Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Mechanistic Study of $CsPbBr_3$ Superstructure Formation

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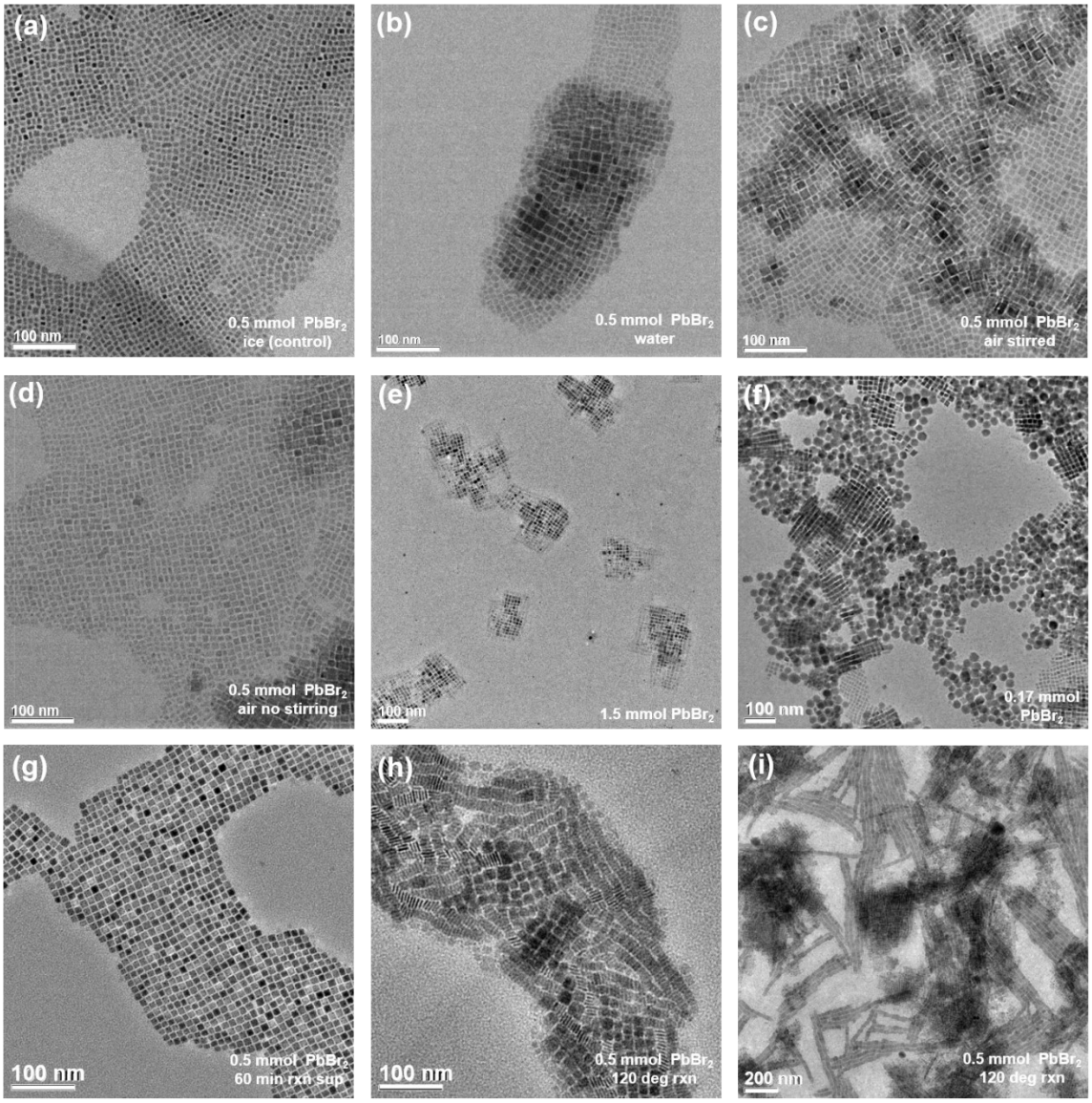

