

Supporting Information

# Stable Yellow Light-Emitting Devices Based on Ternary Copper Halides with Broadband Emissive Self-Trapped Excitons

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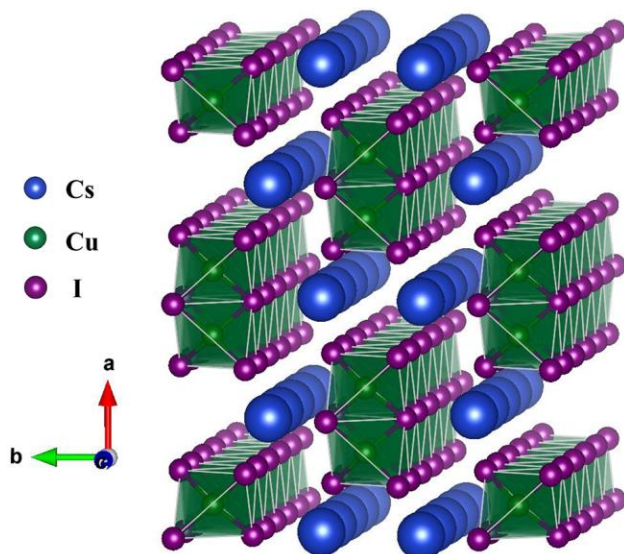
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## Crystal structure of $\text{CsCu}_2\text{I}_3$



**Figure S1. One-dimensional (1D) crystal structure of  $\text{CsCu}_2\text{I}_3$  (blue: Cs atom; purple: I atom; green: Cu atom; dark green octahedron: Cu-I tetrahedron).**

## Spin-coating speed-time profile

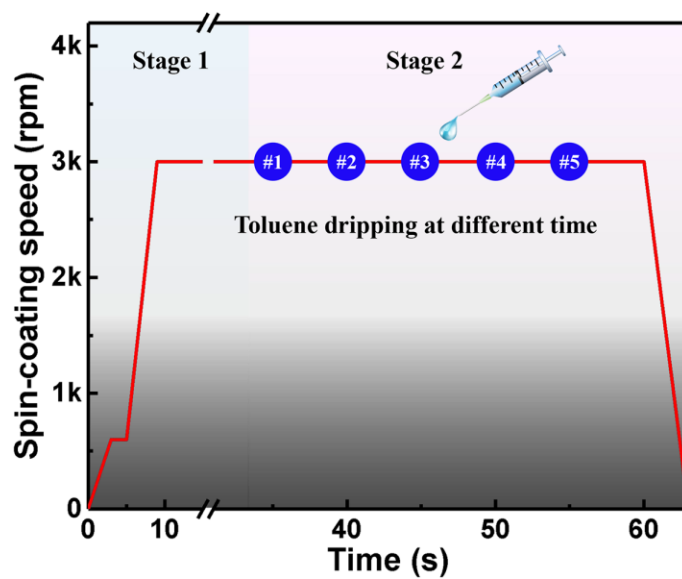
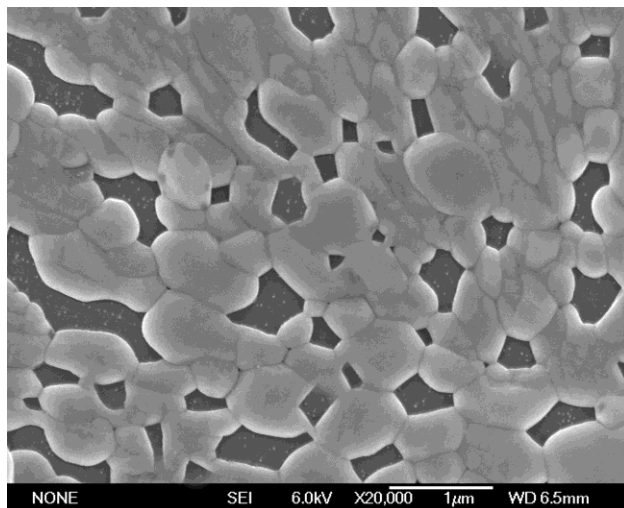


Figure S2. Spin-coating speed-time profile for preparing CsCu<sub>2</sub>I<sub>3</sub> thin films.

