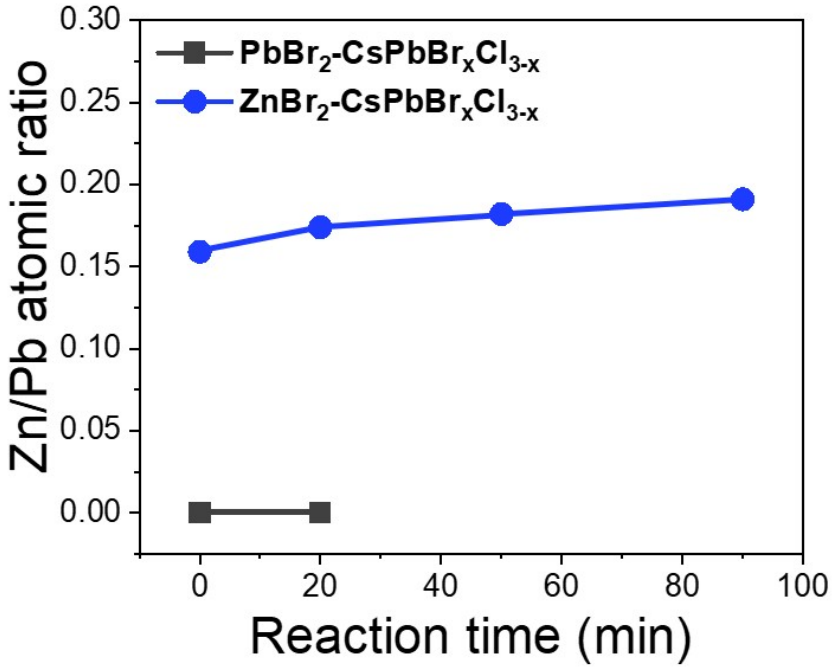


Fig. S5. Zn/Pb atomic ratio obtained from XPS anaylsis for $ZnBr_2$-$CsPbBr_xCl_{3-x}$ NCs and $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs from XPS at different reaction times.

