

Supporting Information

Centimeter-Scale $\text{Gua}_3\text{SbBr}_6$ Single Crystals for White Light-Emitting Diodes Enabled by Inhibition of Multi-Site Nucleation

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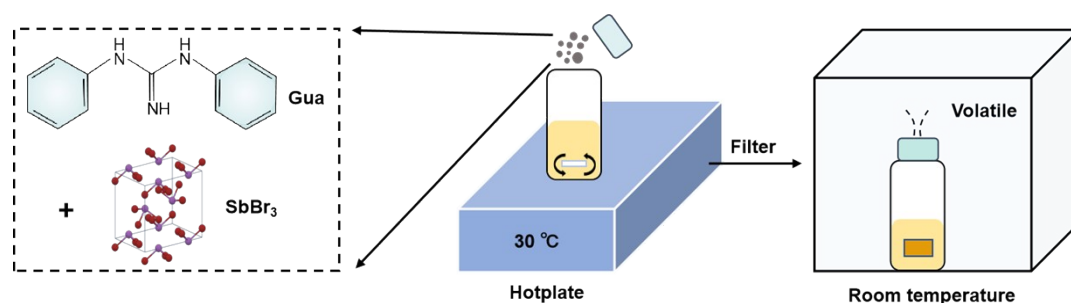


Figure S1: Schematic illustration of the solvent evaporation method of $\text{Gua}_3\text{SbBr}_6$ SC.

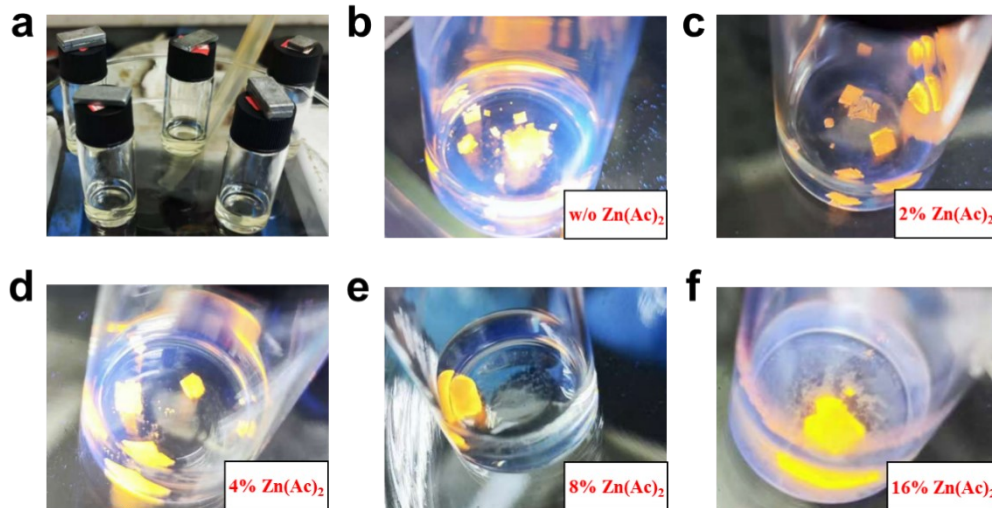


Figure S2: Photos of $\text{Gua}_3\text{SbBr}_6$ SC growth process without $\text{Zn}(\text{Ac})_2$ and with different percentages of $\text{Zn}(\text{Ac})_2$ (2%, 4%, 8% and 16%). (a) The initial precursor solution Photos of all samples. Photos of the precursor solution (b) without $\text{Zn}(\text{Ac})_2$, (c) 2% $\text{Zn}(\text{Ac})_2$, (d) 4% $\text{Zn}(\text{Ac})_2$, (e) 8% $\text{Zn}(\text{Ac})_2$ and (f) (d) 8% $\text{Zn}(\text{Ac})_2$ under UV light after standing for 24 hours.

