Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supporting Information

One-pot synthesis of $Cs_3Cu_2I_5$ nanocrystals based on thermodynamic equilibrium

Xudong Hu, Yuelei Li, Ye Wu, Weiwei Chen, Haibo Zeng and Xiaoming Li *

Key Laboratory of Advanced Display Materials and Devices, Ministry of Industry and Information Technology, Institute of Optoelectronics & Nanomaterials, School of Material Science and Engineering, Nanjing University of Science and Technology. ,Nanjing 210094, P. R. China.

* Corresponding author.

E-mail addresses: lixiaoming@njust.edu.cn.

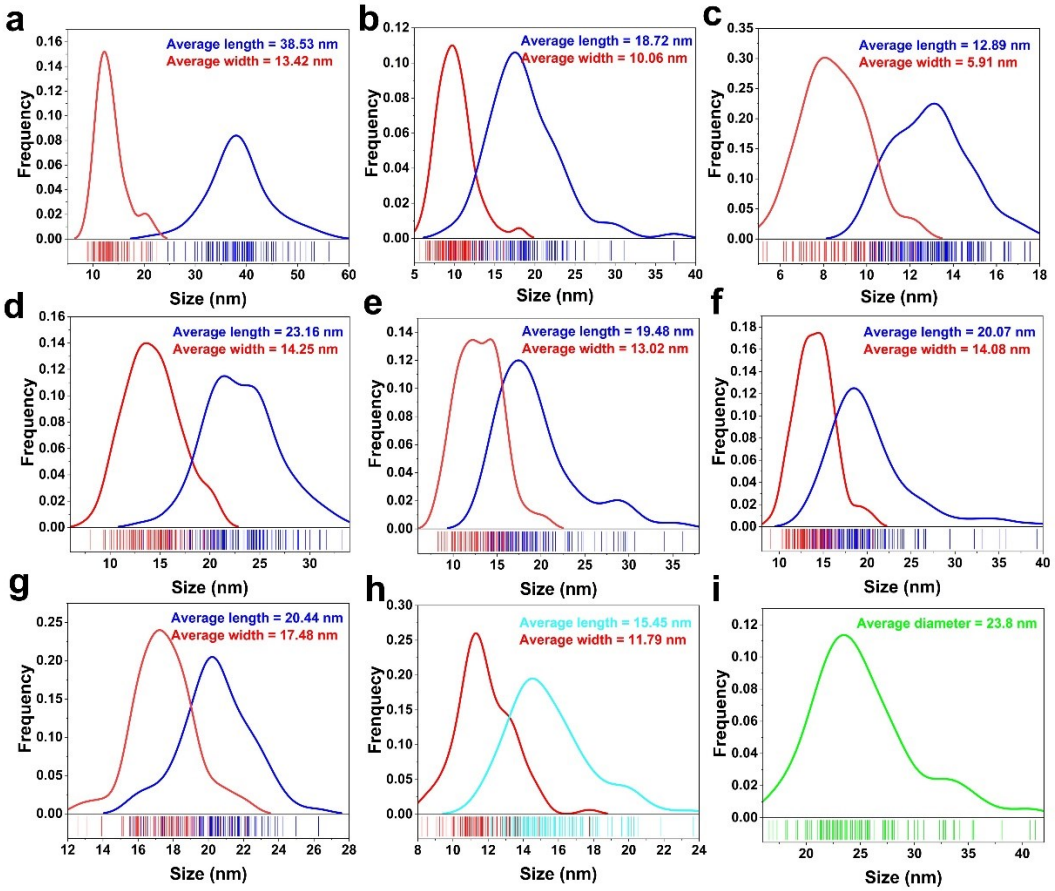

Fig. S1. The particle size distribution of $Cs_3Cu_2I_5$ NCs at differernt amount of ZnI_2 and different temperature. (a) 0.4 mmol, 100 °C. (b) 0.8 mmol, 100 °C. (c) 1.2 mmol, 100 °C. (d) 1.6 mmol, 100 °C. (e) 1.2 mmol, 120 °C. (f) 1.2 mmol, 140 °C. (g) 1.2 mmol, 160 °C. The particle size distribution of $Cs_3Cu_2X_5$ (X = Br, Cl) NCs with (h) 1.2 mmol $ZnBr_2$ and (i) $MnCl_2$ at 100 °C.

