

Supplemental Information

Optimization of Synthetic Parameters for Efficient NIR Luminescence in Ytterbium-doped CsPbCl₃ Perovskite Quantum Dots

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Experimental method

Materials. Lead acetate trihydrate $[\text{Pb}(\text{OAc})_2 \cdot 3\text{H}_2\text{O}]$ (99.99%, Aladdin), cesium acetate (CsOAc) (99.9%, Aladdin), ytterbium acetate hydrate $[\text{YbCl}_3 \cdot 6\text{H}_2\text{O}]$ (99.9%, Aladdin), chlorotrimethylsilane (TMS-Cl) (98%, Aladdin), 1-octadecene (ODE) (90%, Aladdin), oleylamine (OAm) (80%-90%, Aladdin), oleic acid (OA) (AR, Aladdin), and cyclohexane (99%, Aladdin) were used as received unless otherwise noted.

Synthesis of Yb-doped PQDs: $\text{Pb}(\text{OAc})_2 \cdot 3\text{H}_2\text{O}$ (0.123 mmol), $\text{YbCl}_3 \cdot 6\text{H}_2\text{O}$ (0.369 mmol), OA (2 mL), OAm (2 mL), ODE (10 mL) were mixed in a 50 ml three-necked flask. The reaction was carried out at 113°C under nitrogen protection for 30 minutes. The temperature was then rapidly raised to 205°C. Upon reaching this temperature, a mixture of 0.05 mL TMS-Cl and 0.5 mL ODE was promptly injected. Under continued nitrogen protection, 0.615 mL of CsOAc was injected at 250°C. Immediately after injection for 10 seconds, the flask was cooled to room temperature using a water bath. The reaction solution was transferred to a centrifuge tube, where the solution was centrifuged at 8000 rpm for 5 min. The supernatant was discarded, and the pellet was resuspended in cyclohexane. The solution was centrifuged at 6000 rpm for 5 min again, and the supernatant was the target product. The synthesis parameters including reaction temperature, precursor stoichiometry, OA/OAm ratio, and ligand content were optimized for efficiently doping Yb into PQDs with other synthetic process unchanged.

Characterization: X-ray diffraction (XRD) patterns were recorded using a D2 PHASER XRD diffractometer from Bruker Corporation, Germany, employing monochromatic Cu $K\alpha$ radiation (λ

= 1.54184 Å). Transmission electron microscopy (TEM) testing was conducted using a Tecnai G2 F20 TEM from FEI Company. During testing, the original solution was first dispersed in cyclohexane before proceeding with the analysis. Absorption spectra (Abs) were measured in the wavelength range of 250–500 nm using a Shimadzu UV-3600 ultraviolet-visible spectrophotometer. Using a 75W xenon lamp as the excitation source and an Ocean Optics QE Pro fiber-optic spectrometer to monitor the photoluminescence (PL) spectrum of the sample. Fluorescence decay lifetimes were measured using the FLS1000 Steady-State and Transient Fluorescence Spectrometer, with the excitation wavelength set to 365 nm. The photoluminescence quantum yield (PLQY) was measured using the UV-NIR absolute PL quantum yield spectrometer C13534 series equipped with a 150W xenon lamp and an integrating sphere. It was calculated by directly measuring the number of photons emitted and absorbed by the sample using the integrating sphere under the following formula:

$$PLQY = \frac{N^{em}}{N^{abs}} = \frac{\int I_{sample}^{em}(\lambda) - I_{ref}^{em}(\lambda) d\lambda}{\int I_{ref}^{scatter}(\lambda) - I_{sample}^{scatter}(\lambda) d\lambda} \quad (1)$$

where I^{em} indicates the spectrally corrected intensity of the emitted light, $I^{scatter}$ indicates the spectrally corrected intensity of the excitation light.

