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$CsCu_2I_3$ Thin Films Prepared by Different Deposition Methods for Ultraviolet Photodetectors with Imaging Capability

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Theoretical details

The Vienna ab-initio simulation package (VASP) 6.1.2 code with the projector-augmented-wave(PAW) potential are adopted to perform the first-principles calculations. The HSE06 hybrid functional is put to use in the calculations of the electronic properties for the dielectric function. There are 24 atoms in the unit cell. The 3×3×3 Γ-centered k-mesh of Brillouin zone (BZ) are employed in integration, but the band structure are calculated with additional 8 special k points including 140 points. The energy cutoff of the plane-wave basis sets is 500 eV to ensure the calculations to reach convergence. The energy convergent criterion is 10^{-6} eV. In the relaxation calculation, all the force is smaller than 0.01 eV/Å for the equilibrium structures. By using the obtained $\varepsilon(\omega)$, we evaluate the optical absorption coefficient α with an equation as follows:

$$\alpha(\omega) = \sqrt{2}\omega\sqrt{({\varepsilon_r}^2(\omega) + {\varepsilon_i}^2(\omega))^{0.5} - \varepsilon_r(\omega)}$$

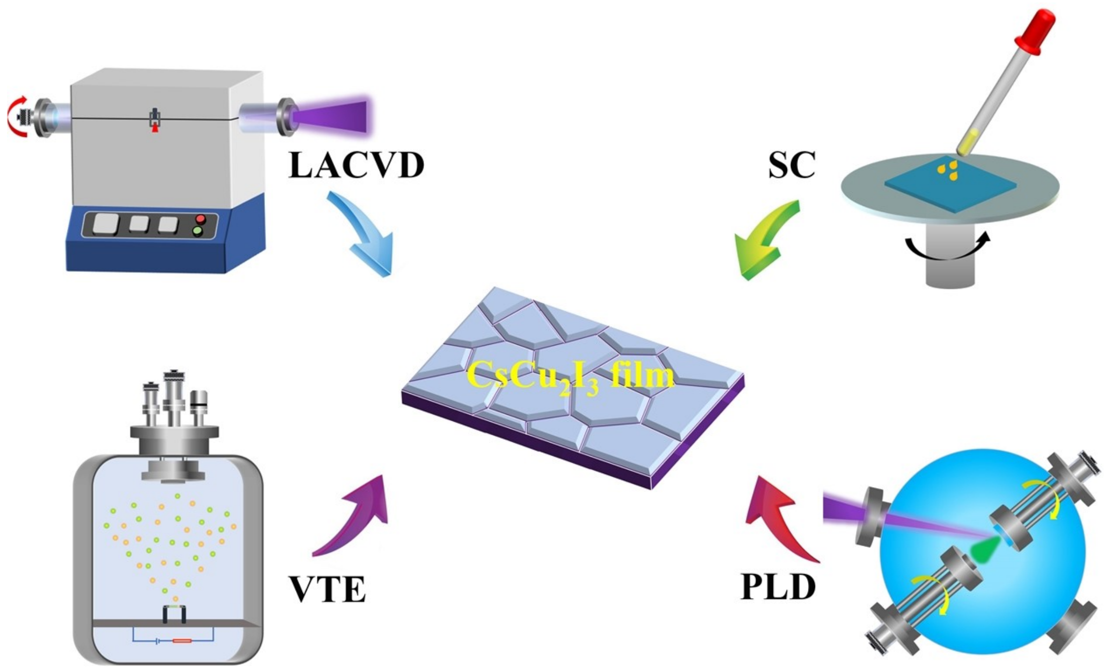

Fig. S1 Schematic diagram for the fabrication of $CsCu_2I_3$ films by LACVD, SC, VTE and PLD utilized in this work.