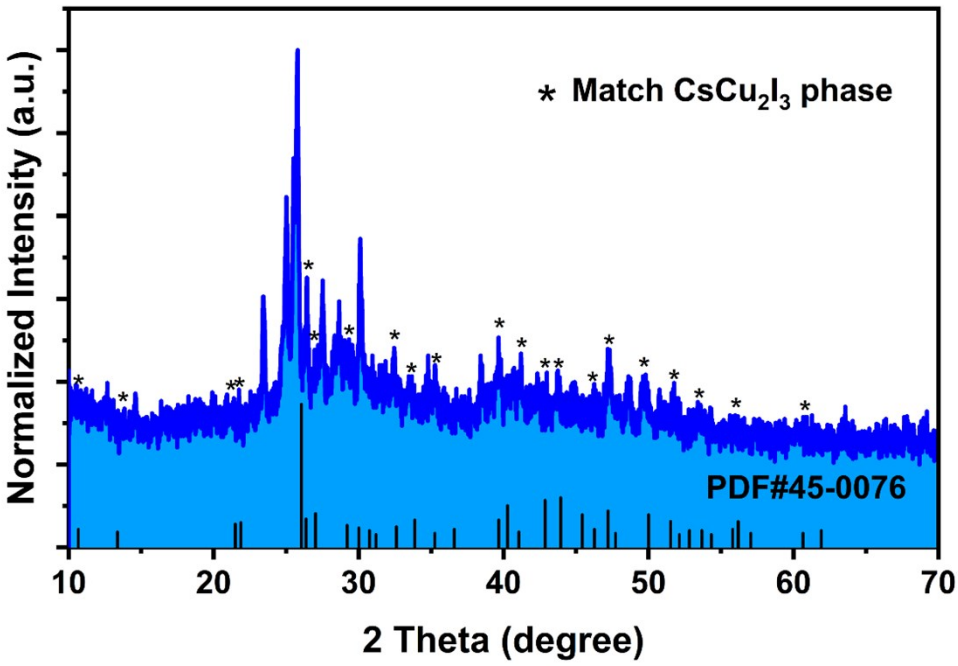

Fig. S2. XRD pattern of the precipitation at 1.6 mmol of ZnI_2. Obvious $CsCu_2I_3$ phase was observed.

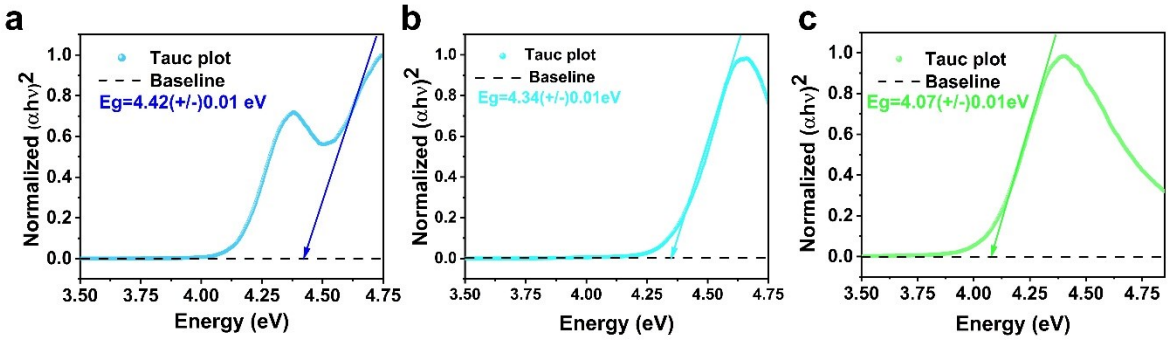

Fig. S3. Band gaps of (a) $Cs_3Cu_2I_5$ NCs, (b) $Cs_3Cu_2Br_5$ NCs, and (c) $Cs_3Cu_2Cl_5$ NCs calculated by Tauc plot.

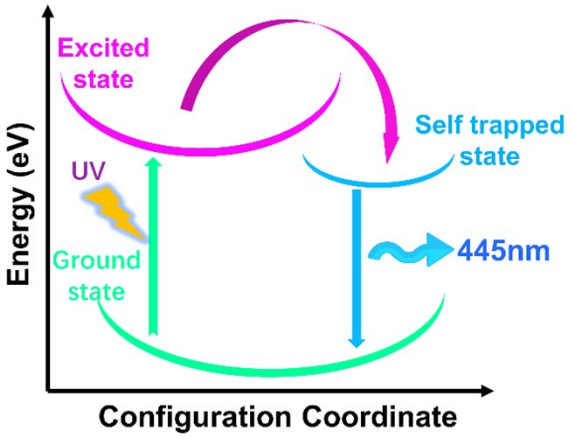

Fig. S4. Self-trapped exciton model of $Cs_3Cu_2I_5$ NCs.