Supplementary Figures

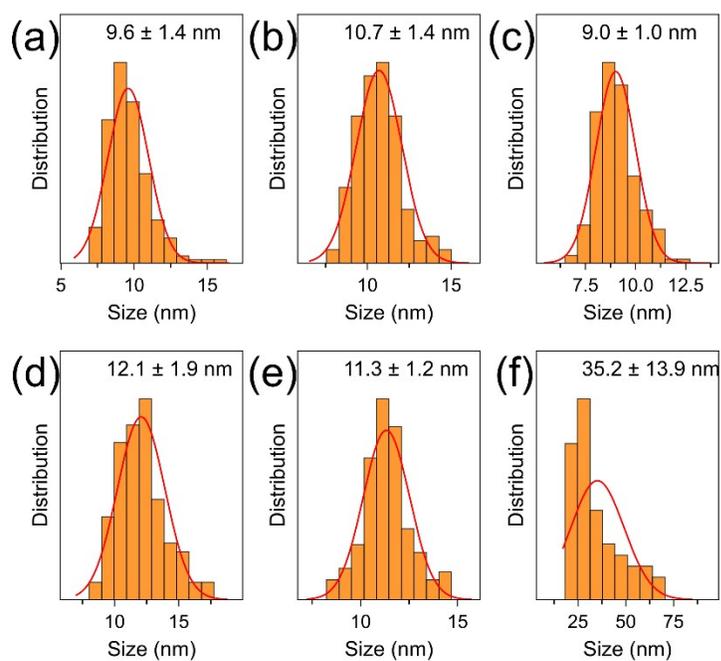


Fig. S1 Size distributions of Yb³⁺ doped CsPbCl₃ PQDs synthesized at the temperature of 190 °C

(a), 210 °C (b), 230 °C (c), 250 °C (d), 270 °C (e), 290 °C (f).

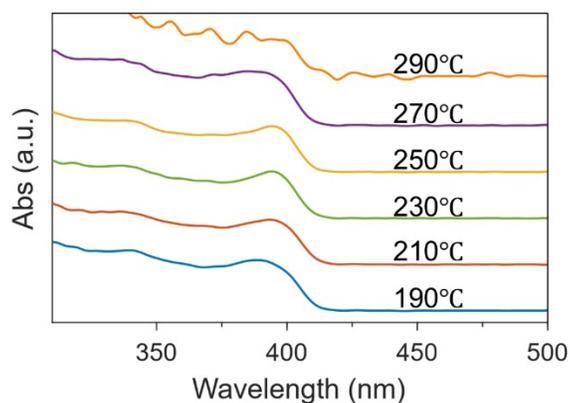


Fig. S2 Absorption spectra of Yb^{3+} doped CsPbCl_3 PQDs synthesized at different temperature.

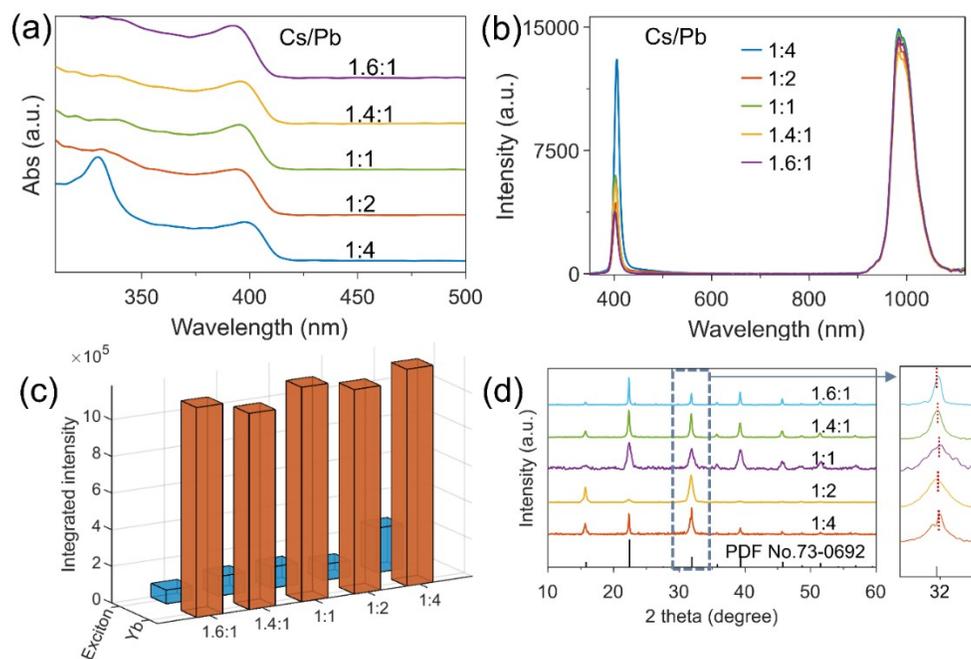


Fig. S3 Structural and optical properties of Yb-doped CsPbCl_3 PQDs synthesized at different Cs/Pb ratio. The absorption spectra (a), PL spectra (b) and corresponding integrate intensity (c). (d) XRD pattern. All PL spectra are obtained under 365 nm excitation.