Figure S1. TEM images of samples synthesized using 0.5 mmol $PbBr_2$ (180 °C) and cooled down using (a) ice-water bath; (b) water bath; (c) air cooling with stirring; and (d) air cooling without stirring. TEM images of ice-water bath cooled samples synthesized (at 180 °C) using (e) 1.5 mmol of $PbBr_2$; and (f) 0.17 mmol $PbBr_2$. TEM images of samples synthesized using 0.5 mmol $PbBr_2$ (g) at 180 °C for 60 min with stirring and immediately air cooled without stirring; and (h) at 120°C and immediately air cooled without stirring. (i) TEM image of SCs formed by samples synthesized at 120°C using 0.5 mmol $PbBr_2$ and immediately air cooled without stirring.

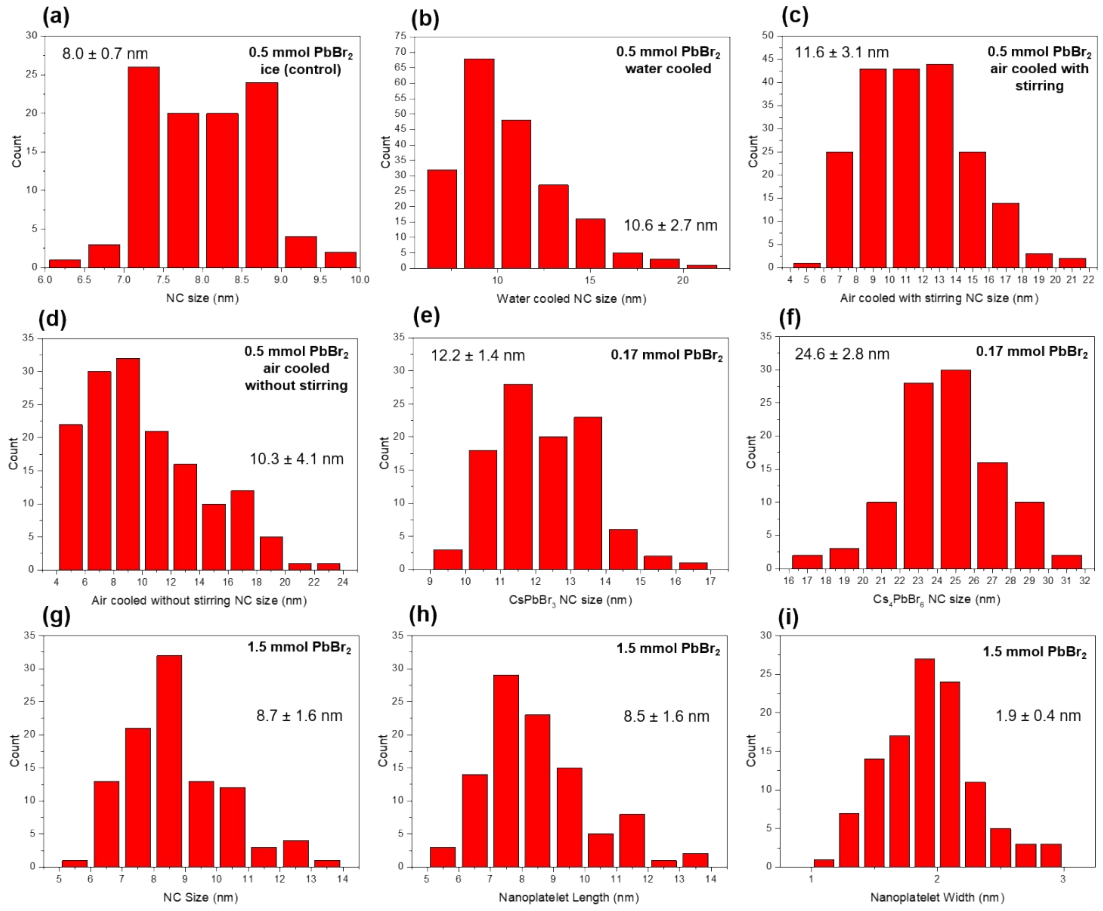

Figure S2. Particle size distributions of samples synthesized using 0.5 mmol $PbBr_2$ (180°C) and cooled down using (a) ice-water bath; (b) water bath; (c) air cooling with stirring; and (d) air cooling without stirring. Particle size distributions of samples