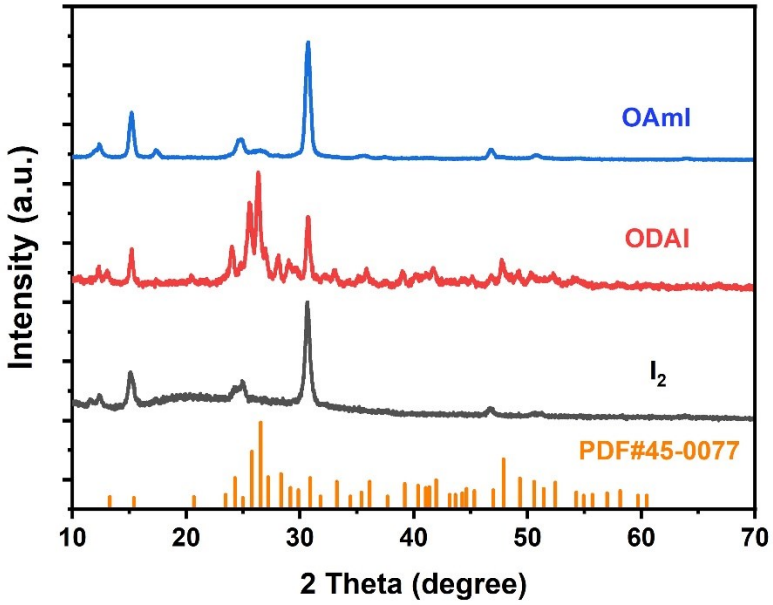

Fig. S5. XRD patterns of $Cs_3Cu_2I_5$ NCs prepared with OLA-I, ODA-I, and I_2.

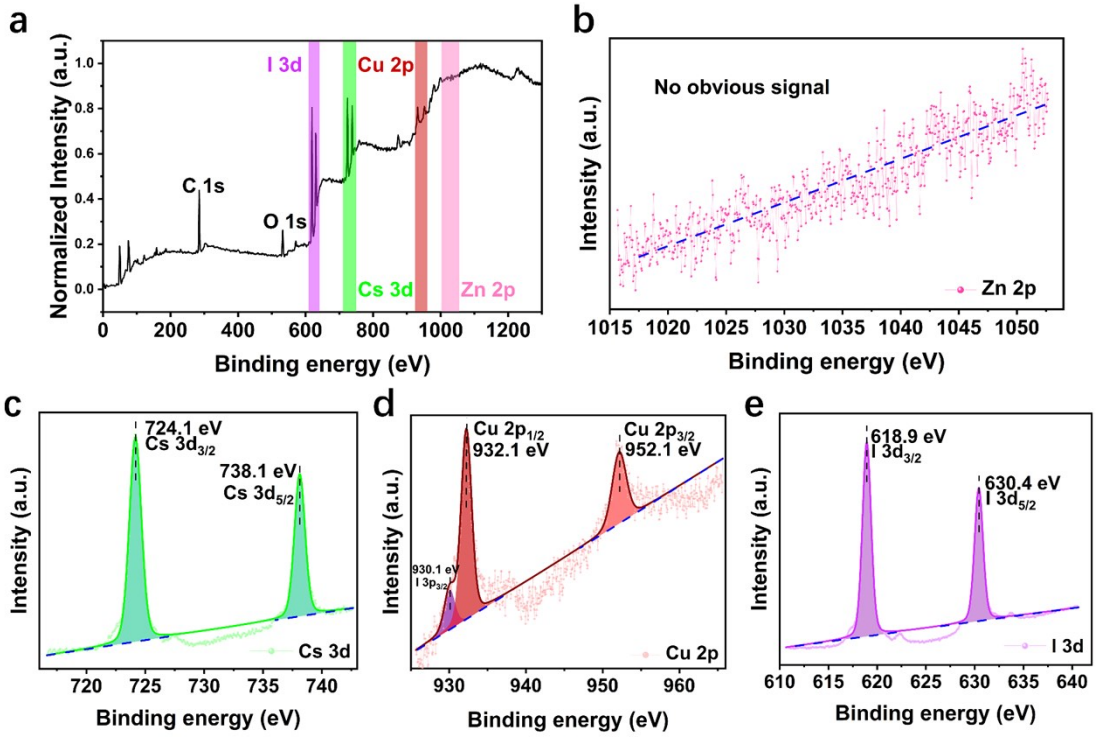

Fig. S6. The XPS survey of $Cs_3Cu_2I_5$ NCs. (a) Full spectra. (b) Zn 2p. (c) Cs 3d. (d) Cu 2p. (e) I 3d.

