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Supporting Information

Insights into the Interparticle Mixing of $CsPbBr_3$ and $CsPbI_3$ Nanocubes: Halide Ion Migration and the Kinetics

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Table S1. The nominal volume ratio of $CsPbBr_3$ and $CsPbI_3$ NCs is displayed along with the absorption coefficients and interplanar distances corrected ratio and the corresponding composition is shown.

Previous ratio $CsPbBr_3$:$CsPbI_3$	**Corrected with absorption coefficients and interplanar distances**		
	$CsPbBr_3$:$CsPbI_3$	x in $CsPbBr_{3-x}I_x$	Composition $CsPbBr_{3-x}I_x$
1:0	1:0	0	$CsPbBr_3$
3:1	1.73:1	1.10	$CsPbBr_{1.90}I_{1.10}$
2:1	1.16:1	1.39	$CsPbBr_{1.61}I_{1.39}$
1:1	1:1.73	1.90	$CsPbBr_{1.1}I_{1.90}$
1:2	1:3.46	2.33	$CsPbBr_{0.67}I_{2.33}$
1:3	1:5.19	2.52	$CsPbBr_{0.48}I_{2.52}$
0:1	0:1	3	$CsPbI_3$

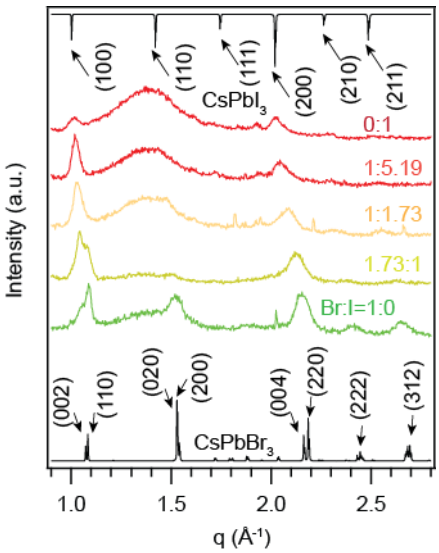

Figure S1. XRD pattern of differently mixed NCs collected at synchrotron in grazing incidence mode. The patterns are compared with standard bulk orthorhombic $CsPbBr_3$ and bulk cubic $CsPbI_3$. The XRD peak shifts towards lower angle with increasing $CsPbI_3$ concentration in mixing.

