

Electronic Supplementary Information

Tuning optical properties of perovskite nanocrystals by supermolecular mercapto- β -cyclodextrin

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Experimental Section

Reagents and Chemicals

Cs₂CO₃ and PbBr₂ were obtained from Sinopharm Chemical Reagent Co., Ltd (Shanghai, China). Octadecene (90%) and Oleic acid (OA, 90%) were purchased from Sigma-Aldrich Co. (St. Louis, MO, USA). Oleylamine (OLA, 80-90%) were purchased from Acros Organics (Belgium). Thiolated β -cyclodextrins (SH- β -CD) was purchased from Shandong BinzhouZhiyuan Biotechnology Co., Ltd (Binzhou, China). All other reagents were of analytical reagent grade and used without further purification.

Synthesis of CsPbBr₃ NCs

Synthesis of CsPbBr₃ NCs from Cs₂CO₃ and PbBr₂ followed literature previously reported by Protesescu.¹ Cs₂CO₃ (0.407g,) was added into 50 mL 3-neck flask along with octadecene (20mL) and OA (1.25 mL), and then heated under N₂ to 150 °C until all Cs₂CO₃ dissolved. The Cs-oleate precursor solution was kept at 100 °C to prevent precipitation before injection. In another 50 mL 3-neck flask, ODE (5 mL) and PbBr₂ (0.188 mmol 0.069g), were dried under N₂ for 1h at 130 °C. 0.5 hour later, OLA (0.5 mL) and OA (0.5 mL) were

injected into the mixture. The temperature was changed to 150 °C after complete solubilisation of the PbBr₂. And then hot Cs-oleate solution (0.4 mL) was injected quickly and the reaction mixture was immediately cooled by the ice-water bath 5s later. The obtained CsPbBr₃ NCs could be purified by centrifugation at high speed (10000 rpm 25 min), and then redispersion in toluene.

CsPbBr₃ NCs treated by SH-β-CD

0.5 mL of crude CsPbBr₃ NCs were dispersed in 5 mL of toluene, and different quantities (normally ranging from 0 to 8 mg) of SH-β-CD was added in the above colloidal solution.

Transmission Electron Microscopy (TEM)

TEM observations were conducted on a JEM-2100 transmission electron microscope (JEOL Ltd.) with a thermionic gun operating at 200 kV of accelerating voltage. The encapsulated CsPbBr₃ NCs@SH-β-CD with different quantities SH-β-CD (0, 4, and 8 mg) were diluted in toluene and then dropping onto carbon-coated 200 mesh copper grids with subsequent solvent evaporation.

Spectroscopy Characterization

The UV-vis spectra were taken on a Shimadzu UV-2450 spectrophotometer (Tokyo, Japan) and the fluorescence (FL) measurements were performed by a Fluoromax-4 fluorescence spectrofluorometer (Horiba, USA). The encapsulated CsPbBr₃ NCs@SH-β-CD with different quantities SH-β-CD (ranging from 0, 2, 4, 6 and 8 mg) were diluted in toluene (50 μL in 1 mL), in 1 cm path length quartz cuvettes. The FT-IR spectrum of SH-β-CD, CsPbBr₃ NCs and CsPbBr₃@SH-β-CD NCs were obtained from a Nicolet 5700 (USA) IR spectrometer in the range of 400–4000 cm⁻¹. Fluorescence lifetime were measured with Fluorolog 3-TSCPC. (Horiba Jobin Yvon Inc., France)

Photoluminescence quantum yield (PLQY) measurements

The absolute value of the PLQY was measured with Fluorolog 3-TSCPC. (Horiba Jobin Yvon Inc., France) Use of an integrating sphere with a short-pass filter allowed us to simultaneously measure absorbance corrected to reflectance and scattering losses. The encapsulated CsPbBr₃ NCs@SH-β-CD with different quantities SH-β-CD were diluted in toluene (50 μL in 1 mL), in 1 cm path length quartz cuvettes.

X-ray powder diffraction (XRD)

The XRD analysis was performed on Ultima IV multipurpose X-ray diffraction system using Copper X-ray tube (standard) radiation at a voltage of 40 kV and 40 mA, and X'Celerator RTMS detector. The diffraction pattern was scanned over the angular range of 10-60 degree (2θ) with a step size of 0.02, at room temperature.

