Electronic Supplementary Information

Bromobenzene Aliphatic Nucleophilic Substitution Guided Controllable and Reproducible Synthesis of High Quality Cesium Lead Bromide Perovskite Nanocrystals

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Methods

Chemicals and reagents

Oleylamine (OAm, 90%, AR), octadecene (ODE, 90%, AR), lead stearate, Cs_2CO_3 (99.9%), n-octylamine, acetyl bromide, N-methylformamide were purchased from Aladdin (Shanghai, China). Dodecylamine were purchased from Sigma Addrich. Benzyl bromide, α,α'-dibromo-p-xylene, 1, 3, 5-tris (bromomethyl) benzene and were purchased from Energy Chemical. ODE and OAm were dried under vacuum for 1h at 120 ºC before use.

Synthesis of $CsPbBr_3$ and $CH_3NH_3PbBr_3$ PNCs

Typically, for the synthesis of $CsPbBr_3$ PNCs, 5 ml ODE, 0.75 ml OAm, 0.016 g Cs_2CO_3 and, 0.0387 g lead stearate, 0.071 g 1, 3, 5-tris (bromomethyl) benzene were sequentially loaded into 25 ml 3-neck flask under vigorous stirring of 2500 rpm and the temperature was raised to 160 ºC under ambient atmospheric conditions, and the reaction mixture was cooled by the ice-water bath. The mixture were purified by ethyl acetate / hexane and then were separated by centrifugation at 10000 rpm for 10 min for three times before further characterization. Gram scale synthesis of $CsPbBr_3$ PNCs could be easily carried out just by amplified 30 folds. Similar to the synthesis of $CsPbBr_3$ PNCs, the $CH_3NH_3PbBr_3$ PNCs could be synthesized just using 30 uL of N-methylformamide instead of Cs_2CO_3.

Characterization

The fluorescence emission spectra were recorded by a FL4500 spectrophotometer. Shimadzu UV-2550 spectrophotometer with one pair of 10 mm quartz cell was employed for the absorption spectra recording. FEI Tecnai-G2-F30 Transmission Electron Microscopic (TEM) was employed to obtain TEM images (at 200 kV). The X-ray diffractometer (Bruker D8 Advance, Bruker AXS, Germany) was operated at 40 kV and 15 mA, and Nickel-filtered Cu Kα radiation was used in the incident beam.

Determination of HCl

5ul of HCl stock solutions of different concentrations from 0 to 36% were added into 1ml of $CsPbBr_3$

PNCs hexane solutions under vigorous shaking for 1min. Then the PL were recorded. The sample of HCl solutions of certain concentrations were detected according to the procedure mentioned above.