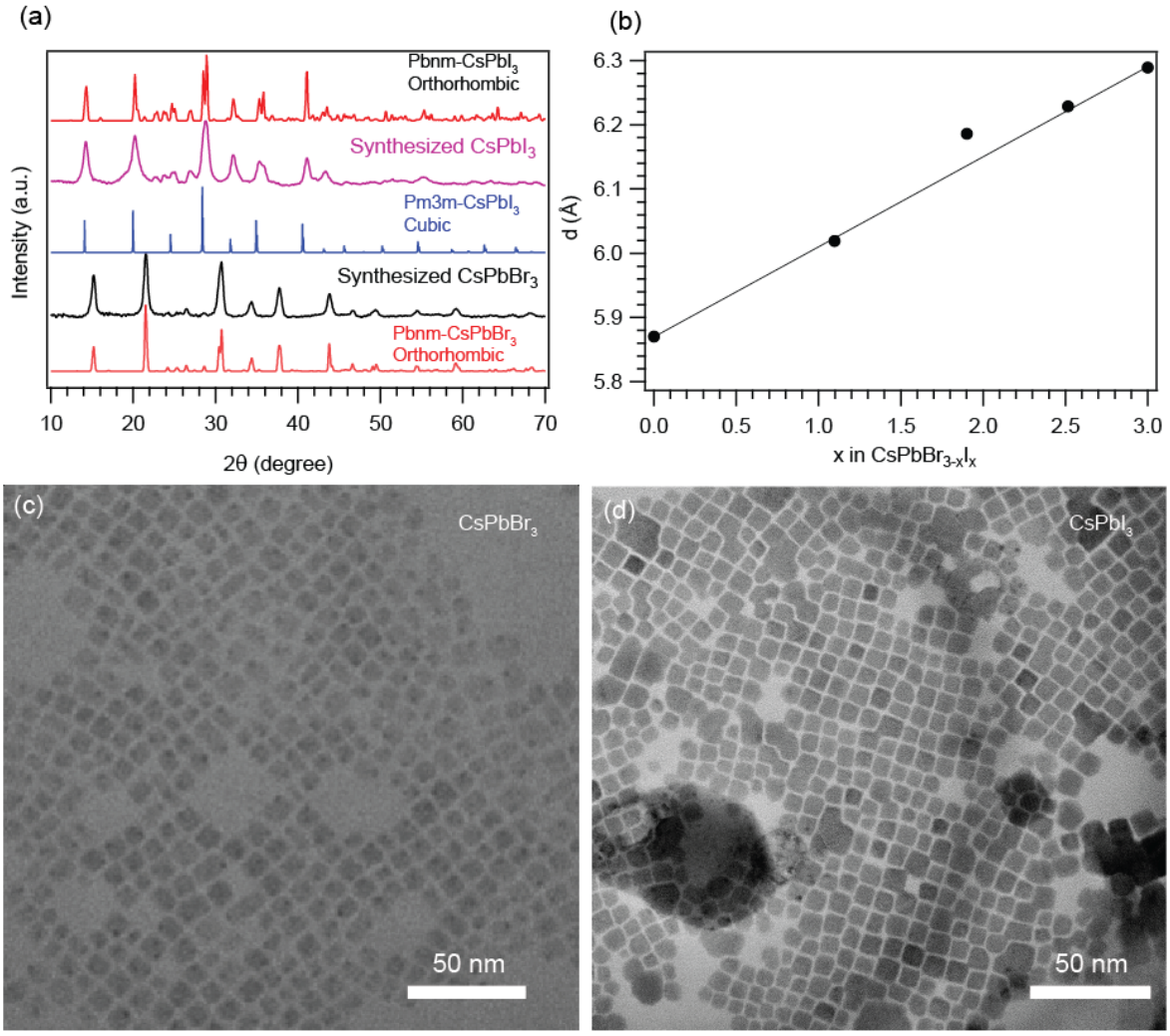

Figure S2. (a) Powder XRD pattern on washed $CsPbBr_3$ and $CsPbI_3$ NCs and comparison with standard cubic and orthorhombic phases. (b) Lattice spacing variation, derived from (110/002) as a function of composition shows the incorporation of the iodide ions increases the lattice spacing. (c) TEM images of (c) $CsPbBr_3$ and (d) $CsPbI_3$ NCs. The scale bar in both the images is 50 nm.