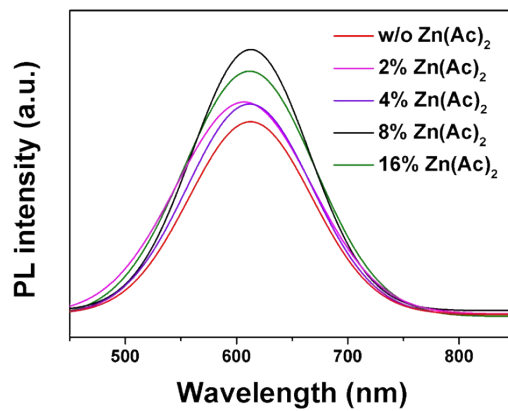


Figure S3: PL spectrum of $\text{Gua}_3\text{SbBr}_6$ SC untreated and treated with 2%, 4%, 8% and 16% $\text{Zn}(\text{Ac})_2$.

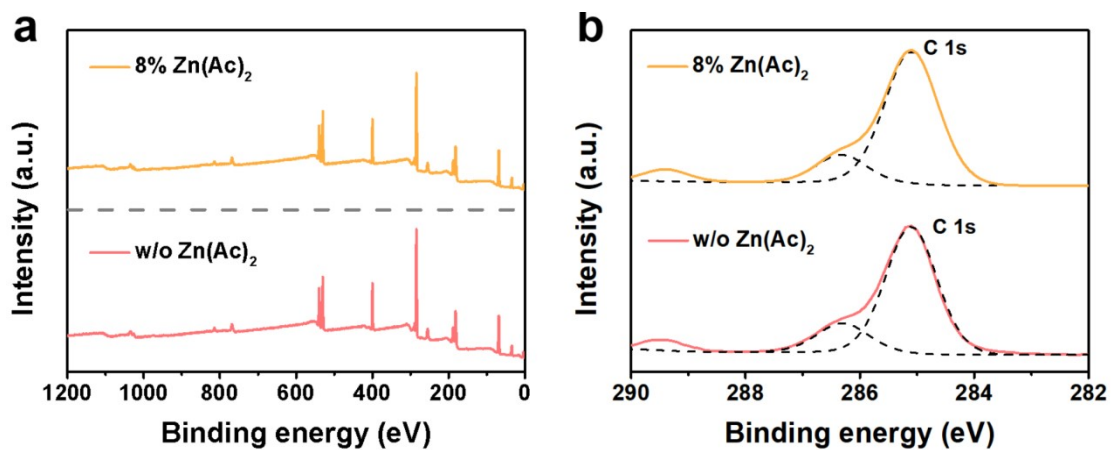


Figure S4. XPS spectra of (a) whole XPS spectrum and (b) C 1s of both samples.

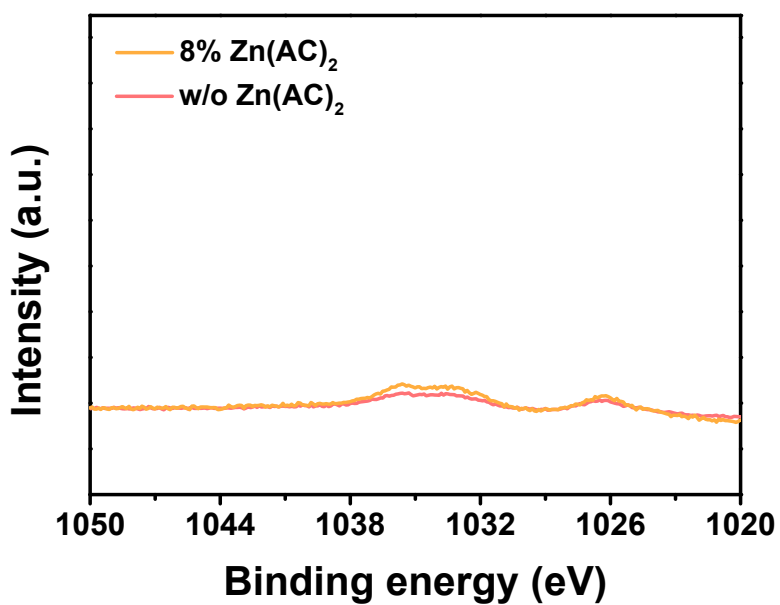


Figure S5. The corresponding Zn 2p XPS spectra of Gua₃SbBr₆ powers without and with 8% Zn(Ac)₂.