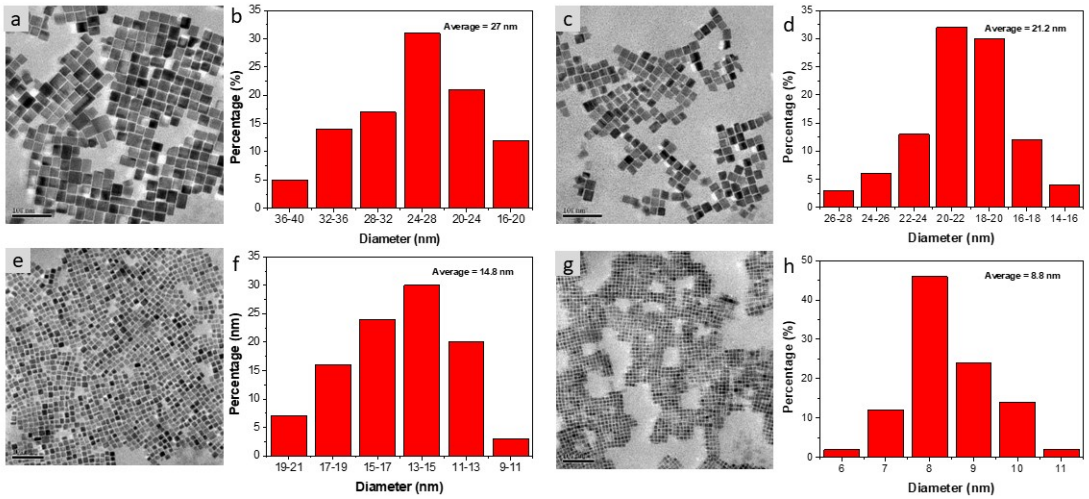

Figure S1. TEM images of $CsPbBr_3$ PNCs and their corresponding histograms of size distributions of different concentrations of OAm from 0.25 ml (a, b); 0.5 ml (c, d), 0.75 ml (e, f) and 1.0 ml (g, h), which reacted with 16.2 mg of Cs_2CO_3, 37.7 mg of lead stearate and 71.2 mg of TBB under continuous heating to 160 ^oC under vigorous stirring.

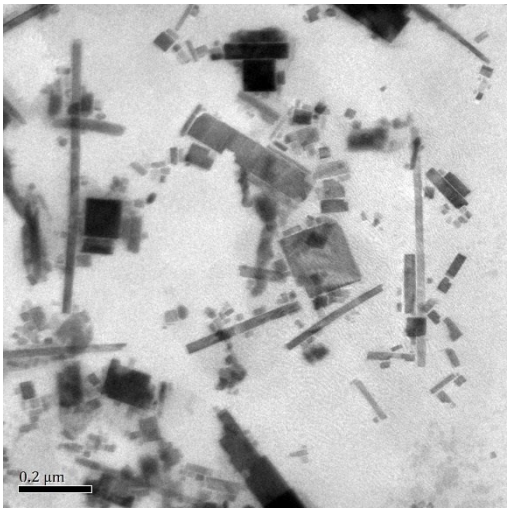

Figure S2. TEM images of $CsPbBr_3$ PNCs obtained from stoichiometric ratio of 1 : 1 : 3 that 8.1 mg of Cs_2CO_3, 38.7 mg of lead stearate and 35.6 mg of TBB were put into 5 ml of octadecene containing 0.75 ml of OAm at room temperature and then heated to 200 ^oC in the open air under vigorous stirring.

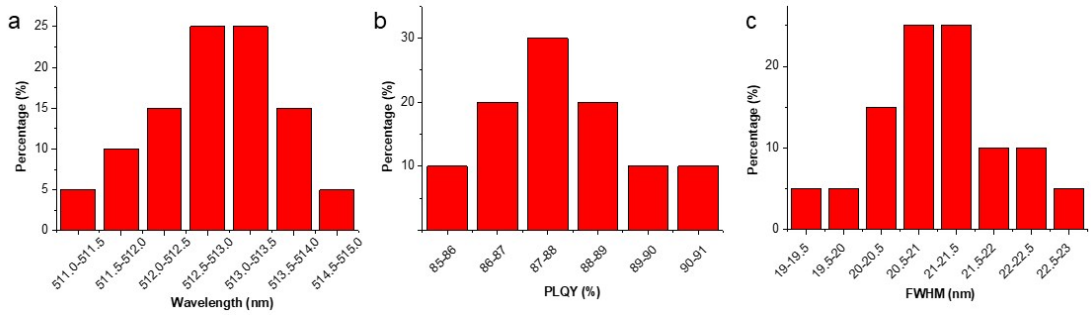

Figure S3. Histograms of emission wavelength, PLQY and FWHM among twenty batches produced by three different experimenters. (16.3 mg of Cs_2CO_3, 38.7 mg of lead stearate and 71.3 mg of TBB were put into 5 ml of ODE containing 0.75 ml of OAm at room temperature and then heated to 160 ^oC in the open air under vigorous stirring.