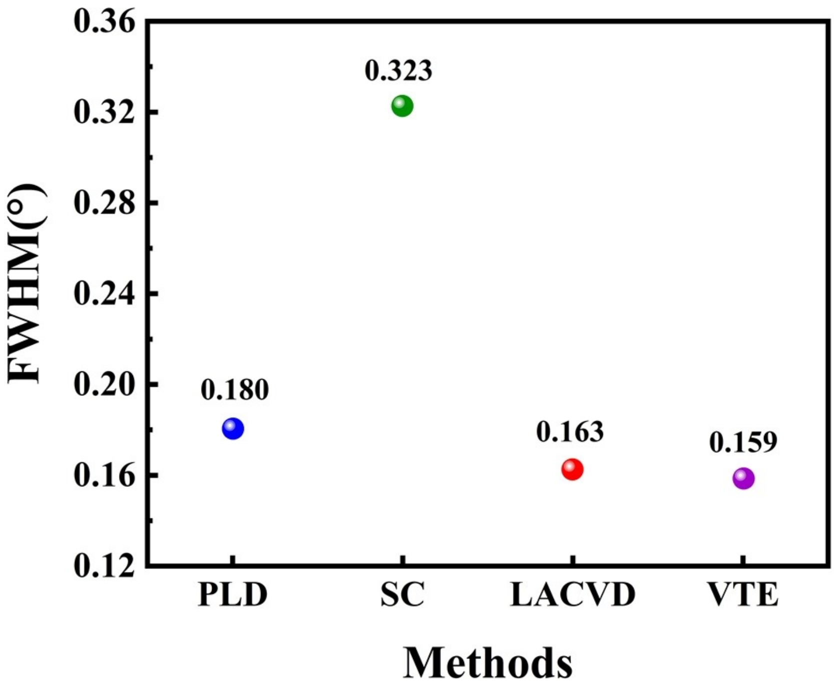

Fig. S2 FWHM of $CsCu_2I_3$ films by LACVD, SC, VTE and PLD.

