

## Electronic Supplementary Material

### Ultrasound-assisted nucleation and growth of hydroxyl-protected and ligand-free $\text{Cs}_3\text{Cu}_2\text{X}_5$ nanocrystals with bright luminescence

Zhiquan Xu<sup>1</sup> †, Dengfeng Luo<sup>2,5</sup> †, Pei Wu<sup>3</sup>, Bo Hou<sup>1</sup>, Zhihao Zhang<sup>1</sup>, Shuqiang Wang<sup>4</sup>,  
Teng Gao<sup>4</sup>, Guobin Huang<sup>4,\*</sup>, Lan Fang<sup>1,\*</sup>

<sup>1</sup>Suzhou Chien-shiung Institute of Technology, Taicang, 215411, China

<sup>2</sup>Peng Cheng Laboratory, Shenzhen 518055, China

<sup>3</sup>University of Chinese Academy of Sciences, Beijing, 100049, China

<sup>4</sup>Institute of Food Safety and Environment Monitoring, Fuzhou University, Fuzhou, 350108, China

<sup>5</sup>Department of Electrical and Electronic Engineering, Southern University of Science and Technology, Shenzhen, 518055, China

**\* Corresponding author:**

Lan Fang; E-mail address: fanglanlan0813@163.com

Guobin Huang; E-mail address: 211310028@fzu.edu.cn

**† These authors contributed equally to this work.**

## 1. Experimental section

### 1.1 Instrumentation.

The X-ray diffraction (XRD) patterns were recorded on an Ultima IV (Rigaku, Japan) diffractometer and Cu K $\alpha$  radiation ( $\lambda = 0.154$  nm) from 10° to 60°. The photoluminescence excitation (PLE) and photoluminescence (PL) spectra were acquired utilizing an F-4600 fluorescence spectrophotometer (Hitachi, Japan). The time-resolved PL spectra (TRPL) and photoluminescence quantum yields (PLQYs) of samples were determined by using an FLS-980 spectrometer (Edinburgh, U.K.). The ultraviolet-visible absorption spectra were examined employing a UV-2600i UV-vis spectrophotometer (Shimadzu, Japan). The transmission electron microscopy (TEM) images and elemental mapping spectrum were obtained using a JEOL JEM-2100 F system (Rigaku, Japan). Chemical states were measured using a K-Alpha+ X-ray photoelectron spectroscopy (Thermo Fisher Scientific, U.S.A.). An ultrasound-assisted crusher (KMH1-720U) with a nominal frequency of 40 kHz and a net output power of 800 W was used for the synthesis of Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub> halide solutions.

### 1.2 DFT calculations section.

The Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub>, CsX, and CuX unit cell was used for periodic DFT investigations using the VASP code<sup>[1-3]</sup>. They were treated as valence electrons, and their interactions were described by the projected augmented wave (PAW) approach<sup>[4]</sup>. The binding energies ( $E_b$ ) of different solvents with precursors surface were calculated as  $E_{\text{precursors/solvents}} - E_{\text{precursors}} - E_{\text{solvents}}$ , where  $E_{\text{precursors/solvents}}$ ,  $E_{\text{precursors}}$ , and  $E_{\text{solvents}}$  are the total energies of the adsorption system, the precursors system and solvents crystals, respectively. The generalized gradient approximation (GGA) Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was applied<sup>[5]</sup>. The K points considered about the symmetry of the crystal structures were used to sample the Brillouin zone, and the cutoff energy of the plane-wave basis was set to 500 eV.