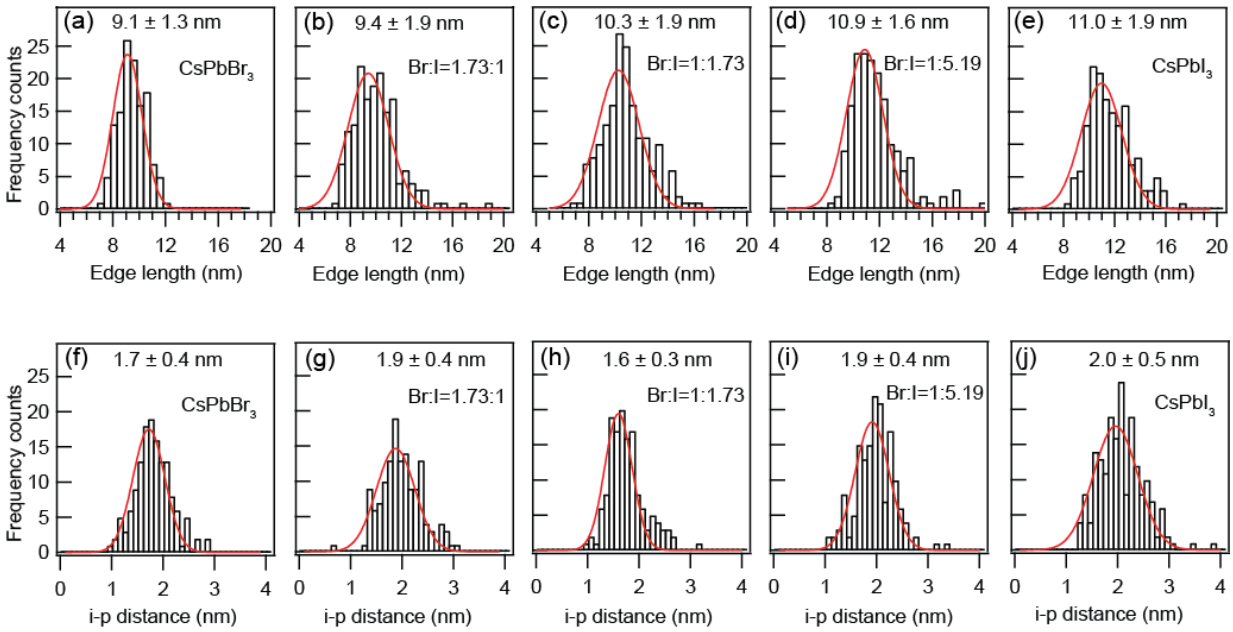

Figure S3. (a-e) Size distribution histogram from TEM image of $CsPbBr_3$, $CsPbI_3$ NCs and the mixing NCs in 1.73:1, 1:1.73, and 1:5.19 ratios (absorption coefficients and interplanar distances corrected). The average edge length and half width half maximum is mentioned in the figure only. (f-j) Corresponding inter-particle (i-p) distance histogram.

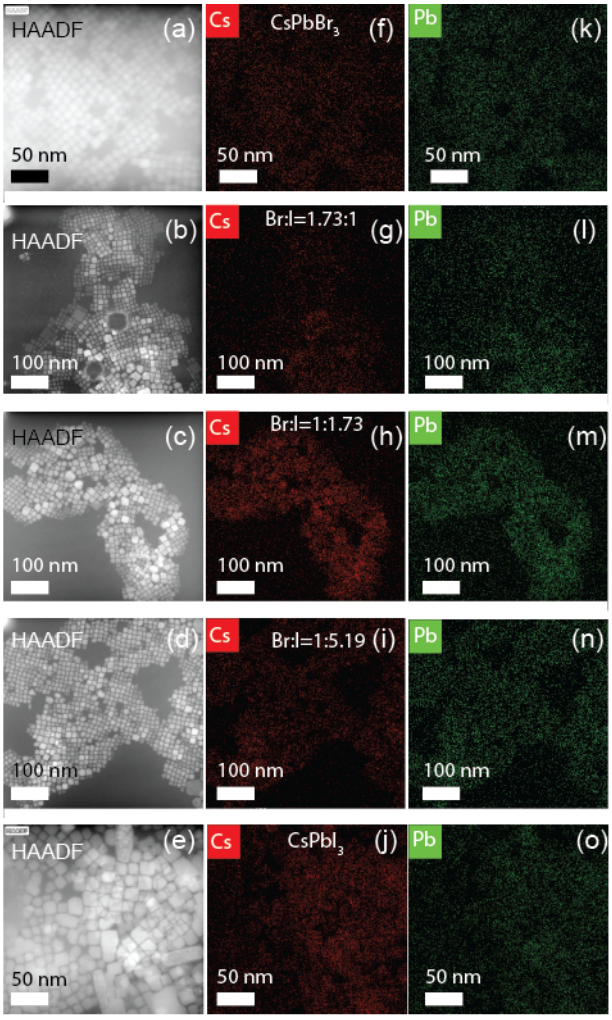

Figure S4. (a-e) HAADF-STEM image of $CsPbBr_3$, 1.73:1, 1:1.73, 1:5.19, and $CsPbI_3$ NCs (absorption coefficients and interplanar distances corrected ratios). Corresponding elemental mapping images for Cs and Pb are presented in (f-j) and (k-o). Cs is shown by red color and Pb is shown by green color.

