Supporting Information

Enhance Luminescence or change morphology: The effect of doping method on Cu^{2+}-doped $CsPbBr_3$ perovskite nanocrystals

Meng Li, Yang Song*, Feiyong Chen*

Resources and Environment Innovation Institute, Shandong Jianzhu University, Jinan, 250101, P. R. China

Table S1 Preparation conditions of sample prepared by hot injection method

Sample	$PbBr_2$ (mmol)	$CuBr_2$ (mmol)	Molar ratio of Cu/Pb	Temperature (ºC)
HI-1	0.188	0	0	140
HI-2	0.188	0.376	2	140
HI-3	0.188	0	0	160
HI-4	0.188	0.376	2	160
HI-5	0.188	0	0	180
HI-6	0.188	0.376	2	180
HI-7	0.188	0.564	3	180

Table S2 Preparation conditions of samples prepared by cation exchange reaction

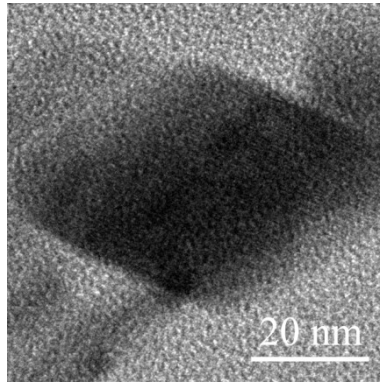| Sample	$CsPbBr_3$ (0.1 µM)	$CuBr_2$ (5 mM)	Adding Rate
CE-1	2 mL	50 µL	2 µL/ min
CE-2	2 mL	100 µL	2 µL/ min
CE-3	2 mL	150 µL	2 µL/ min
CE-4	2 mL	200 µL	2 µL/ min
CE-5	2 mL	250 µL	2 µL/ min
CE-6	2 mL	300 µL	2 µL/ min

Figure S1 The enlarged image of rhombohedral specimens in Fig. 1 (a).
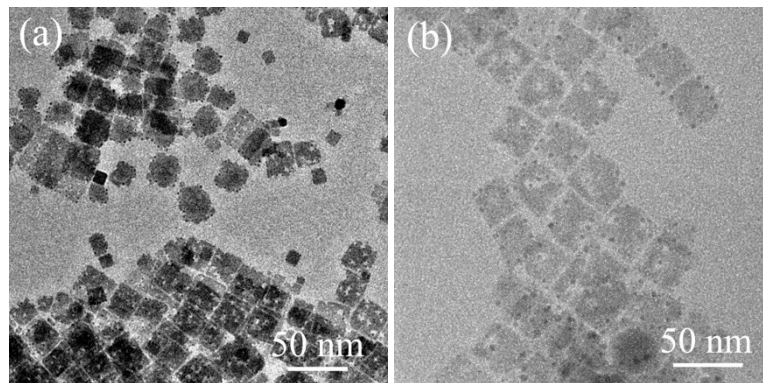

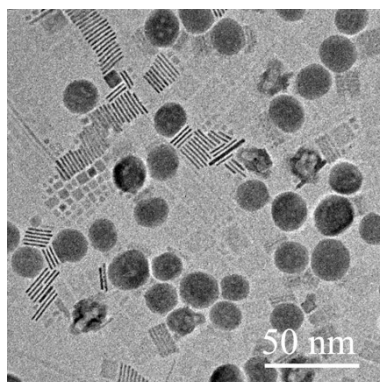Figure S2 TEM image of sample HI-2 (a) and HT-4 (b) at low concentration.
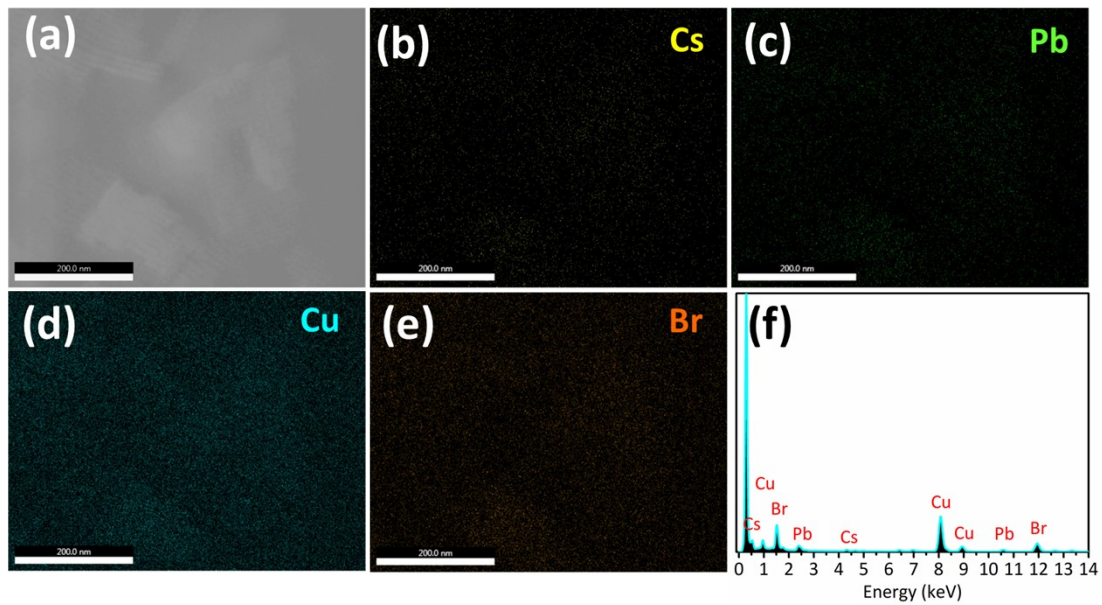