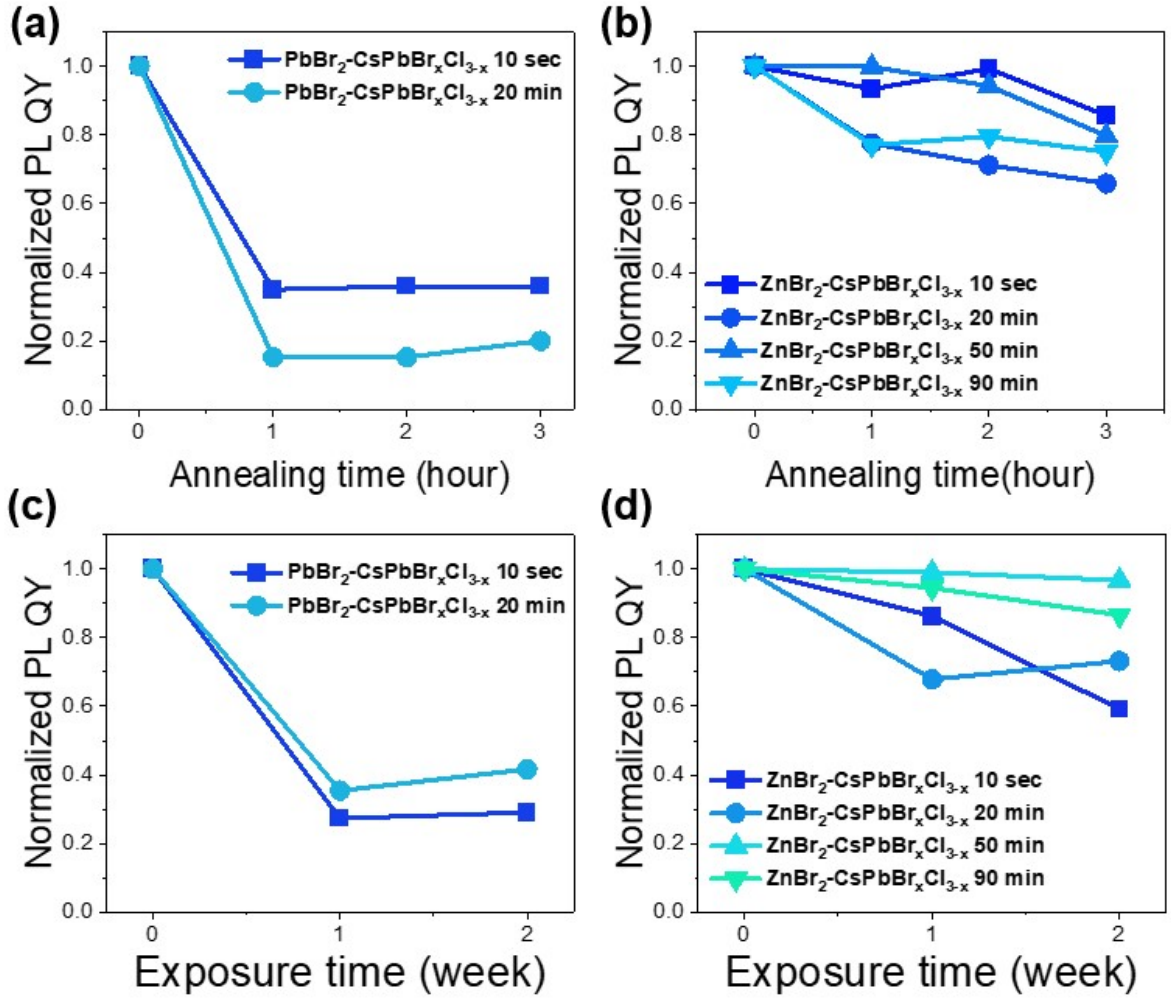
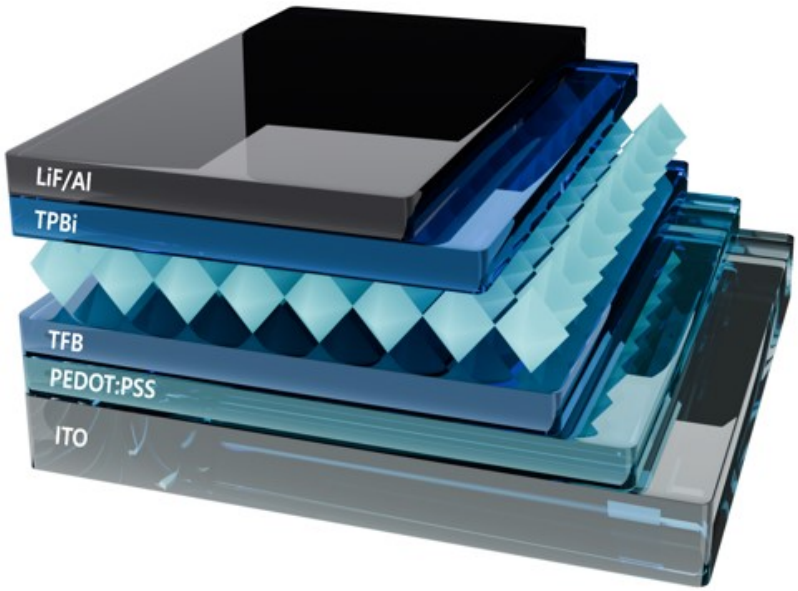


Fig. S6. (a-b) Thermal stability at 70°C and (c-d) air stability results of $CsPbBr_xCl_{3-x}$ NCs depending on reaction time.



Scheme S2. Schematic illustration for the structure of electroluminescent LED devices which employed in our study.

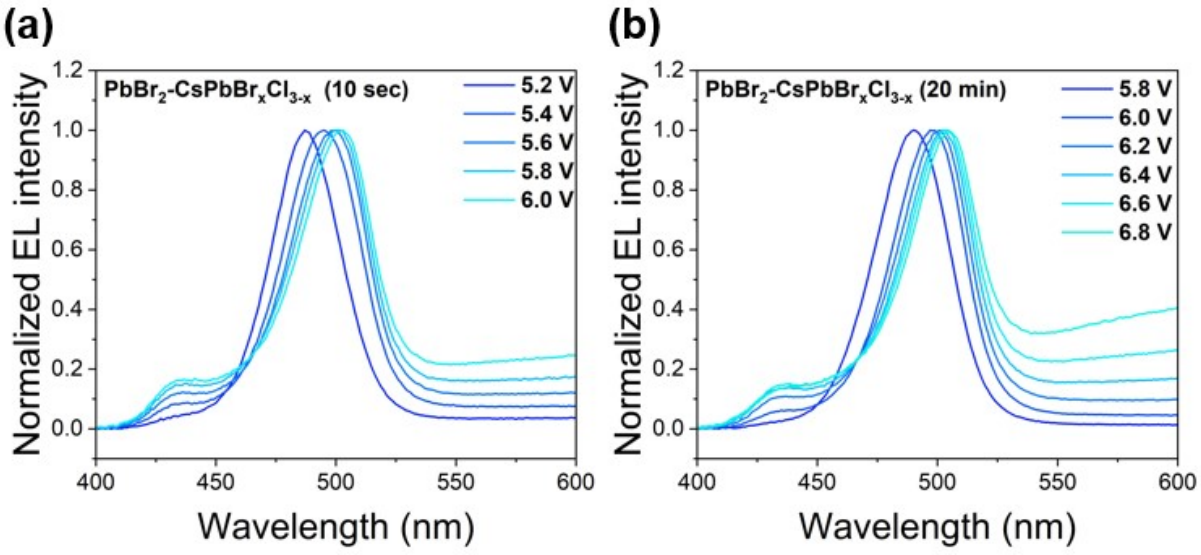


Fig. S7. Normalized EL spectra of LEDs based on $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs prepared with the reaction time of (a) 10 sec and (b) 20 min, respectively, at various operating voltage.