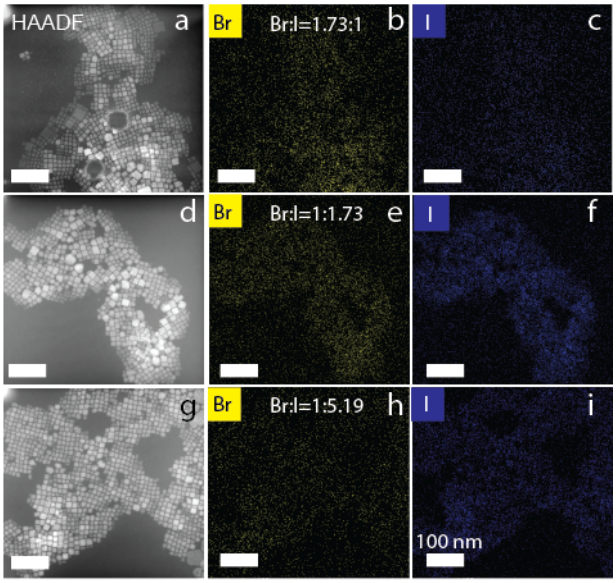

Figure S5. (a, d, g) HAADF-STEM image of the mixing of $CsPbBr_3$ and $CsPbI_3$ NCs in 1.73:1, 1:1.73 and 1:5.19 ratio (absorption coefficients and interplanar distances corrected). The elemental mapping of Br and I is shown by yellow and blue color.

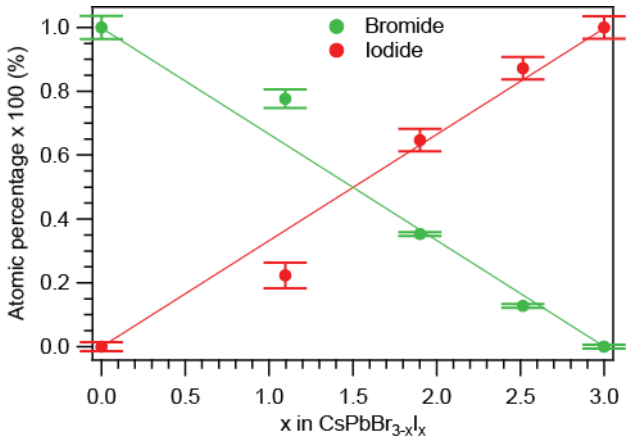

Figure S6. Relative atomic percentage of Br and I from the EDX of STEM elemental mapping of final composition after mixing of $CsPbBr_3$ and $CsPbI_3$ NCs in 1.73:1, 1:1.73 and 1:5.19 ratio (absorption coefficients and interplanar distances corrected). Br and I is shown by green and red solid circles. The dotted line represents the experimental data is slightly deviated from the linear line.

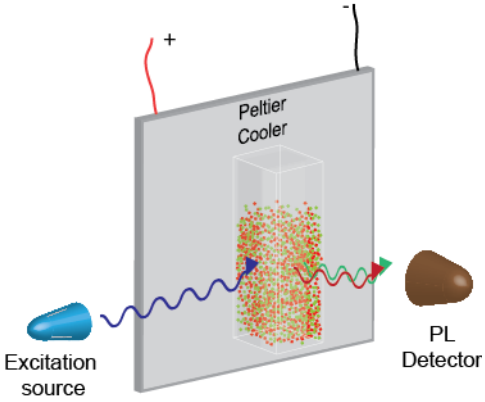

Figure S7. Schematic diagram of the PL experiment stage for in-situ mixing reaction of $CsPbBr_3$ and $CsPbI_3$ NCs at different temperatures. The temperature was controlled by Peltier cooler system by applying a constant bias.

