

Cyclodextrin–Induced Phase Transformation of Cesium Copper Bromide Perovskite

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Chemicals and materials

CuBr (99.0%), CsBr (99.5%), α -cyclodextrins (α -CD, 98%), N, N-dimethylformamide (DMF, 99.5%), diethyl ether (Et₂O, 99.5%), were purchased from Aladdin (Shanghai, China) and used as received without further purification.

Synthesis of Cs₃Cu₂Br₅ and transformed CsCu₂Br₃ powders

0.1 mmol CuBr and 0.15 mmol CsBr were dissolved in 5 mL DMF and diethyl ether (volume ratio = 5:1), and then completely dissolved by ultrasonic and stirred for 1 h at room temperature before use. Glass substrates soaked in Pinaha solution at 60 °C for 30 min, rinsed with water and dried. Then, placed the treated glass substrates on the hot plate (75 °C), and transferred the mixture onto the glass substrate and heated it under the fume hood. After the solvent evaporated completely, stopped heating and collected the powders to obtain Cs₃Cu₂Br₅ microcrystal when the temperature dropped to room temperature. For the Synthesis of CsCu₂Br₃, different concentrations of α -CD were dissolved in DMF and diethyl ether (volume ratio = 5:1) to form α -CD solution, then added the α -CD solution to the Cs₃Cu₂Br₅ powders and evaporated the solvent, collected the powders after the solvent evaporated completely.

Characterization

The photoluminescence (PL) and photoluminescence excitation (PLE) spectra and fluorescence lifetime of samples were recorded by a FLS1000 fluorescence spectrometer (Edinburgh Instruments, UK). Photoluminescence quantum yields (PLQYs) were measured with a

FLS1000 fluorescence spectrometer with an integrating sphere attachment. The excitation and emission light from all directions of the sample surface was homogenized by the integrating sphere, and light at the exit port entered the monochromator for detection by the detector. Scanning electron microscopy (SEM) images were obtained on a JSM-7800F (JEOL, Japan). X-ray powder diffraction (XRD) measurements were conducted by using an XRD-6000 X-ray diffractometer (Shimadzu, Japan) with Cu K α radiation running at 40 kV and 35 mA. Fourier transform infrared (FTIR) spectra were recorded with a Nicolet iS50 spectrometer (Thermo Fisher Scientific, USA). X-ray photoelectron spectroscopy (XPS) measurements were performed using a EscaLab 250Xi (Thermo Fisher Scientific, USA) with an achromatic Al K α source (1486.6 eV). Nuclear magnetic resonance (NMR) data were performed on a AVANCE NEO 400 MHz spectrometer (Bruker, Switzerland).

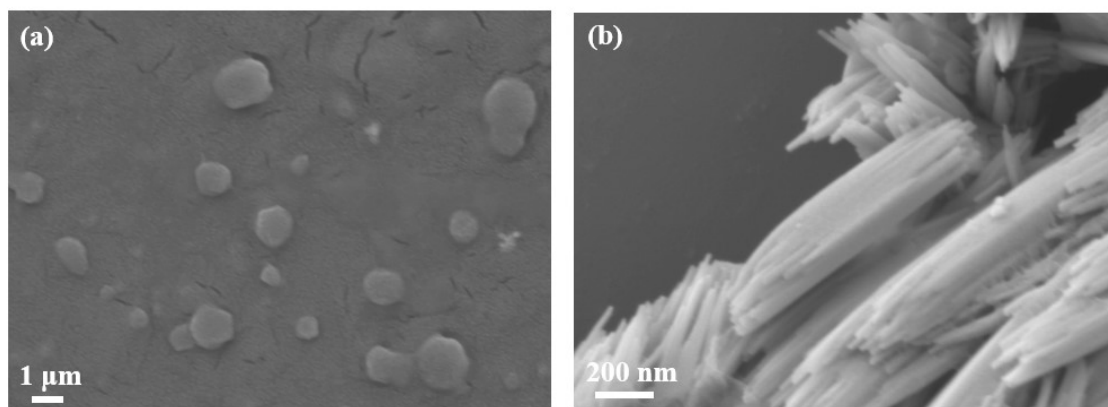


Figure S1 SEM image of (a) Cs₃Cu₂Br₅ powder and (b) transformed CsCu₂Br₃ powder.

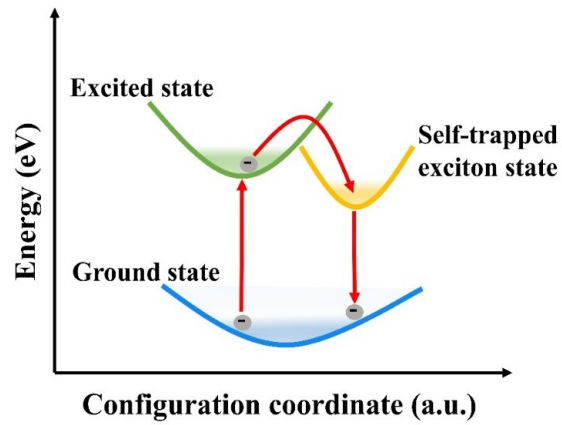


Figure S2 Configuration coordinate diagram for the STEs' dynamic mechanism of the $\text{Cs}_3\text{Cu}_2\text{Br}_5$ and CsCu_2Br_3 .

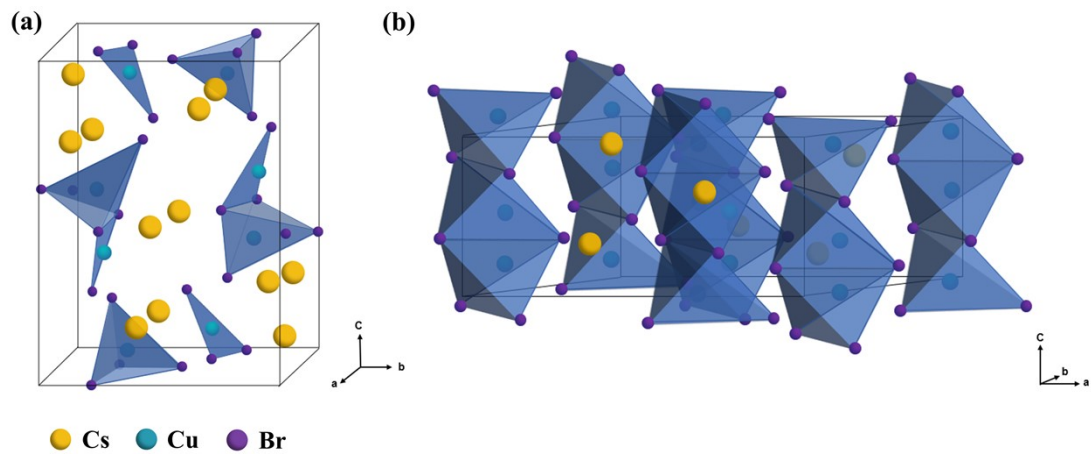


Figure S3 Crystal structure of (a) $\text{Cs}_3\text{Cu}_2\text{Br}_5$ and (b) CsCu_2Br_3 . The yellow, cyan and purple spheres represent Cs, Cu, and Br atoms, respectively.