synthesized using 0.17 mmol $PbBr_2$ (180 °C) for (e) $CsPbBr_3$; and (f) Cs_4PbBr_6 NCs. Particle size distributions for samples synthesized using 1.5 mmol $PbBr_2$ (180 °C) for (g) NCs; (h) NP length; and (i) NP width.

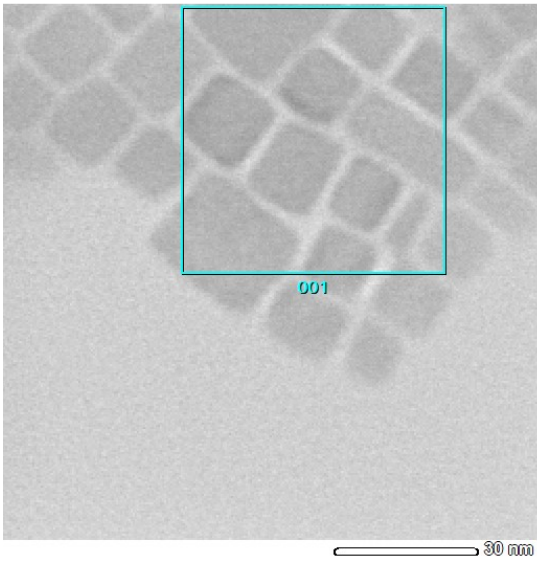

Figure S3. STEM image of samples prepared via air cooling without stirring. Square indicates area under EDS scan.

Table S1. Atomic percentages of Cs, Pb and Br within scanned area.

Element	Atom %
Cs	11.52
Pb	17.96
Br	70.51

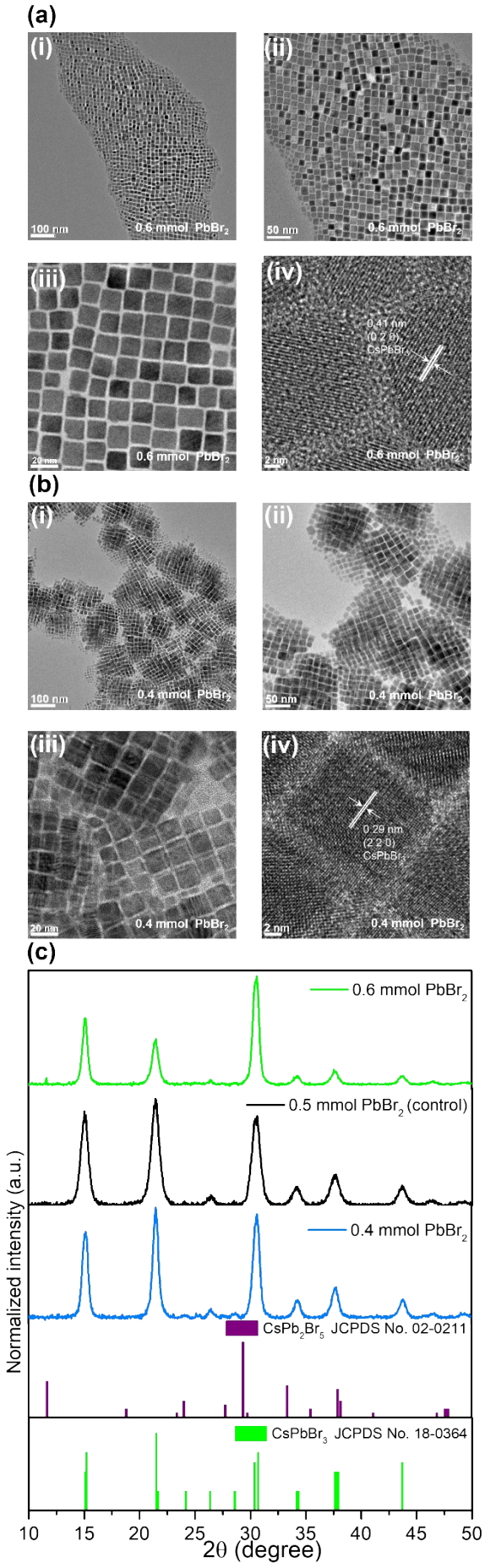
(a)
(i)
100 nm
0.6 mmol PbBr2
(ii)
50 nm
0.6 mmol PbBr2
(iii)
20 nm
0.6 mmol PbBr2
(iv)
0.41 nm
(0 2 0)
CsPbBr3
2 nm
0.6 mmol PbBr2
(b)
(i)
100 nm
0.4 mmol PbBr2
(ii)
50 nm
0.4 mmol PbBr2
(iii)
20 nm
0.4 mmol PbBr2
(iv)
0.29 nm
(2 2 0)
CsPbBr3
2 nm
0.4 mmol PbBr2
(c)
0.6 mmol PbBr2
0.5 mmol PbBr2 (control)
0.4 mmol PbBr2
CsPb2Br5 JCPDS No. 02-0211
CsPbBr3 JCPDS No. 18-0364
Normalized intensity (a.u.)
10
15
20
25
30
35
40
45
50
2θ (degree)