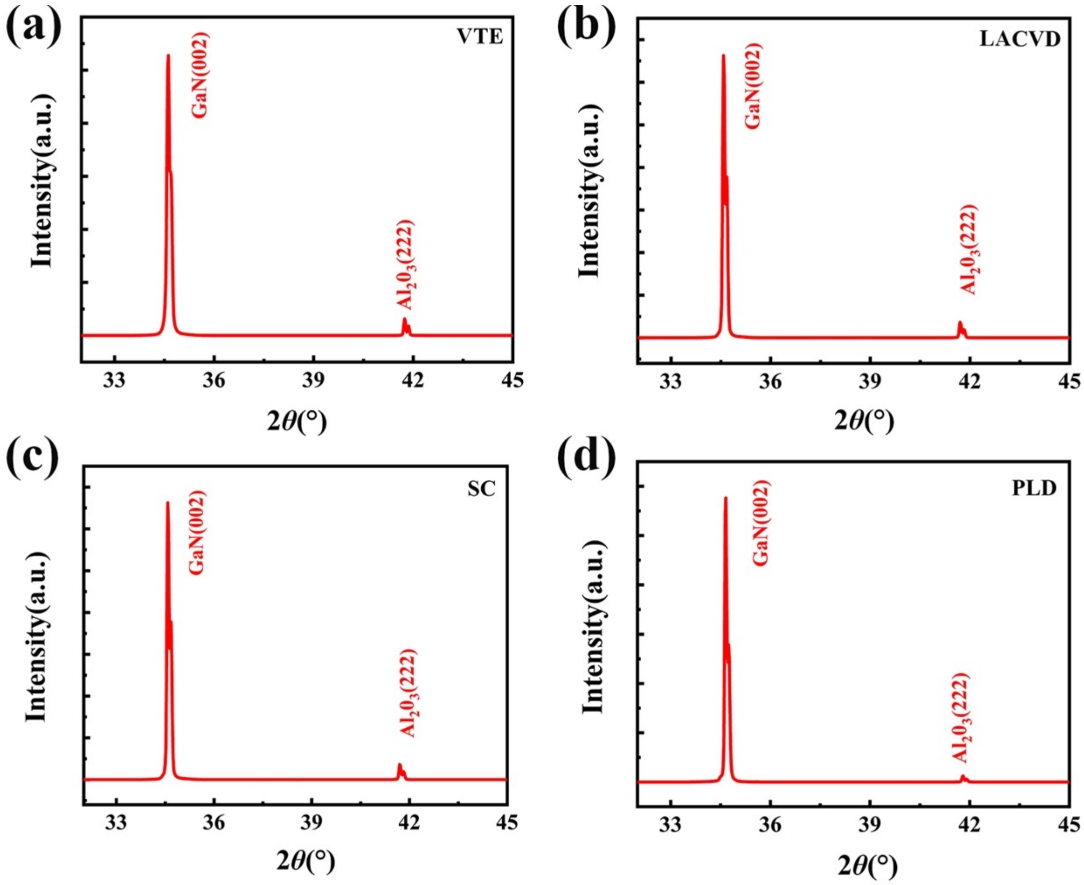

Fig. S3 XRD patterns of $CsCu_2I_3$/GaN (32°-45°).

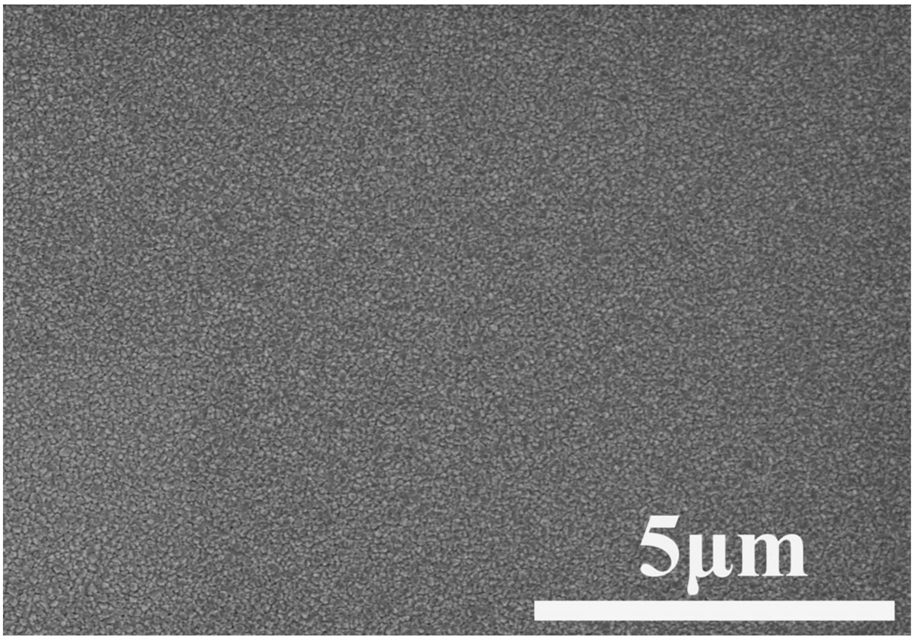

Fig. S4 SEM image of large-area films prepared by VTE.

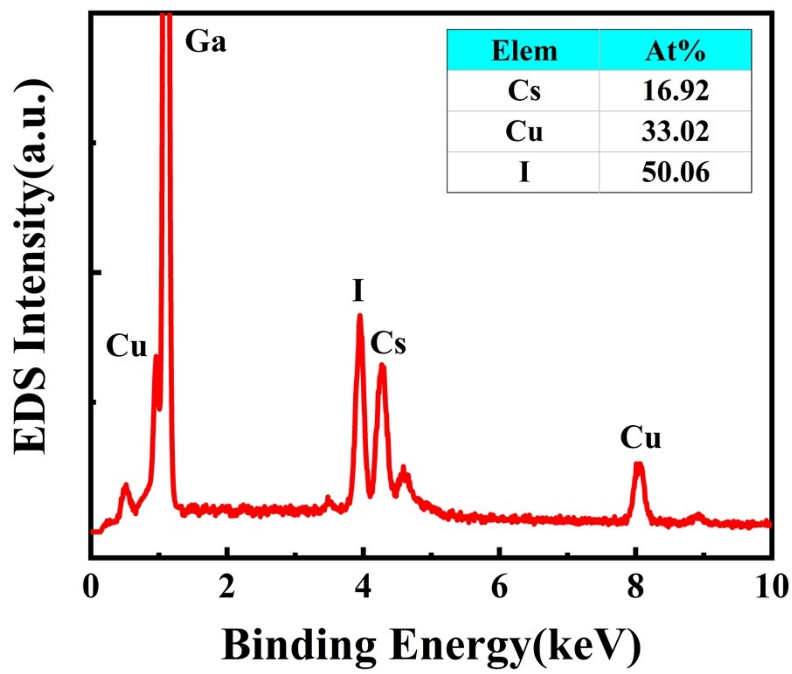

Fig. S5 EDS spectrum of $CsCu_2I_3$ film prepared by VTE.