Thermogravimetry analysis (TGA)

The TGA was carried out using a Mettler Toledo STARe System with an operative temperature range 25-1100 °C and 0.1 microgram sensitivity. The samples were heated from 50 to 800 °C, with an increase of 5 °C/min and under nitrogen flux of 40 mL/min.

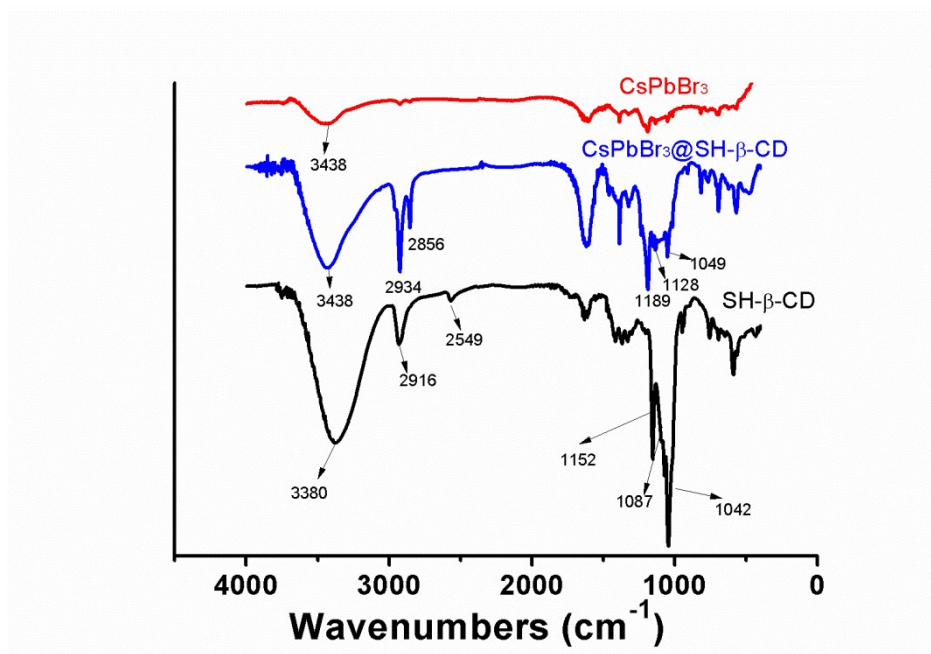


Figure S1. Fourier transform infrared (FT-IR) spectrum of CsPbBr₃ NCs (Red Line), SH-β-CD (Black Line), CsPbBr₃@SH-β-CD (blue Line), respectively.

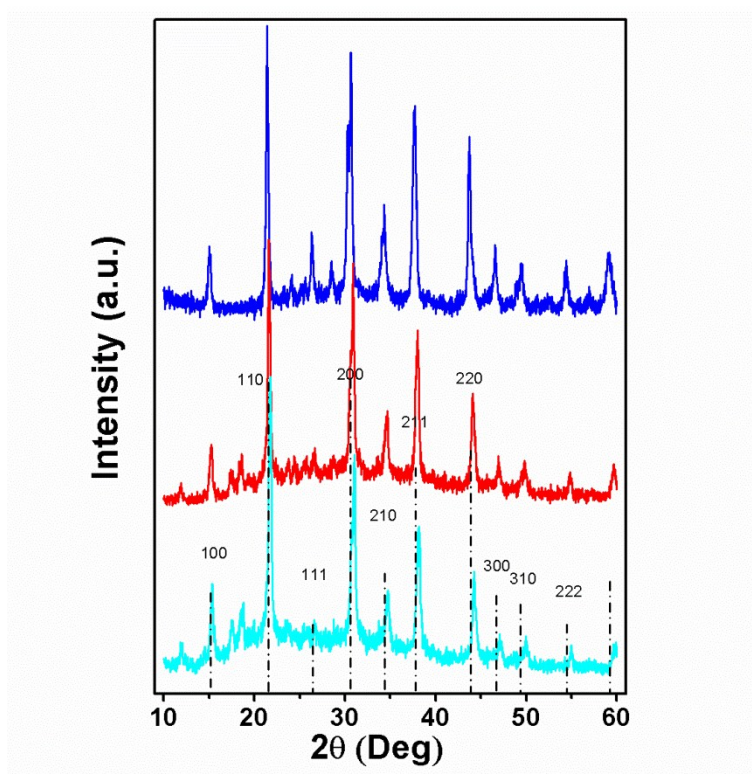


Figure S2. X-ray diffraction patterns for CsPbBr₃ NCs (blue Line), partially (red Line) and fully SH- β -CDs encapsulated CsPbBr₃ (cyan Line), respectively.