Figure S4. TEM and HRTEM images of samples synthesized (a) using 0.6 mmol $PbBr_2$ cooled using ice-water bath at different magnifications; and (b) using 0.6 mmol $PbBr_2$ cooled using ice-water bath at different magnifications. (c) XRD patterns for samples synthesized under the same experimental conditions (180 °C, ice-water bath cooled) using different amounts of $PbBr_2$ precursor.

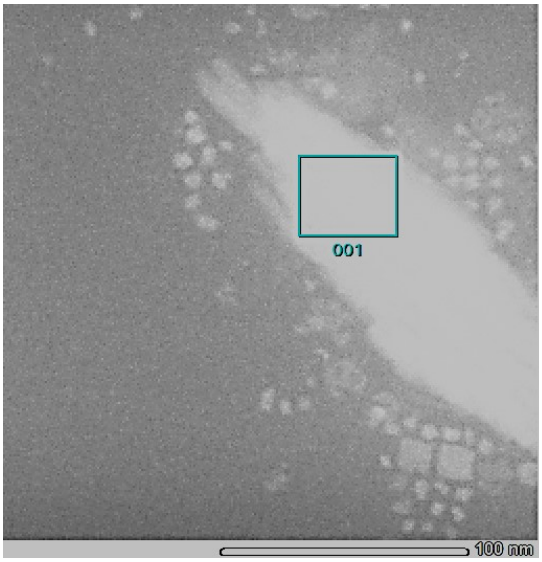

Figure S5. HAADF STEM image of samples prepared using 1.5 mmol $PbBr_2$ at a particular sample location. Square 001 indicates area under EDS scan.

Table S2. Atomic percentages of Cs, Pb and Br within scanned area 001.

Element	001 Atom %
Cs	Not detected
Pb	3.94
Br	96.06

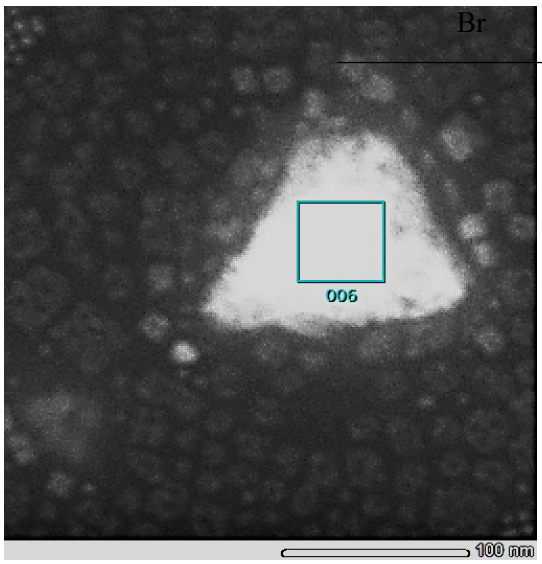

Figure S6. HAADF STEM image of samples prepared using 1.5 mmol $PbBr_2$ at a particular sample location. Square 006 indicates area under EDS scan.