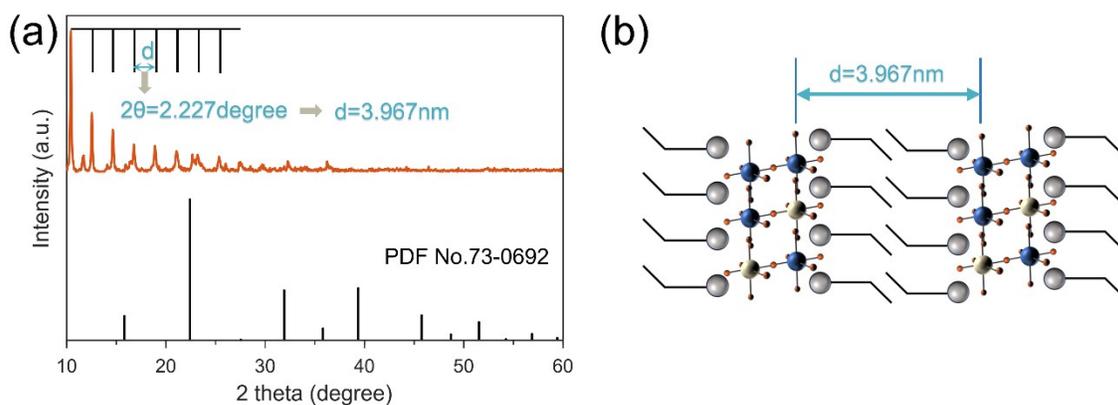


Fig. S4 (a-b) analysis of XRD pattern of Yb^{3+} doped CsPbCl_3 PQDs synthesized at TMS-Cl amount of 1.18 mmol with the Cs/Pb ratio of 1:4.

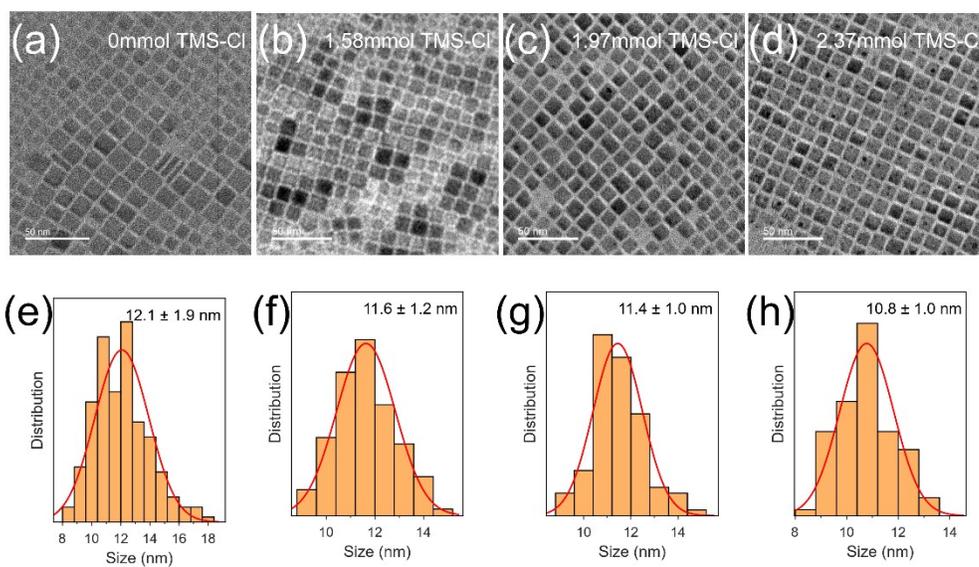


Fig. S5 (a-h) TEM images and corresponding size distributions of Yb^{3+} codoped CsPbCl_3 PQDs synthesized at different amount of TMS-Cl with the Cs/Pb ratio of 1:1.

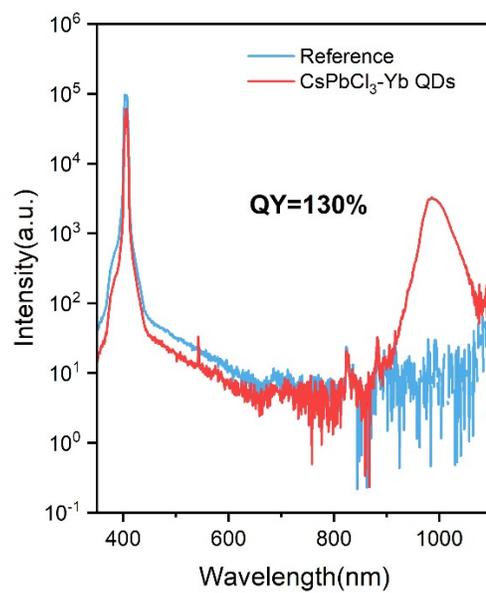


Fig. S6 PLQY of Yb emission in Yb³⁺ doped CsPbCl₃ PQDs synthesized at optimized reaction parameters.