**Morphology of the CsCu<sub>2</sub>I<sub>3</sub> thin films prepared without the antisolvent**



**Figure S3. SEM image of the CsCu<sub>2</sub>I<sub>3</sub> thin films prepared without toluene as the antisolvent.**

## Comparison on the surface roughness of five CsCu<sub>2</sub>I<sub>3</sub> thin films samples

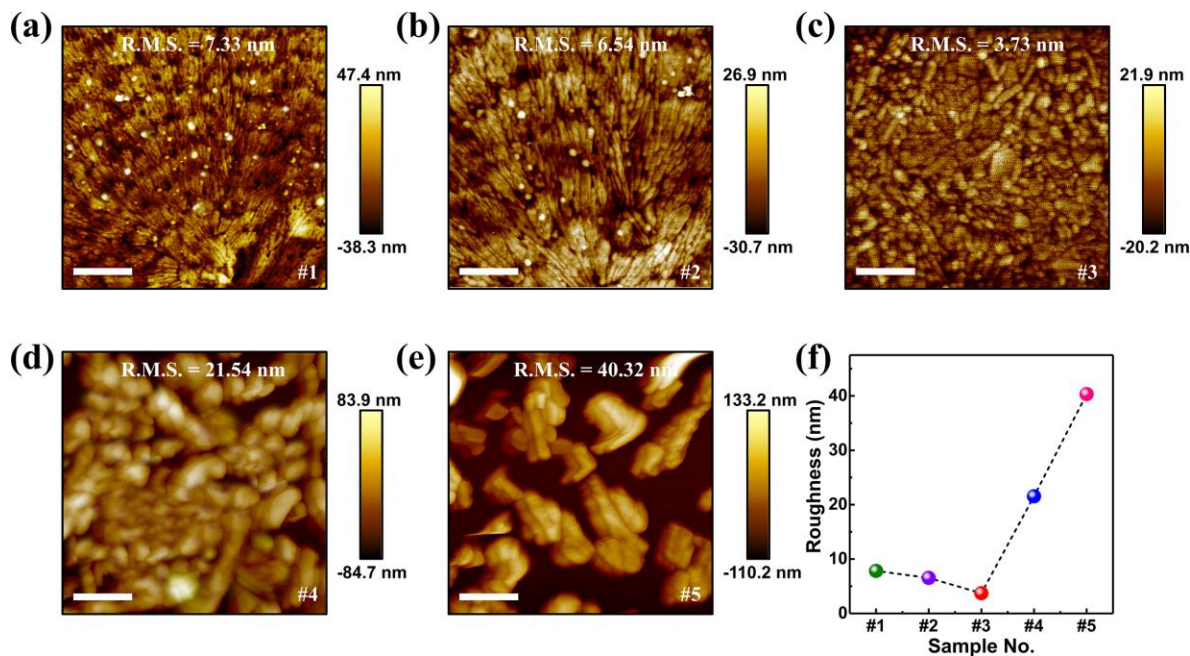
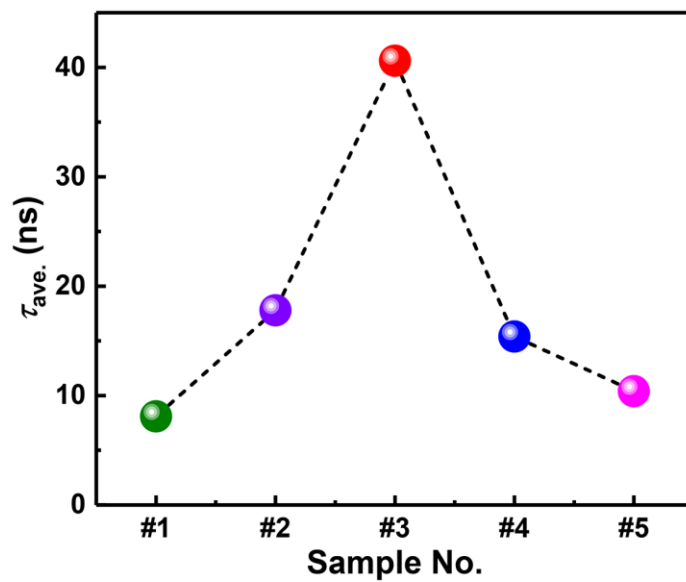