Table S3. Atomic percentages of Cs, Pb and Br within scanned areas 005-008.

Element	006 Atom %
Cs	3.67
Pb	8.03
Br	88.30

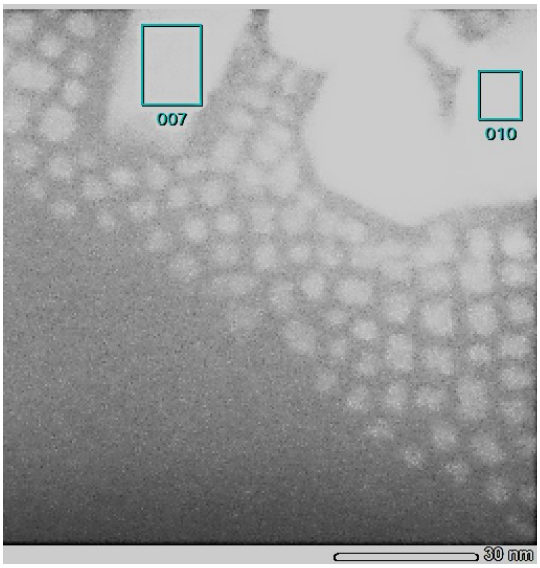

Figure S7. HAADF STEM image of samples prepared using 1.5 mmol $PbBr_2$ at a particular sample location. Squares 007 and 010 indicates area under EDS scan.

Table S4. Atomic percentages of Cs, Pb and Br within scanned areas 007 and 010.

Element	007 Atom %	010
Cs	Not detected	2.33
Pb	15.46	9.73
Br	84.54	87.94

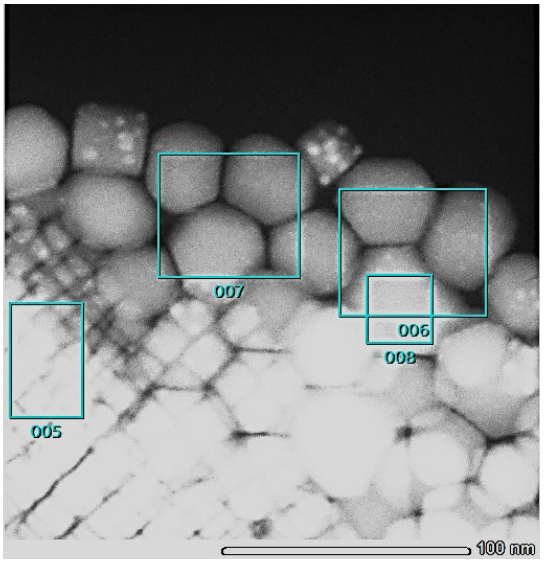

Figure S8. HAADF STEM image of samples prepared using 0.17 mmol $PbBr_2$ at a particular sample location. Squares 005-008 indicate areas under EDS scan.

Table S5. Atomic percentages of Cs, Pb and Br within scanned areas 005-008.