Figure S3 TEM images of sample HI-7.

Figure S4 TEM image (a), elemental mapping of Cs, Pb, Cu, and Br in the scanned area (b–e), and EDX spectrum (f) of sample HI-6.

Table S3 ICP-OES analysis of sample HI-2, HI-6, CE-4

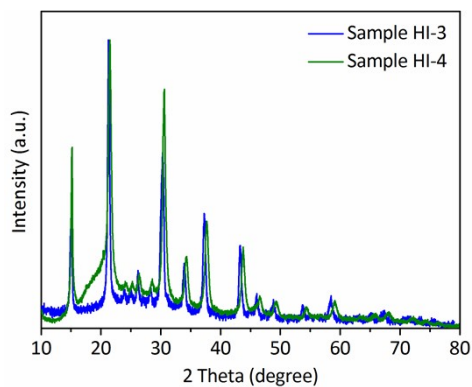| Sample	Cu/Pb feeding ratio	Actual Cu/Pb ratio	Actual Cu doping content (mol %)
HI-2	2	14.93:509.00	2.85
HI-6	2	1.38:31.77.00	4.16
CE-4	5000	18.62:427.18	4.18

Figure S5 XRD patterns of sample HI-3 and HI-4.

Table S4 Ionic radius and calculated tolerance factor (τ) and octahedral parameter (μ)

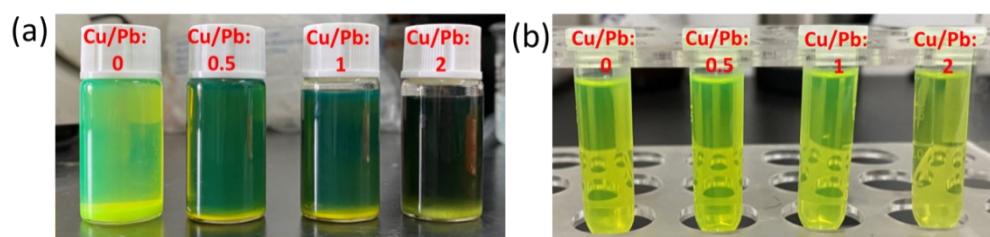| Ion	Ionic radius (pm)	Compound	Caculated τ	Calculated μ
Cs^+	188	$CsPbBr_3$	0.86	0.61
Pb^{2+}	119	$CsPb_{0.5}Cu_{0.5}Br_3$	0.93	0.49
Cu^{2+}	72	$CsCuBr_3$	1.00	0.37
Br^-	196			

Figure S6 The color images of crude solution (a) and purified solution (b) of samples prepared by hot-injection method at 180 oC with the molar ratio of Cu/Pb at 0, 0.5, 1, 2; (b) The purified solution of the above four samples.
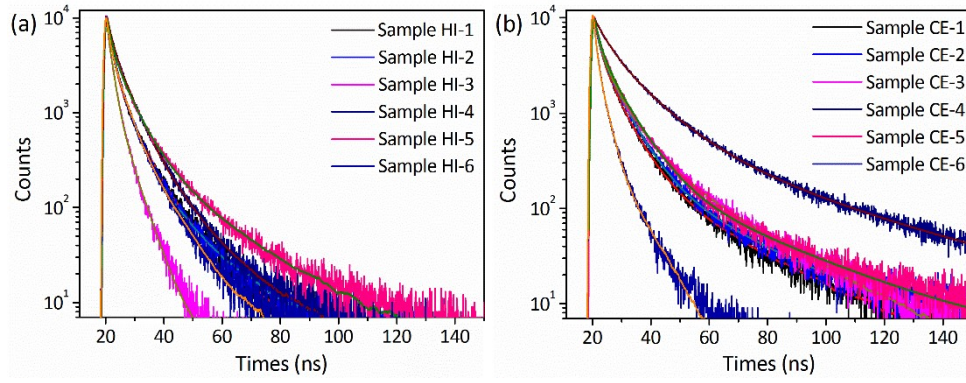
Figure S7 Time-resolved PL decay curves of samples.