Figure S4. AFM images of the CsCu<sub>2</sub>I<sub>3</sub> thin films prepared with different dripping time of the toluene antisolvent: (a) #1, 35 s; (b) #2, 40 s; (c) #3, 45 s; (d) #4, 50 s; (e) #5, 55 s. All scale bars are 1  $\mu$ m. (f) Summary of root-mean-square roughness of the CsCu<sub>2</sub>I<sub>3</sub> thin films prepared with different conditions.

**Comparison on the PL decay behavior of five CsCu<sub>2</sub>I<sub>3</sub> thin films samples**



**Figure S5. Average PL lifetime of the CsCu<sub>2</sub>I<sub>3</sub> thin films obtained with different dripping time of toluene.**

### Dependence of the photon energy on the measured temperature

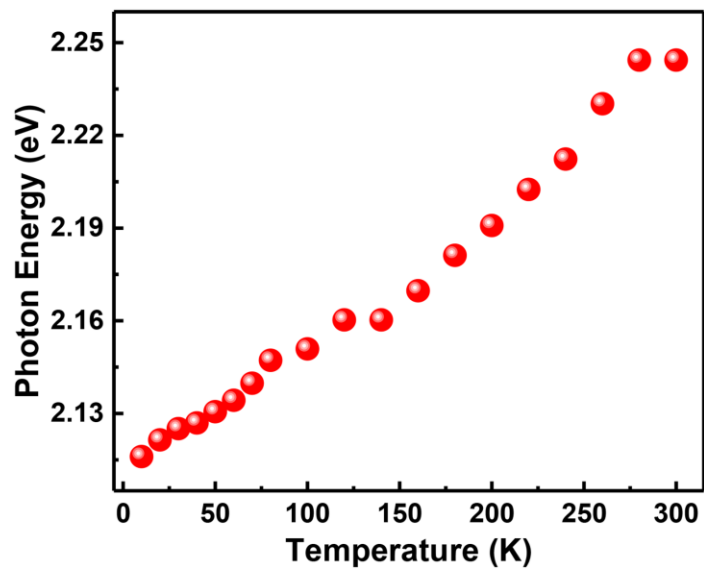


Figure S6. Shift of the photon energy of the CsCu<sub>2</sub>I<sub>3</sub> thin films as a function of measured temperature (10 to 300 K).

## Estimation of the specific formation time of STEs

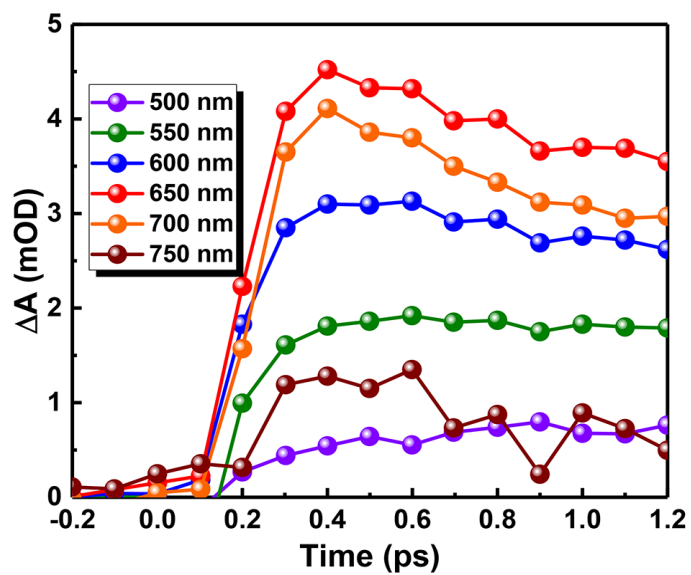


Figure S7. PIA onsets of the CsCu<sub>2</sub>I<sub>3</sub> probed at different wavelengths.