Element	005 Atom %	006 Atom %	007 Atom %	008 Atom %
Cs	14.85	24.16	24.58	24.46
Pb	18.78	9.20	10.81	10.71
Br	66.37	66.65	64.61	64.83

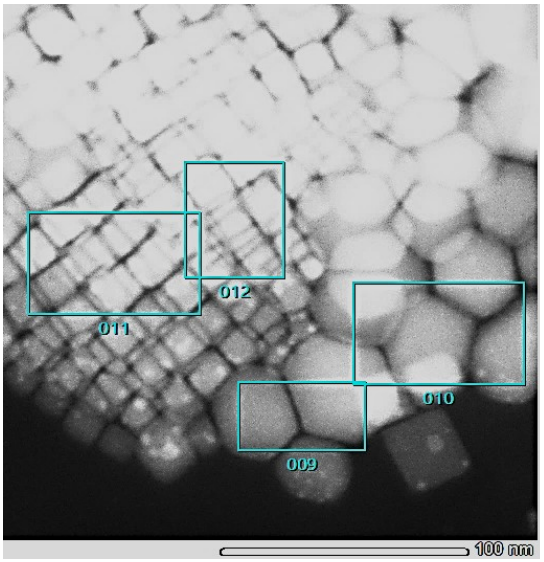

Figure S9. HAADF STEM image of samples prepared using 0.17 mmol $PbBr_2$ at a particular sample location. Squares 005-008 indicate areas under EDS scan.

Table S6. Atomic percentages of Cs, Pb and Br within scanned areas 009-012.

Element	009 Atom %	010 Atom %	011 Atom %	012 Atom %
Cs	24.87	24.40	13.85	13.84
Pb	10.79	9.67	20.40	20.35
Br	64.34	65.94	65.75	65.81

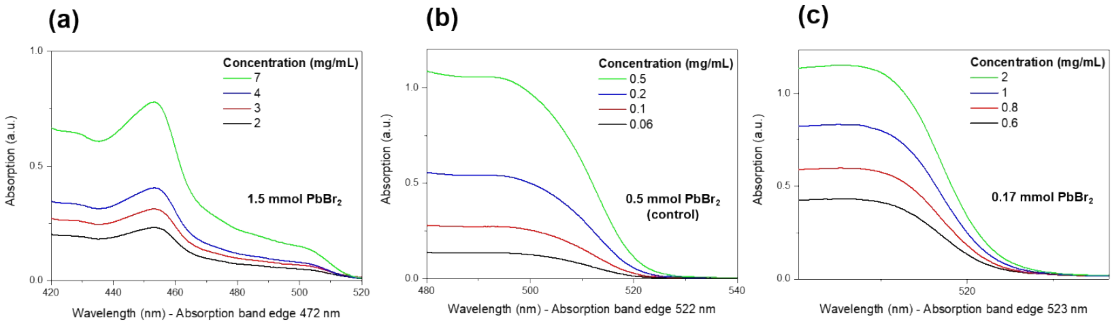

Figure S10. UV-Vis absorption spectra using different concentrations for samples synthesized under the same experimental conditions (180 °C, ice-water bath cooled) using (a) 1.5 mmol $PbBr_2$; (b) 0.5 mmol $PbBr_2$; and (c) 0.17 mmol $PbBr_2$.