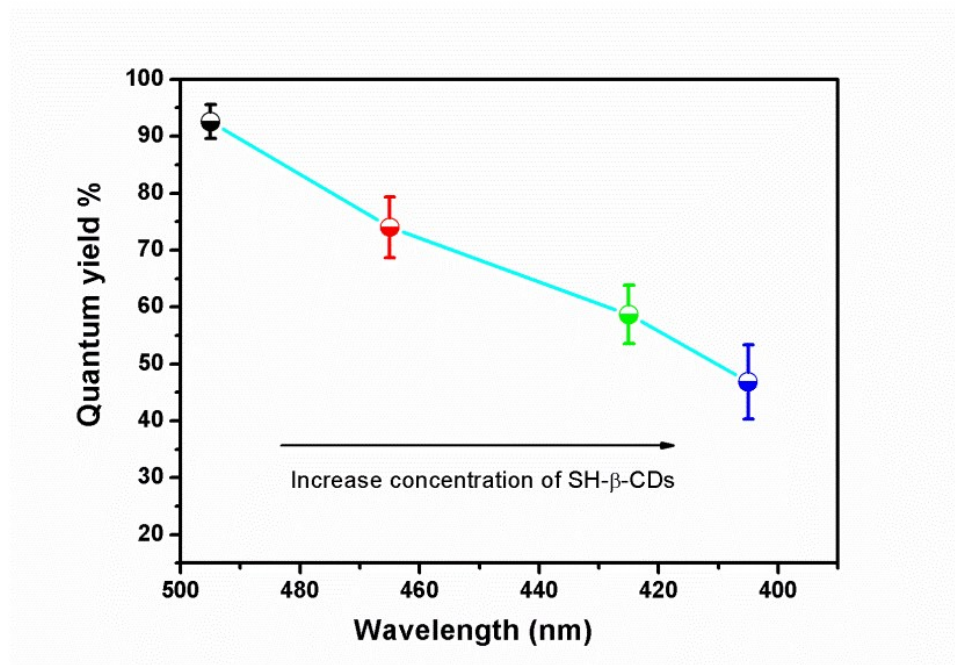


Figure S3. PLQY recorded on the encapsulated CsPbBr₃ NCs with different concentration of SH- β -CDs.