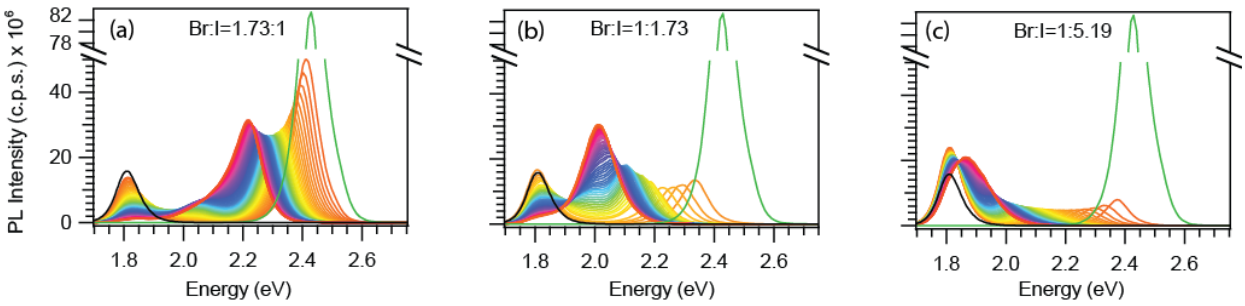

Figure S8. Time dependent PL emission spectra of in-situ mixing reaction of $CsPbBr_3$ and $CsPbI_3$ NCs at three different ratios (absorption coefficients and interplanar distances corrected): (a) 1.73:1, (b) 1:1.73, and (c) 1:5.19 at 24 ℃/297 K temperature. The black solid line is for $CsPbI_3$ and green line is for $CsPbBr_3$ NCs. . The surface plot of these is shown in **Figure 2.**

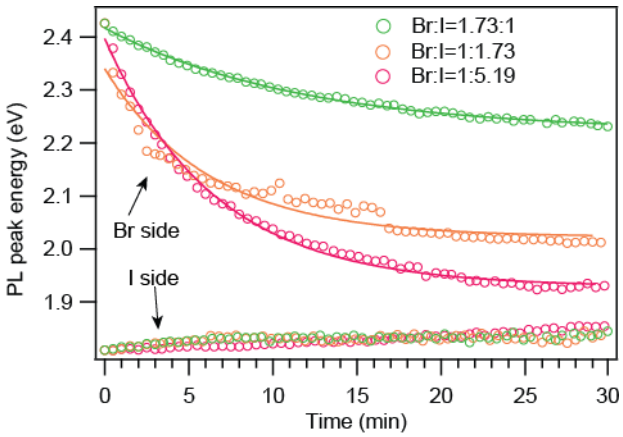

Figure S9. The variation of bromide side and iodide side PL peak energy with time for mixing of $CsPbBr_3$ and $CsPbI_3$ NCs in 1.73:1, 1:1.73, and 1:5.19 ratios (absorption coefficients and interplanar distances corrected). The rate of change of bromide side is becoming slower with increasing $CsPbBr_3$ amount in mixing.