## Investigation on the excitation and emission spectra of the CsCu<sub>2</sub>I<sub>3</sub> thin films

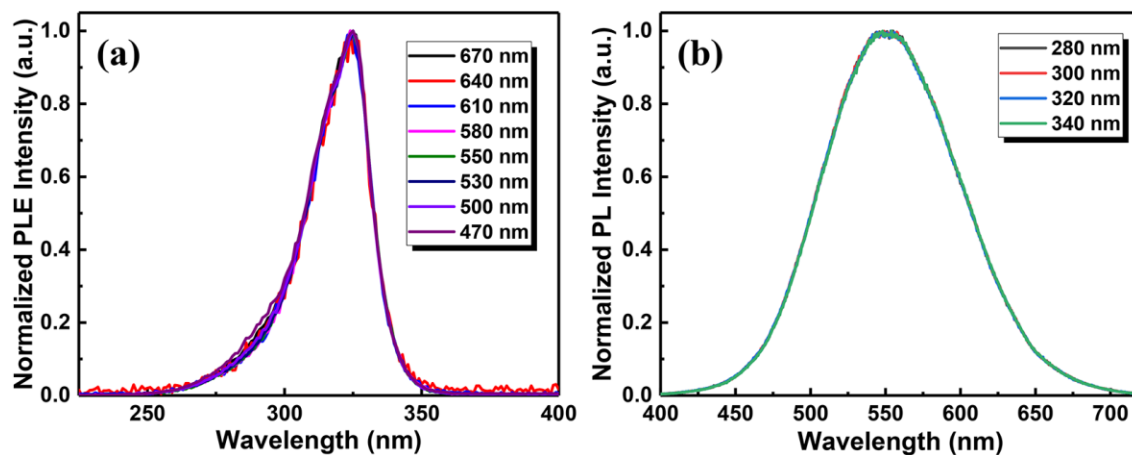


Figure S8. (a) Normalized excitation spectra of the CsCu<sub>2</sub>I<sub>3</sub> thin films for the emission from 470 to 670 nm. (b) Normalized PL spectra of the CsCu<sub>2</sub>I<sub>3</sub> thin films measured at different excitation wavelengths.

### Calculation of the structural distortion of $\text{CsCu}_2\text{I}_3$

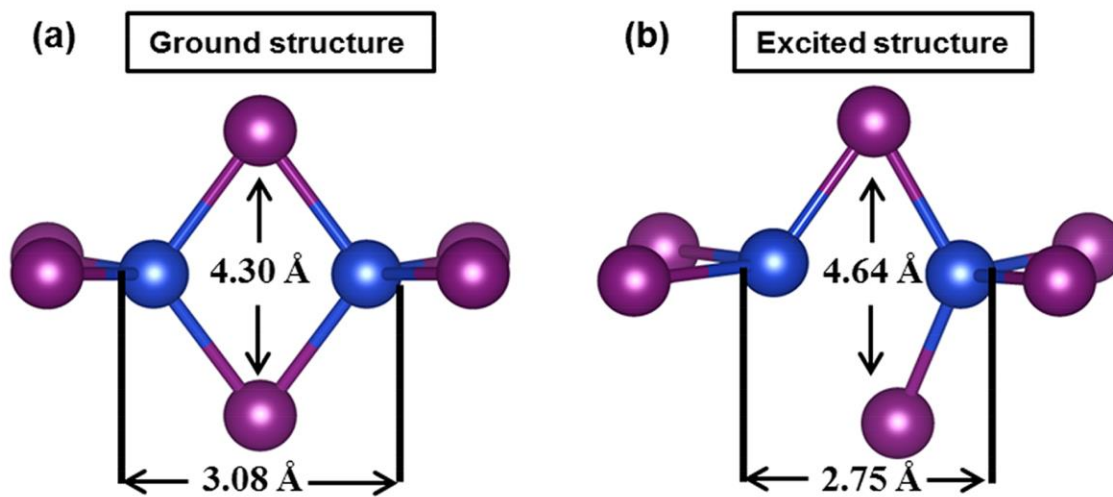
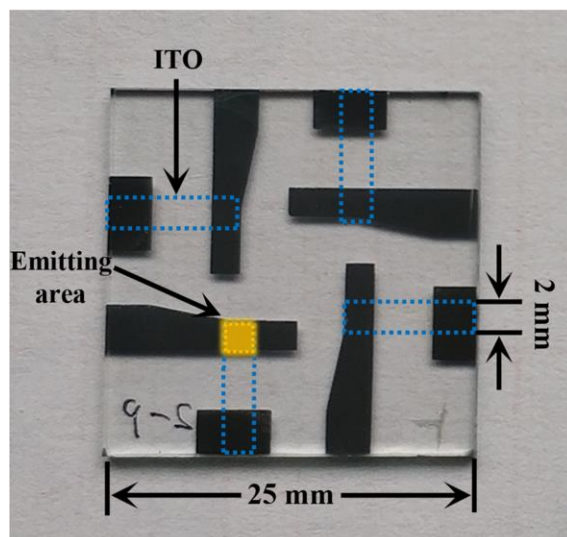