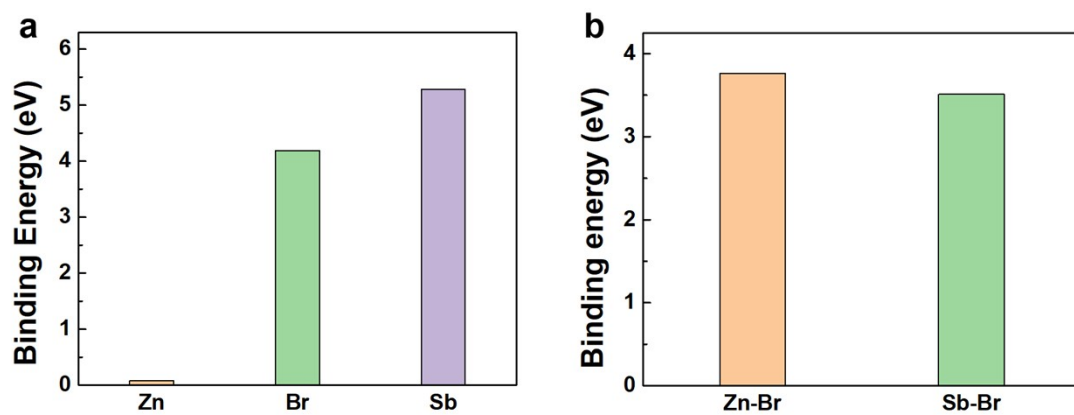


Figure S6. (a)The binding energies of DGP with Zn²⁺, Br⁻, Sb³⁺. (b)The binding energies of Zn-Br and Sb-Br.

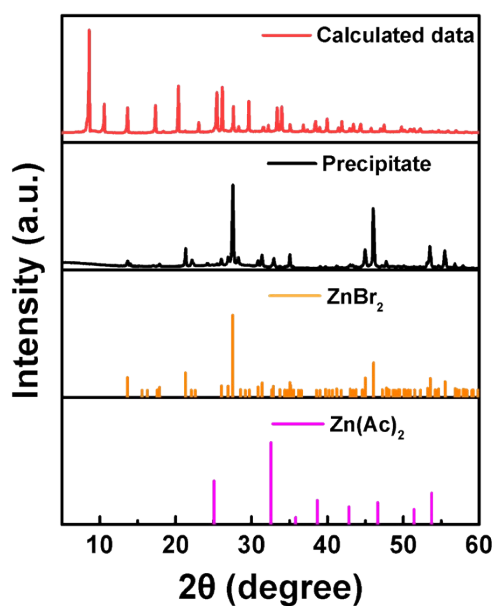


Figure S7. Calculated XRD patterns of Gua₃SbBr₆ SC, measured XRD patterns of precipitate and Standard XRD card of ZnBr₂ and Zn(Ac)₂.

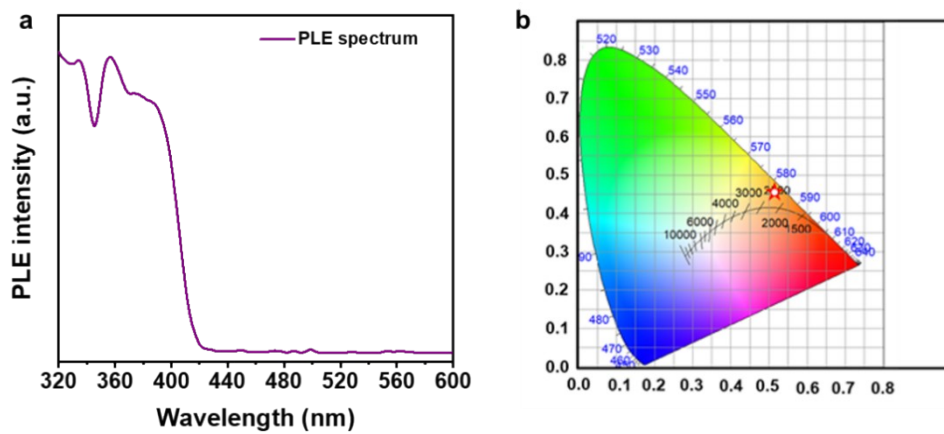


Figure S8. (a) The PLE spectrum and (b) CIE coordinate of Gua₃SbBr₆ SC.