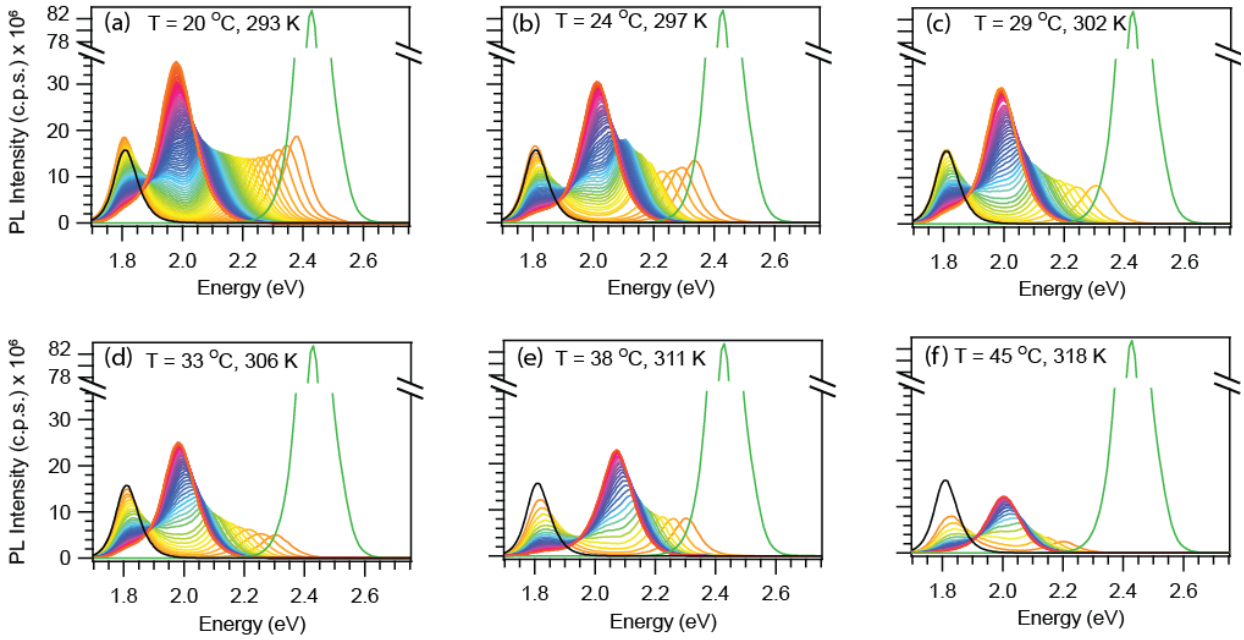

Figure S10. Time dependent PL emission spectra of in-situ mixing reaction of $CsPbBr_3$ and $CsPbI_3$ NCs in 1:1.73 ratio (absorption coefficients and interplanar distances corrected) for different temperatures (a) 20 °C, (B) 24 °C, (c) 29 °C, (d) 33 °C, (e) 38 °C, and (f) 45 °C. The surface plot of these is shown in **Figure 3**. The black solid line is for $CsPbI_3$ and green line is for $CsPbBr_3$ NCs. The iodide peak is slightly blue shifted and intensity goes down where bromide side peak is red shifted and a new intermediate peak emerges merged with the bromide side peak forms a single peak.

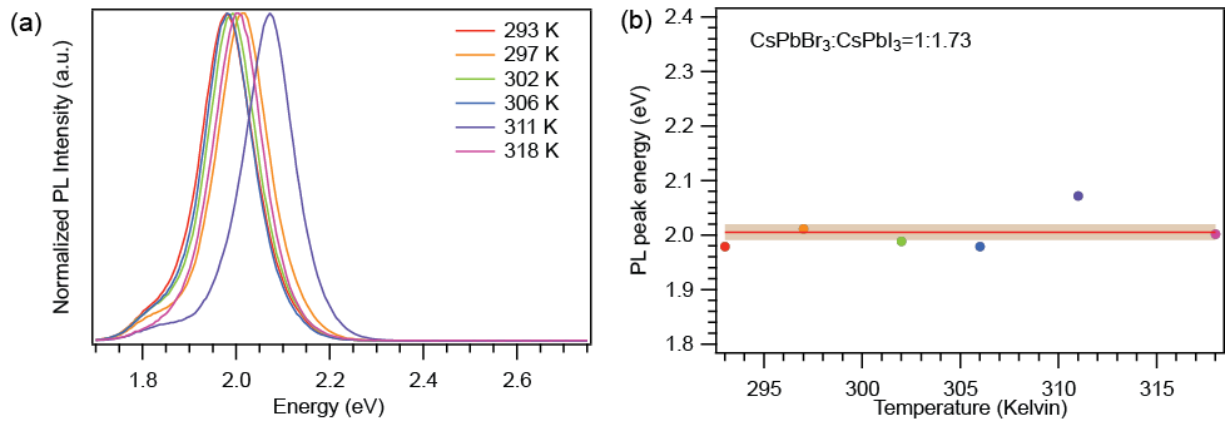

Figure S11. (a) PL emission spectra and (b) corresponding PL peak energy collected before stopping the reactions of $CsPbBr_3$ and $CsPbI_3$ in 1:1.73 (nominal volume ratio 1:1) at different temperatures. The solid red line shows the average peak energy, and the brown band shows the error bar in the average peak energy. The slight variation in the peak position for the reaction at 311 K is probably because (i) the reaction was stopped before it was completed; (ii) slight variations in the volumes of the stock solutions taken during the reaction.