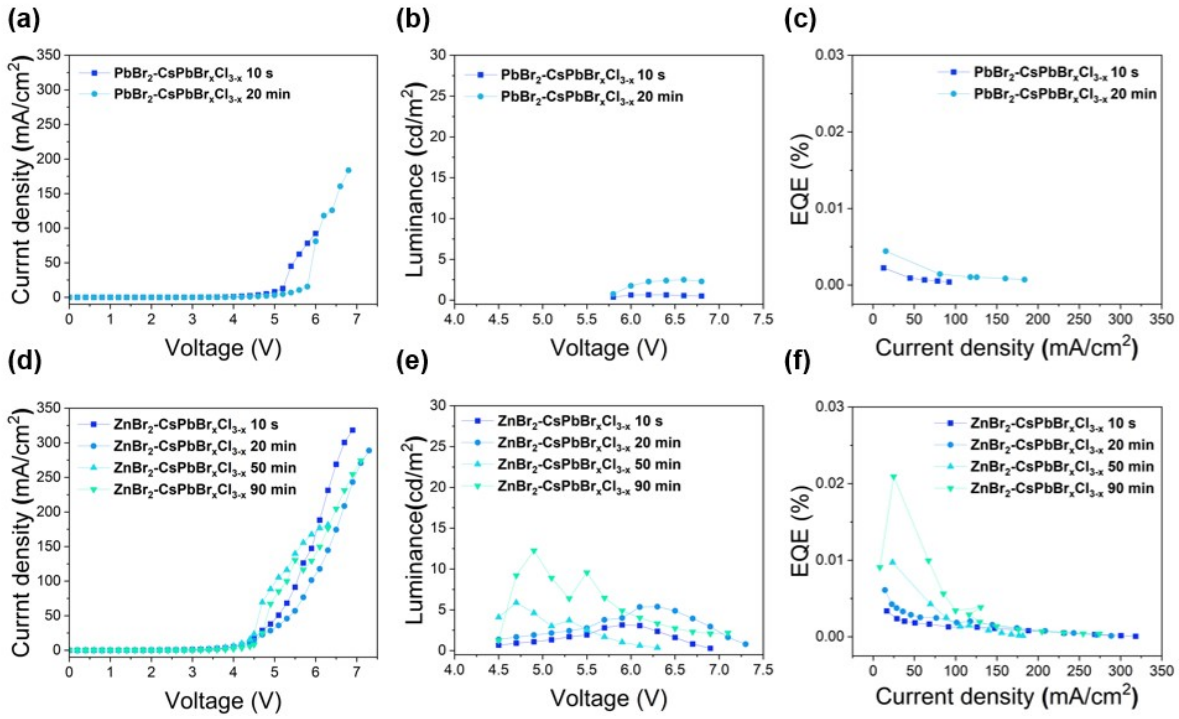


Fig. S8. EL performance of LEDs. The $ZnBr_2$-$CsPbBr_xCl_{3-x}$ NCs of (a) current density-voltage curves, (b) luminance-voltage curves (c) EQE-current density curves and $PbBr_2$-$CsPbBr_xCl_{3-x}$ NCs (d) current density-voltage curves, (e) luminance-voltage curves (f) EQE-current density curves.

Table S2. Summary of TRPL decay data for perovskite nanocrystals with different reaction times.

Perovskite NCs	A_1	τ_1	A_2	τ_2	A_3	τ_3	τ_{avg}
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 10 s	0.4	13.2	0.4	13.2	0.2	44.6	18.7
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 20 min	0.5	14.8	0.5	14.8	0.1	58.7	19.8
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 50 min	0.5	15.3	0.6	15.3	0.1	54.8	19.9
$ZnBr_2$-$CsPbBr_xCl_{3-x}$ 90 min	0.5	13.5	0.4	13.5	0.1	48.2	18.3
$PbBr_2$-$CsPbBr_xCl_{3-x}$ 10 s	0.2	1.8	0.6	8.5	0.2	29.8	11.5
$PbBr_2$-$CsPbBr_xCl_{3-x}$ 20 min	0.3	1.4	0.5	5.9	0.2	16.6	6.9