Table S5 Components B_1/ B_2/ B_3, time constants τ_1 /τ_2/ τ_3, and $\tau_{average}$

Sample	τ_1	τ_2	τ_3	B_1	B_2	B_3	$\tau_{average}$	CHISQ
HI-1	5.44	1.62	15.62	46.68	40.07	13.25	8.98	1.01
HI-2	1.13	4.14	15.33	30.73	56.24	13.02	8.70	1.01
HI-3	1.51	4.60	42.62	62.55	36.37	1.08	9.34	1.05
HI-4	1.27	4.92	13.81	20.21	63.62	16.18	8.29	1.01
HI-5	5.32	1.31	18.62	55.60	24.53	19.87	12.19	1.03
HI-6	3.84	0.98	10.15	56.32	25.20	18.49	6.44	1.01
CE-1	1.43	5.72	21.62	26.60	57.09	16.32	13.31	1.08
CE-2	1.47	6.60	25.26	23.10	61.54	15.36	15.13	1.04
CE-3	6.21	1.66	22.01	49.32	25.71	24.97	15.66	1.08
CE-4	4.37	12.38	40.53	18.23	55.45	26.32	28.42	1.10
CE-5	1.92	7.56	32.47	23.06	62.32	14.62	19.25	1.06
CE-6	0.71	2.52	8.39	34.80	53.14	12.06	4.63	1.04

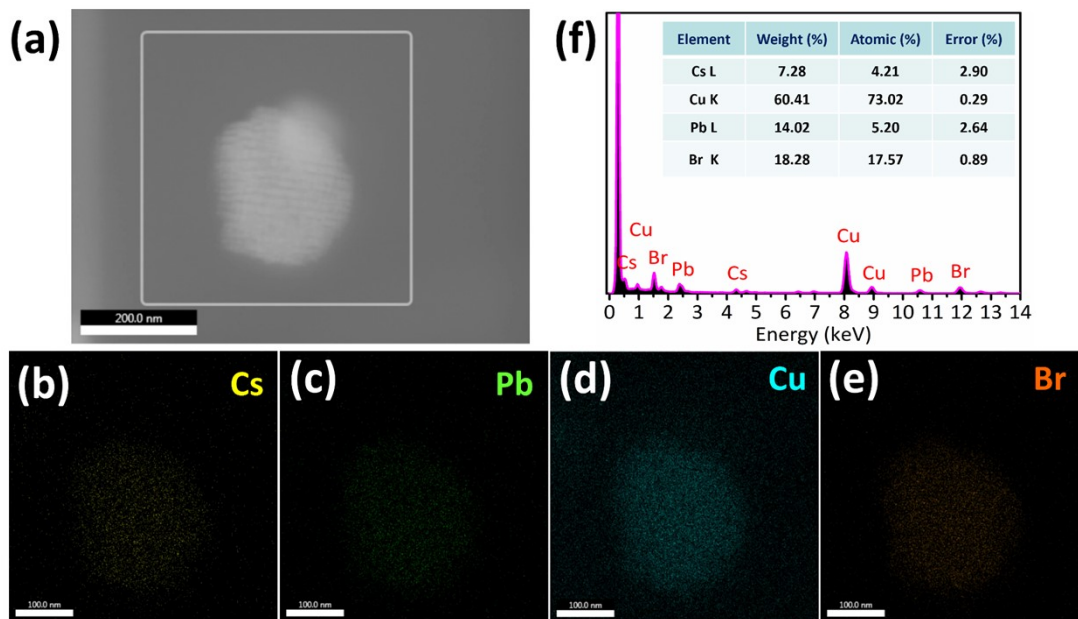| Element	Weight (%)	Atomic (%)	Error (%)
Cs L	7.28	4.21	2.90
Cu K	60.41	73.02	0.29
Pb L	14.02	5.20	2.64
Br K	18.28	17.57	0.89

Figure S8 TEM image (a), elemental mapping of Cs, Pb, Cu, and Br in the scanned area (b–e), and EDX spectrum (f) of sample CE-4.