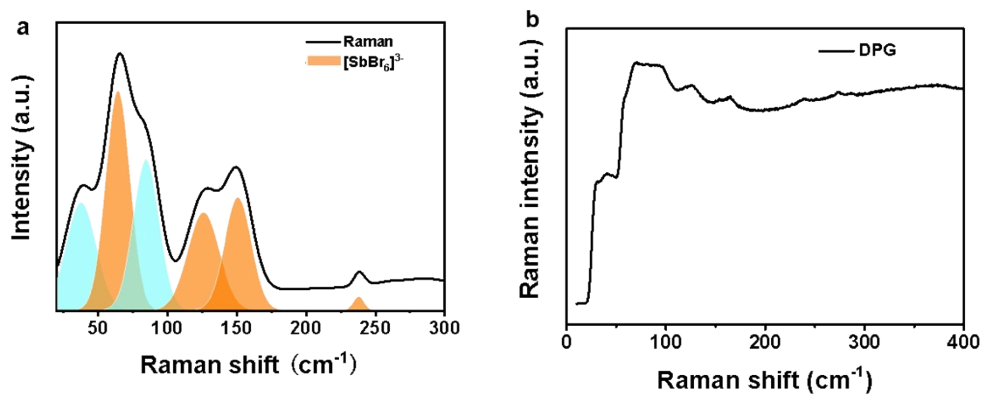


Figure S9. Raman spectrum of (a) Gua₃SbBr₆ and (b) organic Gua powers excited at 633 nm.

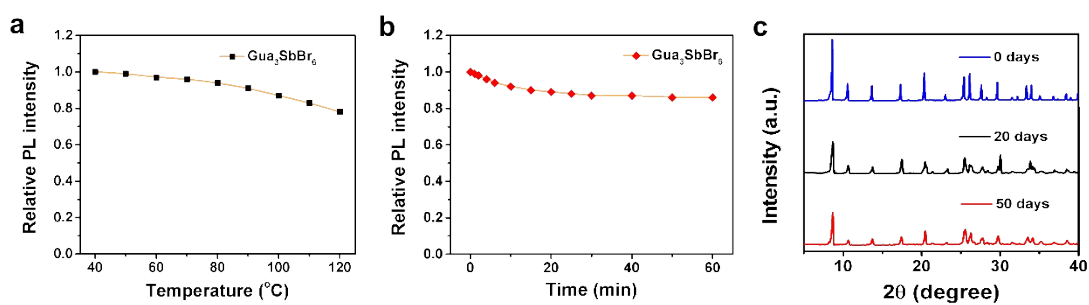


Figure S10. Variation of the relative PL intensities of the $\text{Gua}_3\text{SbBr}_6$ SC with 8% $\text{Zn}(\text{Ac})_2$ placed (a) in a hotplate, (b) under UV light, and (c) prolonged exposure to the air with 70% humidity.

Table 1: Single-crystal X-ray diffraction data of a $\text{Gua}_3\text{SbBr}_6$ SC.

Empirical formula	$(\text{C}_{13}\text{H}_{13}\text{N}_3)_3\text{Sb}_1\text{Br}_6$
Formula weight	
Temperature	150 K
Wavelength	0.71073
Crystal system	P-3
Space group	R3
Unit cell dimensions	$a=16.7199 \alpha=90^\circ$ $b=16.7199 \beta=90^\circ$ $c=14.1411 \gamma=120^\circ$
volume	1238.02
2θ range for data collection	
Reflections collected	4669
Absorption correction	MULTI-SCAN
Max and min transmission	0.009 0.028
Refinement method	Full-matrix least-squares on F^2

Table 2: The performance of the state-of-the-art perovskite-based WLEDs.

Emitter	PL peak (nm)	PLQY (%)	Power efficiency (lm/W)	CRI	Ref
(Gua-DPG) ₃ SbCl ₆	584	100%	-	86.5	1
Cs ₂ NaInCl ₆ :Sb ³⁺	605	92.4%	-	95.4	2
Cs ₂ Cu ₂ Cl ₅ :Zn ²⁺	522	70.19	-	95.8	3
Cs ₃ InCl ₆ :Sb ³⁺ /Mn ²⁺	620	51.38	-	85.5	4
(OTA) _{2+x} SnI _{4+x}	617	92	-	92	5
Cs ₂ NaInCl ₆ :Sb ³⁺ NCs	460	80.1	37.5	80	6
CsPbBr ₃ NCs	517	92	-	86	7
(DPG)₃SbBr₆	611	100	48.6	89	This work

Reference

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