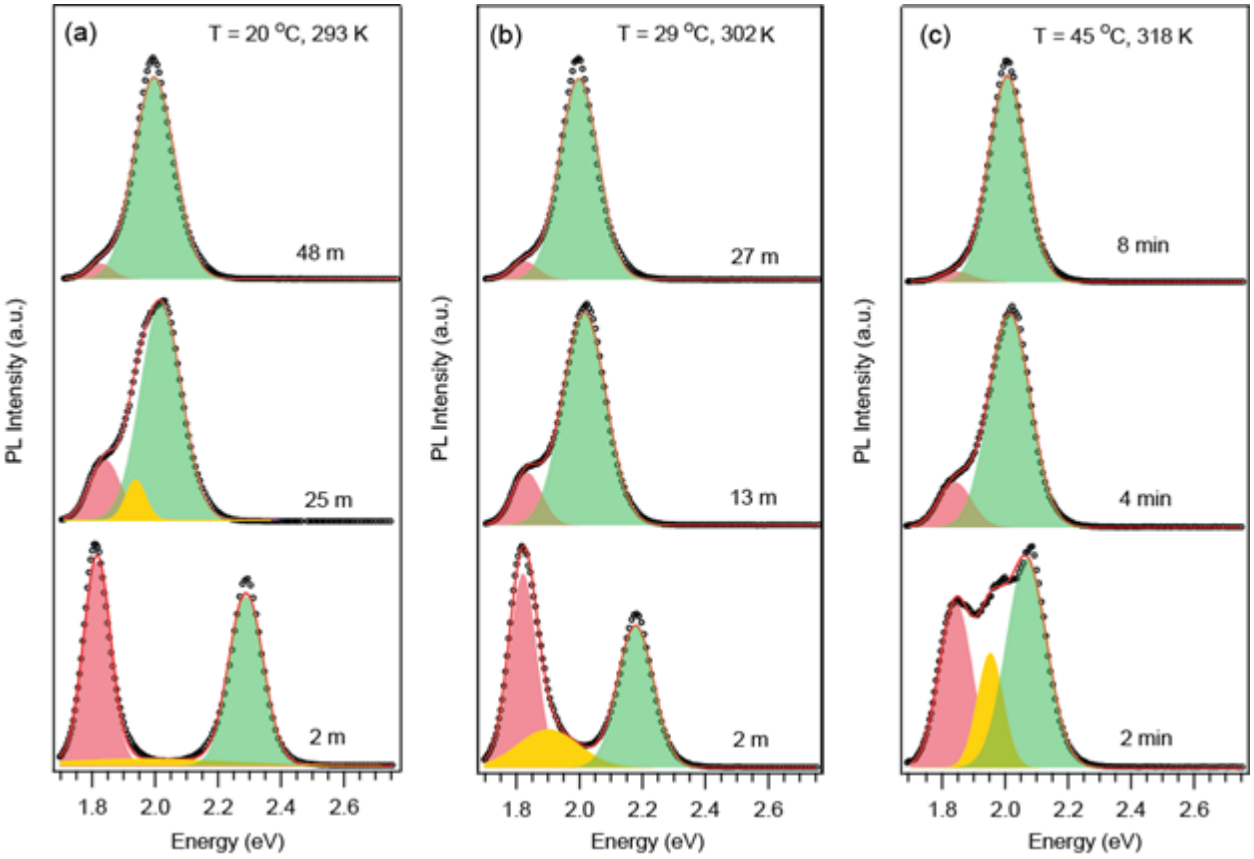

Figure S12. Deconvoluted PL spectra of interparticle mixing of $CsPbBr_3$ and $CsPbI_3$ nanocrystals in 1:1.73 ratio (absorption coefficients and interplanar distances corrected) at different temperatures. (a) 20 °C, (b) 29 °C, and (c) 45 °C. The PL spectra are shifted vertically represents the data of different reaction time. The experimental data are shown by black solid circles; total fit is shown by red solid line. The iodide side, bromide side, and new intermedimate peaks are shown by red, green, and yellow color respectively.