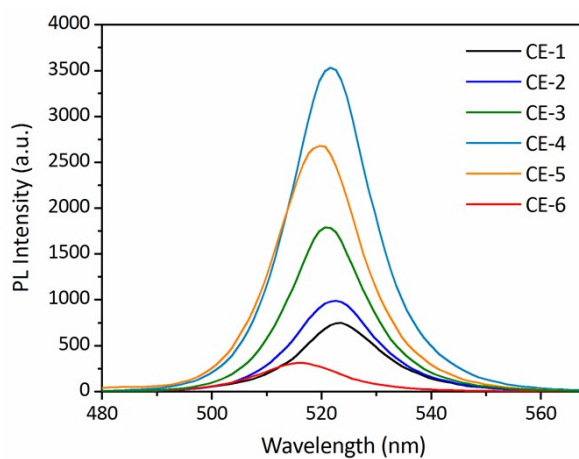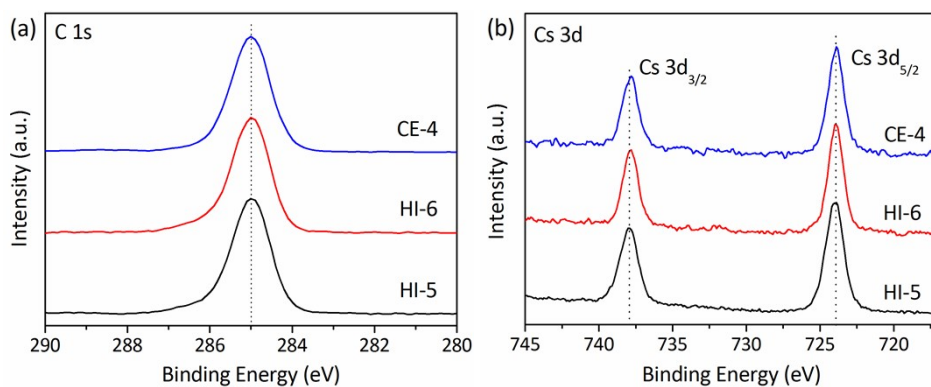Figure S9 PL spectra of sample CE-1 to CE-5.

Figure S10 (a) XPS C 1s spectra after peak calibration at 285 eV. (b) Cs 3d spectrum of sample HI-5, HI-6, CE-4.
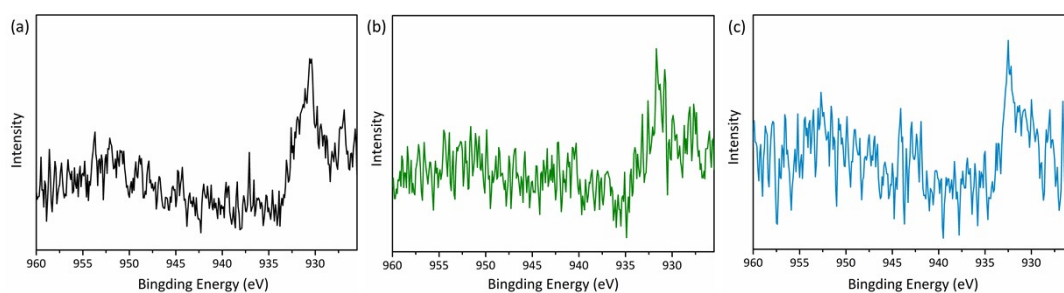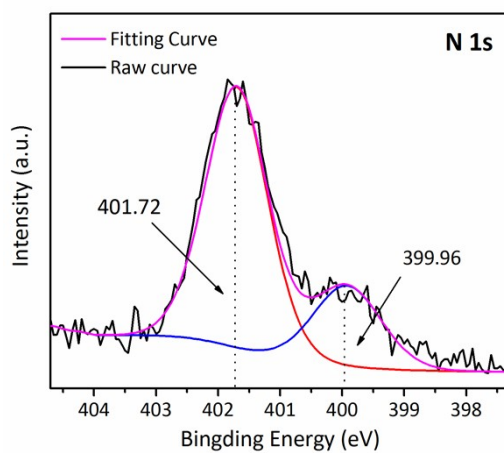

Figure S11 Cu 2p spectrum of sample HI-5 (a), HI-6 (b), CE-4 (c).

Figure S12 N 1s spectrum of sample HI-6.