Figure S9. The geometric (a) ground state, and (b) excited state structures of  $\text{CsCu}_2\text{I}_3$ .

### Photograph of the fabricated device



**Figure S10.** Photograph of the fabricated device consisting of four emitting units. The active area of each unit is  $2 \times 2 \text{ mm}^2$ .

## Comparison of the device performances of five devices

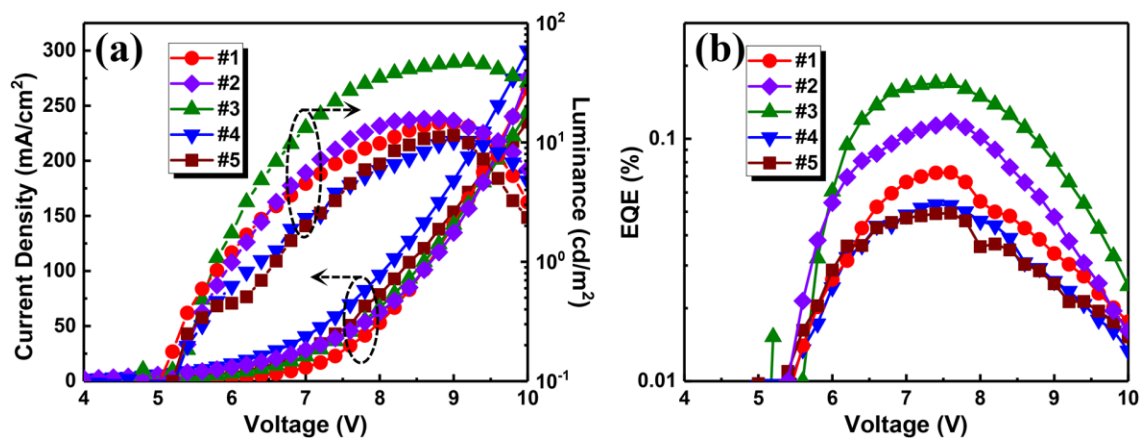


Figure S11. (a) Current density-voltage-luminance, and (b) EQE curves of the LEDs prepared with different dripping conditions of the  $\text{CsCu}_2\text{I}_3$  thin films.