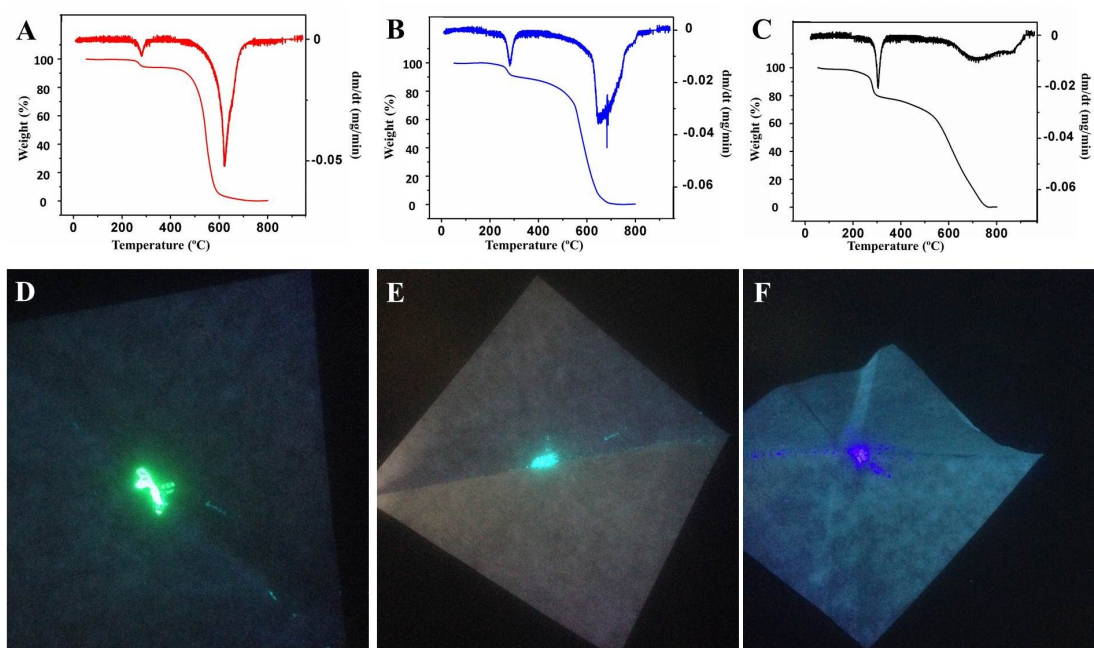


Figure S4. TGA heating curves and the corresponding 1st derivatives curves of CsPbBr₃ NCs (A), partially (B) and fully SH-β-CDs (C) encapsulated CsPbBr₃ NCs powders and photographs of CsPbBr₃ NCs (D), partially (E) and fully SH-β-CDs (F) encapsulated CsPbBr₃ NCs powders under UV lamp, $\lambda = 365$ nm.

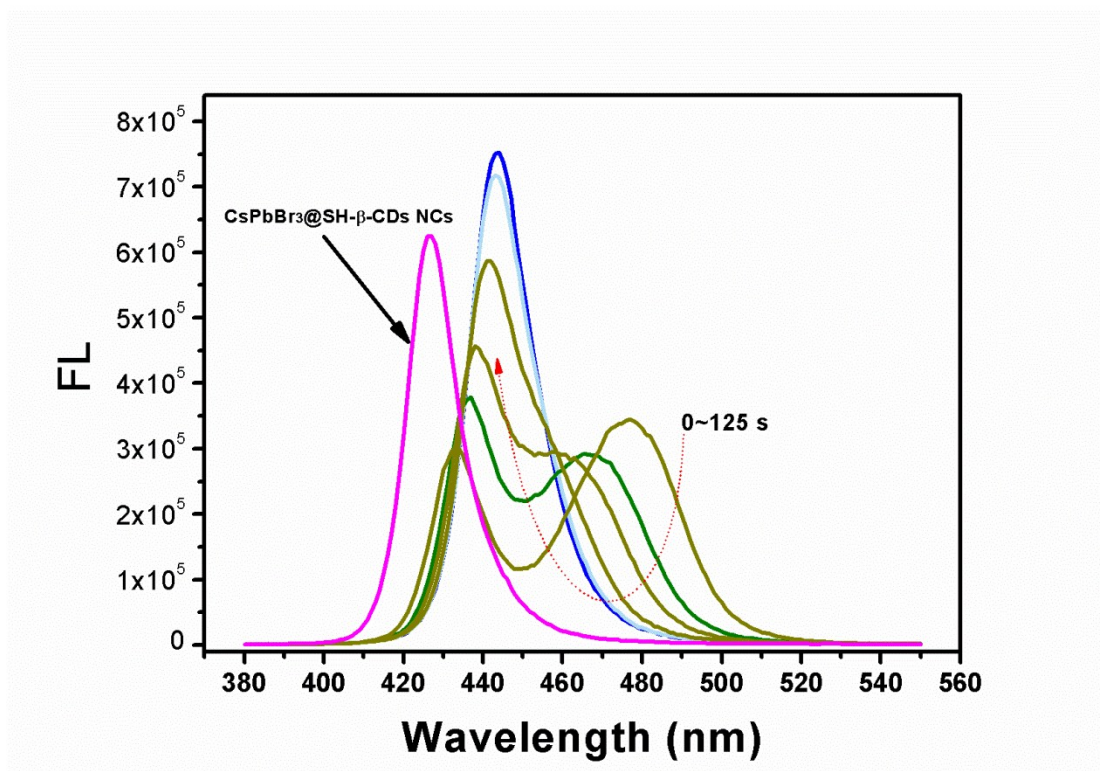


Figure S5. Time-dependent (0, 25, 50, 75, 100, 125 s) PL spectra showing an intermediate stage formed during inter-NCs homogenization after injecting pristine CsPbBr₃ NCs into the encapsulated CsPbBr₃@SH-β-CDs NCs.

References

1. L. Protesescu, S. Yakunin, M. I. Bodnarchuk, F. Krieg, R. Caputo, C. H. Hendon, R. X. Yang, A. Walsh and M. V. Kovalenko, *Nano. Lett.*, 2015, **15**, 3692-3696.