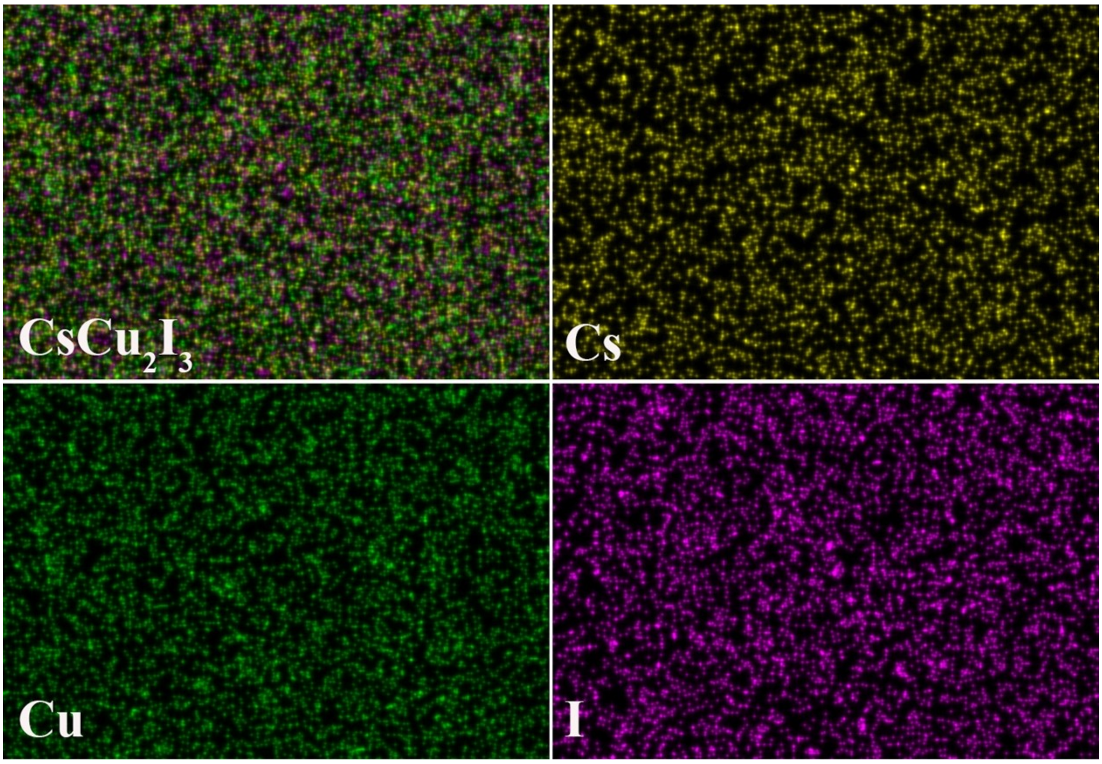

Fig. S6 Elemental mapping of $CsCu_2I_3$ film prepared by VTE.