## Assessment of the reproducibility of the studied LEDs

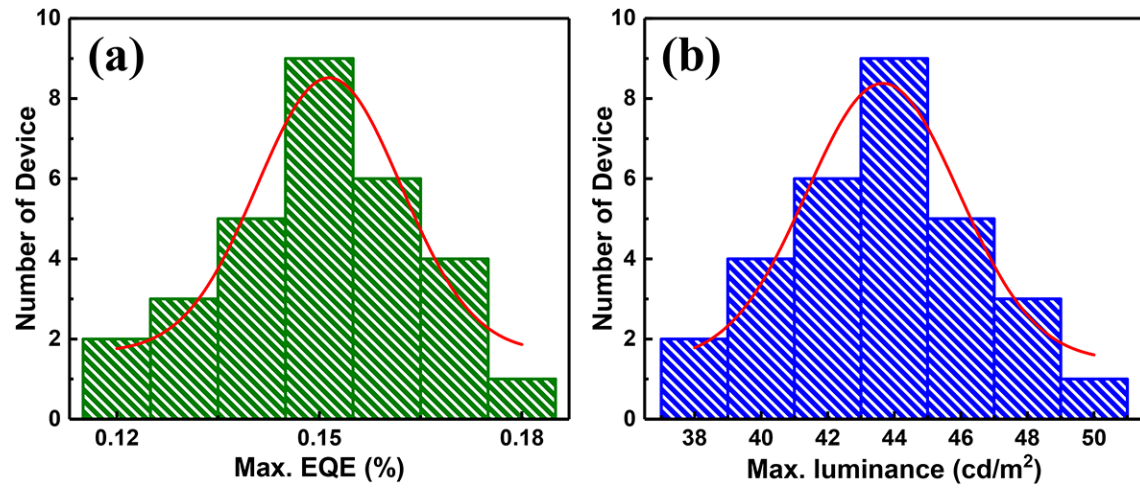


Figure S12. Statistical diagram of the (a) maximum EQE, and (b) maximum luminance measured from 30 devices with the same device structure.

**Investigation on the storage stability of the  $\text{CsCu}_2\text{I}_3$  thin films in air ambient**

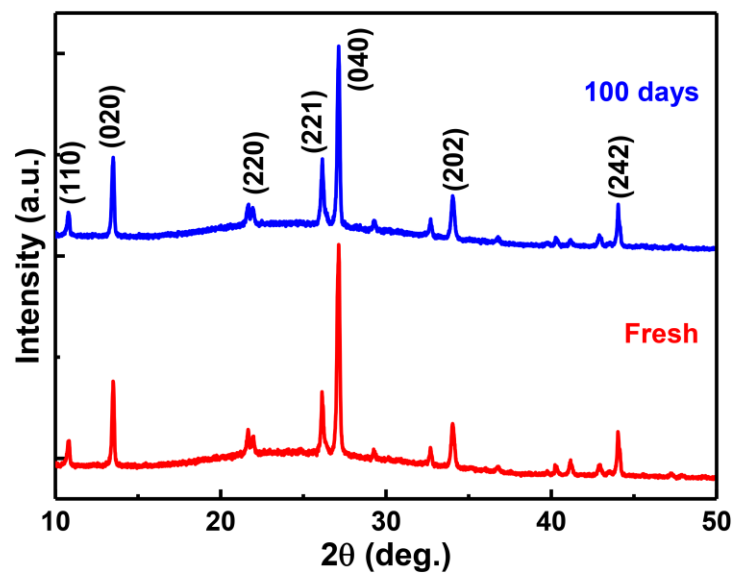


Figure S13. Comparison of the XRD patterns of the  $\text{CsCu}_2\text{I}_3$  thin films before and after storage for 100 days in air ambient.

**Table S1 The calculated bandgap, effective masses of electron and hole, excitation energy, emission energy, and the Stokes shift of CsCu<sub>2</sub>I<sub>3</sub>**

	Bandgap (eV)	Effective mass ( $m_0$ )			Excitation energy (eV)	Emission energy (eV)	Stokes shift (nm)
CsCu <sub>2</sub> I <sub>3</sub>	4.02		$m_e$	$m_h$	4.02	2.37	213.03
		$\Gamma \rightarrow S$	0.22	0.55	(3.82 <sup>a</sup> )	(2.26 <sup>a</sup> )	(224.06 <sup>a</sup> )

<sup>a</sup>The experimental values are also shown in parentheses for comparison.