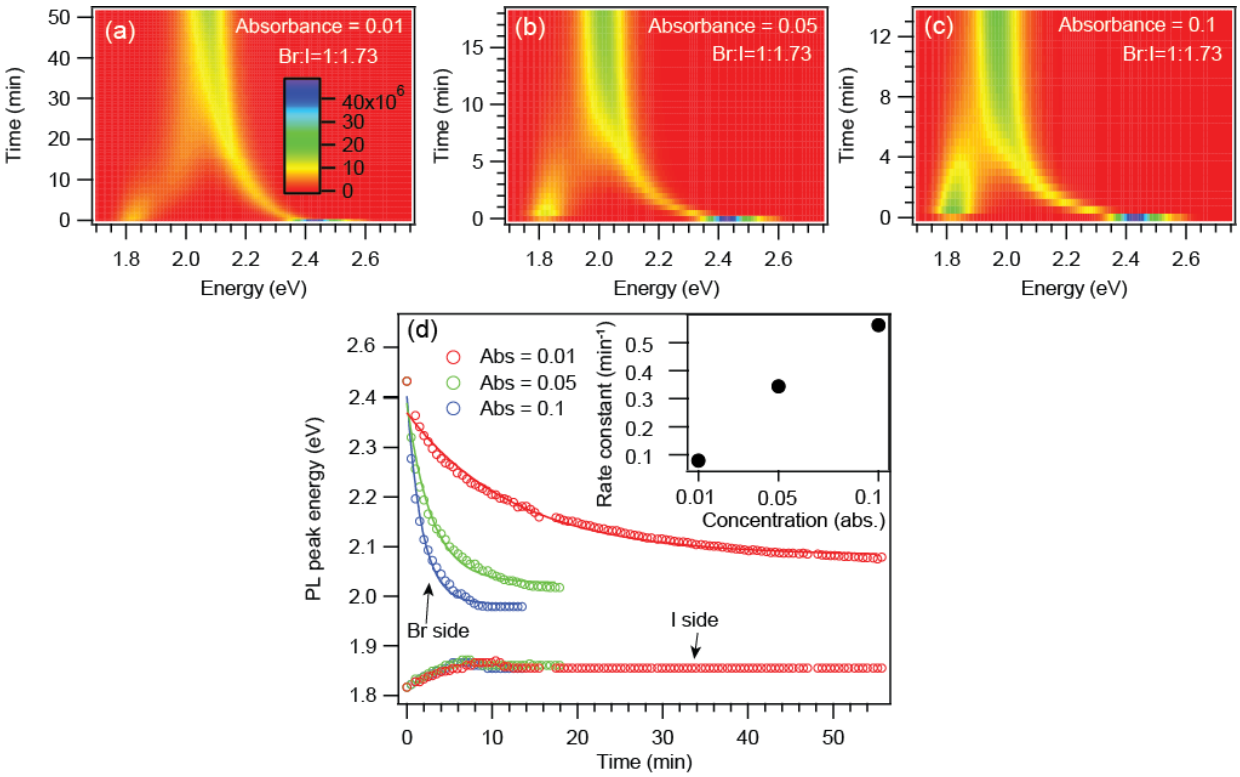

Figure S13. Time evolution of steady-state PL for 1:1.73 ratio (absorption coefficients and interplanar distances corrected) of $CsPbBr_3$ and $CsPbI_3$ at three different concentrations: absorbance (a) 0.01, (b) 0.05, (c) 0.1 at 24 °C/297 K temperature. The energy scale (x-axis) and the PL intensity (color scale) are identical for all concentrations; however, the reaction times, represented by the y-axis are different for each concentration. (d) The variation of PL peak position for bromide side and iodide side with time for different concentration. Inset of the figure shows an increase in concentration, the reaction proceeds faster.