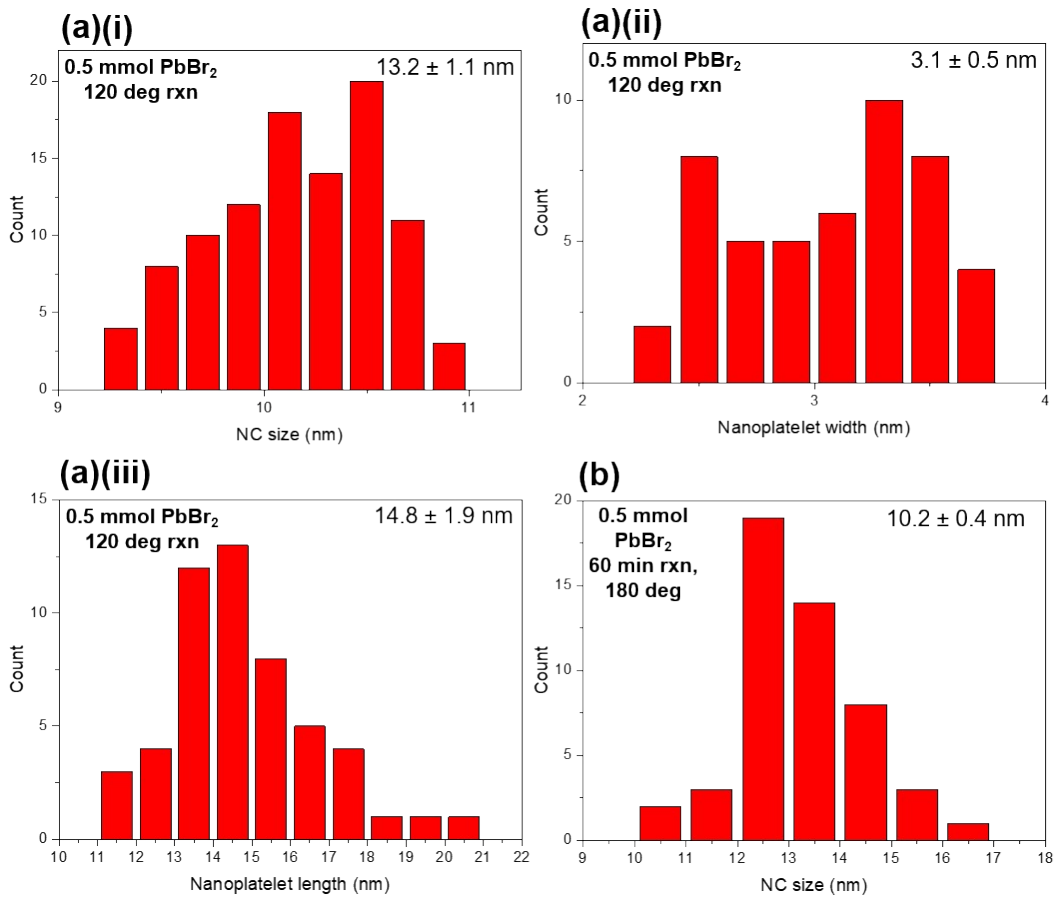

Figure S11. (a) Particle size distributions of samples synthesized using 0.5 mmol $PbBr_2$ at 120 °C and immediately air cooled without stirring (i) NCs; (ii) NPL width; and (iii) NPL length; (b) Particle size distributions of NCs (supernatant) synthesized using 0.5 mmol $PbBr_2$ at 180 °C for 60 min with stirring, followed by air cooling without stirring.

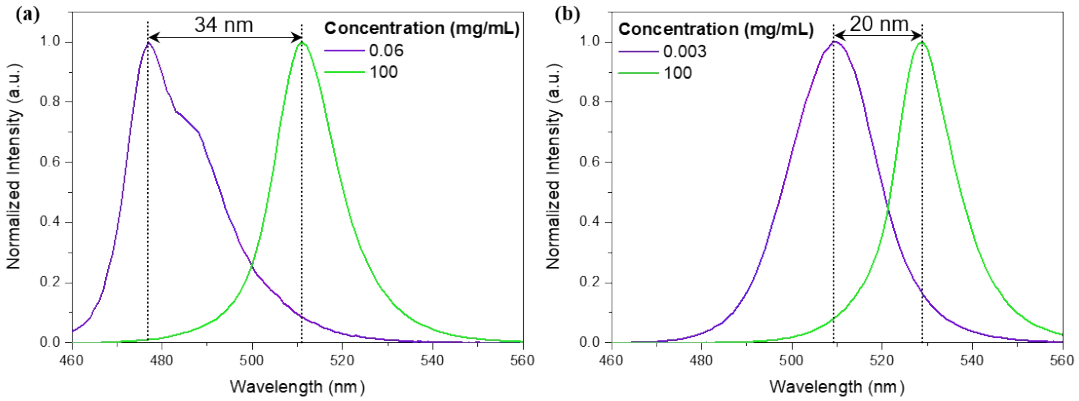

Figure S12. PL spectra at ECP concentration and 100 mg/ml for $CsPbBr_3$ samples prepared at (a) 120 °C with immediate air cooling without stirring after hot-injection and; (b) 180 °C with immediate ice-water bath cooling after hot-injection.