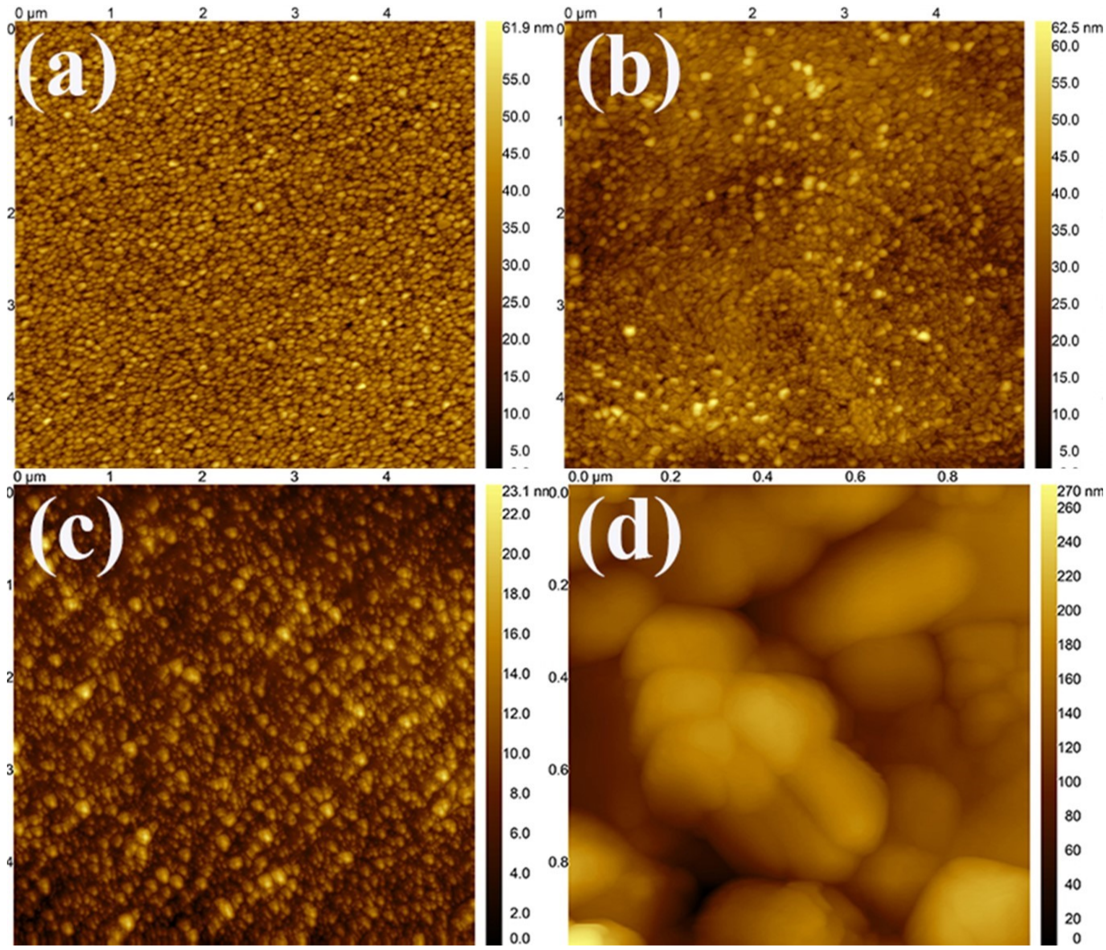

Fig. S7 AFM images of $CsCu_2I_3$ films prepared by PLD, VTE, LACVD and SC.