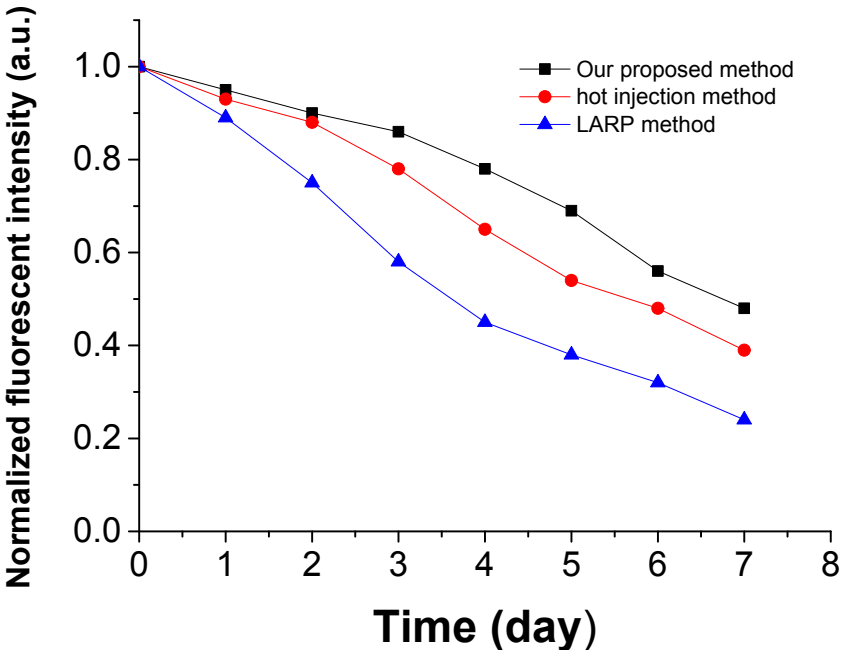

Figure S4. The synthesized $CsPbBr_3$ PNCs stability comparations over time (days) under ambient conditions.

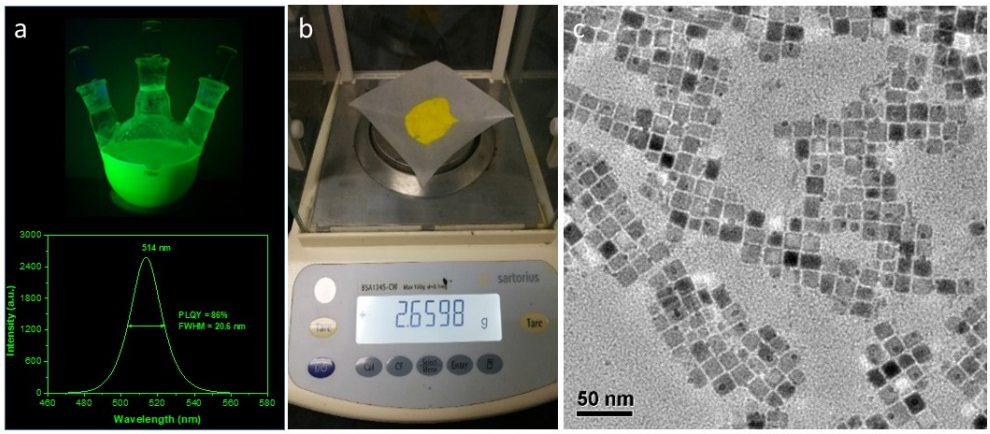

Figure S5. Gram scale synthesis of $CsPbBr_3$ PNCs in one pot. Photographs of the crude solution $CsPbBr_3$ PNCs obtained under UV lamp with λ of 365 nm PL spectrum of $CsPbBr_3$ PNCs obtained with a PL maximum at 514 nm, FWHM of 20.6 nm and PLQY of 86% (a) ; corresponding dried $CsPbBr_3$ PNCs powder (b); and TEM images of the obtained $CsPbBr_3$ PNCs.