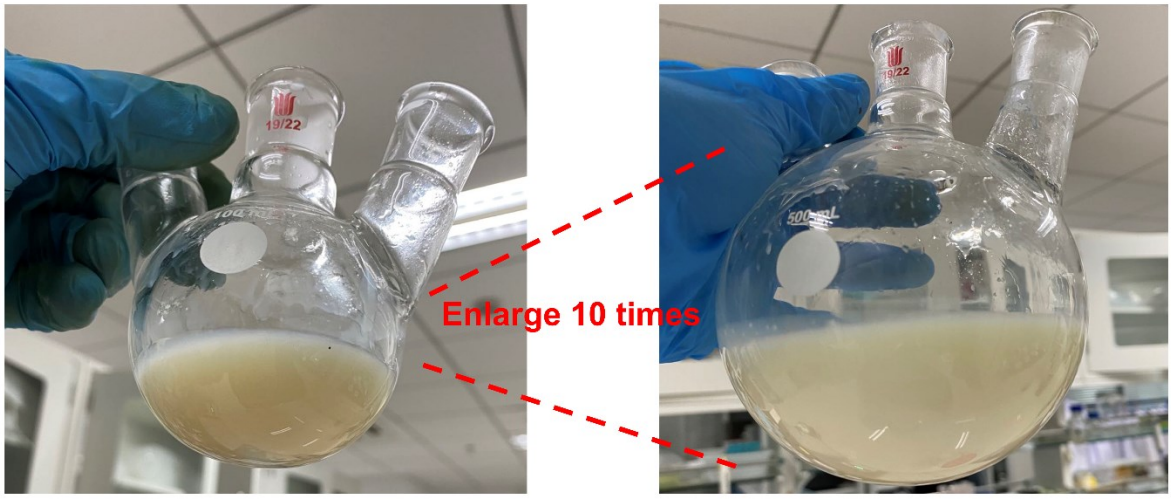

Fig. S7. Mass production of $Cs_3Cu_2I_5$ NCs by enlarging the reactant amount by 10 times.

Exponential fitting of PL decays and calculation. Decay time of the samples was obtained from the decay curves, which is simulated by using a bi-exponential decay function (1):

$$I(t) = A_0 + A_1 e^{\left(-t/\tau_1\right)} + A_2 e^{\left(-t/\tau_2\right)} \quad (1)$$

Where I(t) is the PL intensity at time t, A_i are the weight constants, τ_1 and τ_2 represent the PL decay time. The mean lifetime τ_{ave} is calculated by the formula (2):

$$\tau_{ave} = \frac{A\,\tau_1^2 + B\,\tau_2^2}{A\,\tau_1 + B\,\tau_2} \quad (2)$$

Where A and B represent the ratio of component contribution to the decay.

Table S1. Summary of time-resolved PL decay measurements, where the lifetimes of samples are tested in cyclohexane solution. τ_1 and τ_2 are the detailed recombination lifetimes, A and B represent the ratio of component contribution to the decay.

$Cs_3Cu_2X_5$ NCs	τ_1 (μs)	A (%)	τ_2 (μs)	B (%)	τ_{ave} (μs)
$Cs_3Cu_2I_5$ NCs	0.35	23.45	1.22	76.55	1.15
$Cs_3Cu_2Br_5$ NCs	1.44	29.02	4.65	70.98	4.29
$Cs_3Cu_2Cl_5$ NCs	25.53	39.50	120.74	60.50	109.20

ICP-OES calculation. The element fraction is calculated by the following formula:

$$C_x(mg/kg) = \frac{C_0(mg/L)\, f\, V_0(mL) * 10^{-3}}{m(g) * 10^{-3}} = \frac{C_1(mg/L)\, V_0(mL) * 10^{-3}}{m(g) * 10^{-3}} \quad (1)$$

$$W(\%) = \frac{C_x(mg/kg)}{10^6} * 100\% \quad (2)$$

$$C_1(mg/kg) = C_0(mg/L) * f \quad (3)$$

Where m_0 is the mass of the sample taken for analysis, V_0 is the volume of the sample after digestion, C_0 is the concentration of elements in the test solution, f is the diluted multiples. C_1 is the element concentration of stock solution, C_x is the final test result of the tested element, W is the final percentage of the element.

Table S2. The detail conclulation data measured by ICP-OES.

m_0 (mg)	V_0 (mL)	Element	C_0 (mg/L)	f	C_1 (mg/L)	C_x (mg/kg)	W (%)
48.3	50	Zn	0.78	1	0.78	/	0.08