Electronic Supplementary Information

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

Qi-Le Li\textsuperscript{a}, Wen-Xiu Lu\textsuperscript{a}, Neng Wan\textsuperscript{b} and Shou-Nian Ding\textsuperscript{a}\textsuperscript{*}

\textsuperscript{a}Jiangsu Province Hi-Tech Key Laboratory for Bio-medical Research, School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, China.
\textsuperscript{b}SEU-FEI Nano-Pico Center, Key Laboratory of MEMS of Ministry of Education, School of Electrical Science and Engineering, Southeast University, 210096 Nanjing, China

*E-mail: snding@seu.edu.cn

Experimental Section

Reagents and Chemicals

Cs\textsubscript{2}CO\textsubscript{3} and PbBr\textsubscript{2} 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 CsPbBr\textsubscript{3} NCs

Synthesis of CsPbBr\textsubscript{3} NCs from Cs\textsubscript{2}CO\textsubscript{3} and PbBr\textsubscript{2} followed literature previously reported by Protesescu.\textsuperscript{1} Cs\textsubscript{2}CO\textsubscript{3} (0.407 g) was added into 50 mL 3-neck flask along with octadecene (20mL) and OA (1.25 mL), and then heated under N\textsubscript{2} to 150 °C until all Cs\textsubscript{2}CO\textsubscript{3} 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 PbBr\textsubscript{2} (0.188 mmol 0.069g), were dried under N\textsubscript{2} 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 droppiong 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 CsPbBr$_3$ 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 ºC and 0.1 microgram sensitivity. The samples were heated from 50 to 800 ºC, with an increase of 5 ºC/min and under nitrogen flux of 40 mL/min.

![FT-IR Spectrum](image)

**Figure S1.** Fourier transform infrared (FT-IR) spectrum of CsPbBr$_3$ NCs (Red Line), SH-β-CD (Black Line), CsPbBr$_3$@SH-β-CD (blue Line), respectively.
**Figure S2.** X-ray diffraction patterns for CsPbBr$_3$ NCs (blue Line), partially (red Line) and fully SH-β-CDs encapsulated CsPbBr$_3$ (cyan Line), respectively.

**Figure S3.** PLQY recorded on the encapsulated CsPbBr$_3$ NCs with different concentration of SH-β-CDs.
Figure S4. TGA heating curves and the corresponding 1st derivatives curves of CsPbBr$_3$ NCs (A), partially (B) and fully SH-β-CDs (C) encapsulated CsPbBr$_3$ NC$_S$ powders and photographs of CsPbBr$_3$ NCs (D), partially (E) and fully SH-β-CDs (F) encapsulated CsPbBr$_3$ 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 CsPbBr$_3$ NCs into the encapsulated CsPbBr$_3$@SH-β-CDs NCs.

References