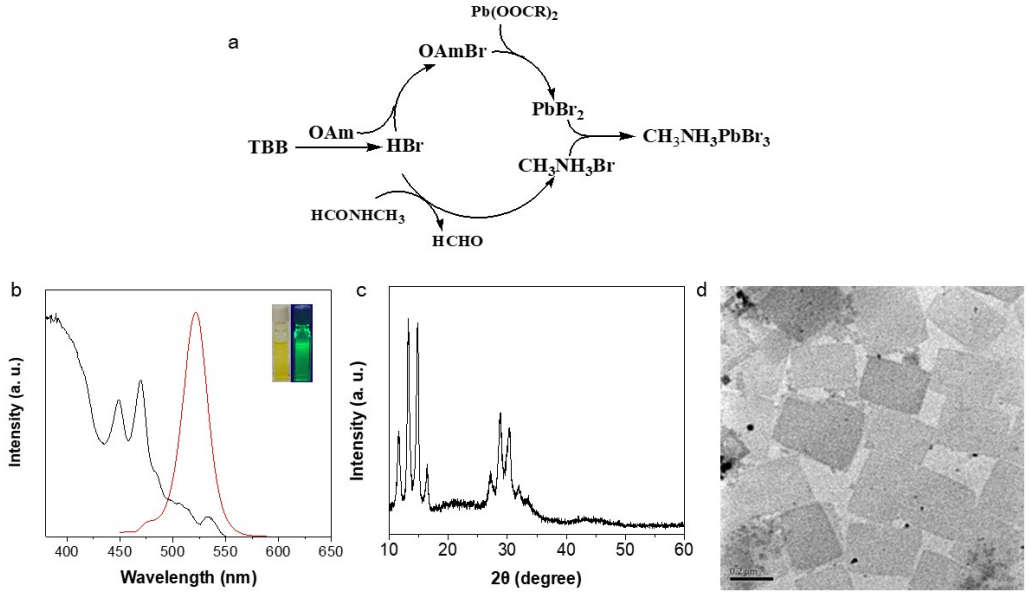

Figure S6. (a) absorption (black line) and PL (red line) spectra of $CH_3NH_3PbBr_3$ PNCs with a PL maximum at 521 nm, FWHM of 27 nm (Inset photograph of $CH_3NH_3PbBr_3$ PNCs in hexane solution under (left) normal white light and (right) a UV lamp with λ of 365 nm); (b) XRD pattern of $CH_3NH_3PbBr_3$ PNCs. (c) TEM images of $CH_3NH_3PbBr_3$ PNCs.

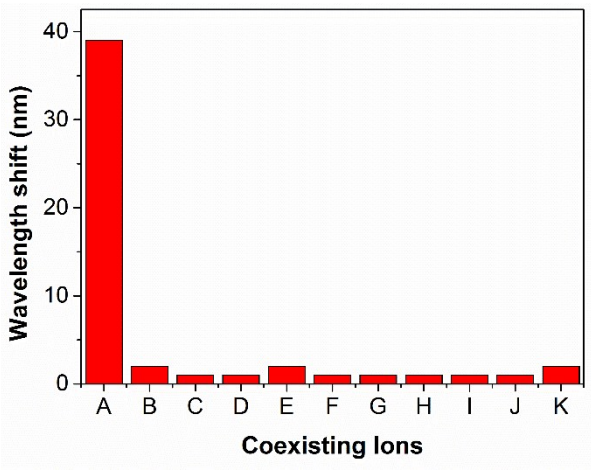

Figure S7. Selectivity of for $CsPbBr_3$ NCs the detection of HCl over other ions: the concentrations of HCl are 6%; the concentration of the other ions is 0.05%. From A to K are Cl^-, NO_3^-, PO_4^{3-}, SO_4^{2-}, CO_3^{2-}, K^+, Na^+, Ca^{2+}, Mg^{2+}, Fe^{3+}, Mn^{2+}.

Table S1. Recovery rates and relative standard deviations (RSD) for detection of HCl in three different samples based on the wavelength shift of $CsPbBr_3$ PNCs

Sample	Average found (%) (n = 3)	HCl added (%)	HCl found (%)	Recovery rate (%)	R.S.D.(%) (n = 3)
1	6.2	5	11.6	103.6%	3.7
2	18.4	5	23.1	98.7	5.6
3	27.9	5	33.2	100.9%	7.2