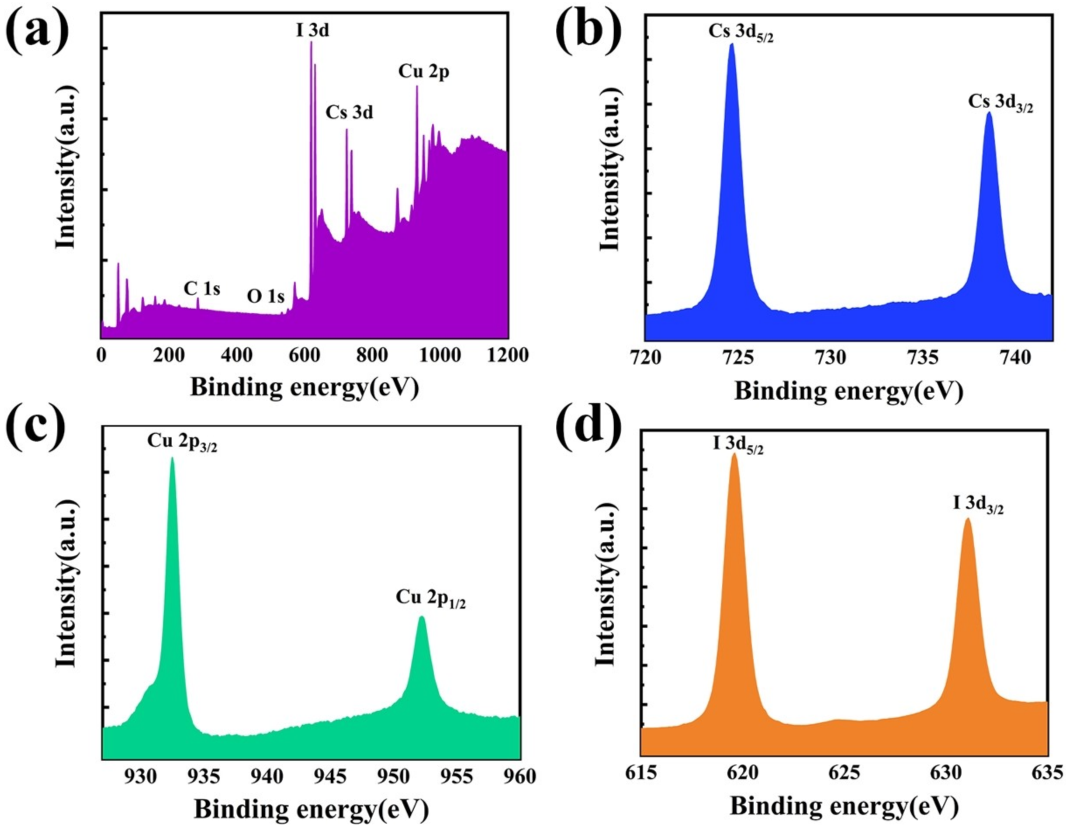

Fig. S8 XPS spectra of $CsCu_2I_3$ film prepared by VTE: (a) total spectrum, (b) Cs 3d (c) Cu 2p (d) I 3d.

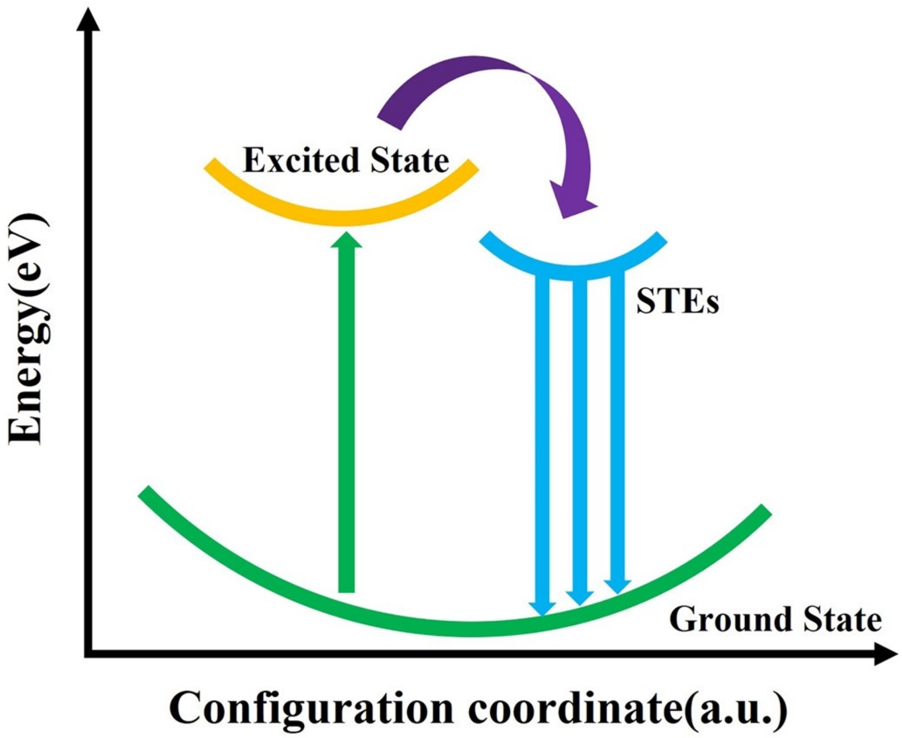

Fig. S9 Self-trapped exciton effect of $CsCu_2I_3$.

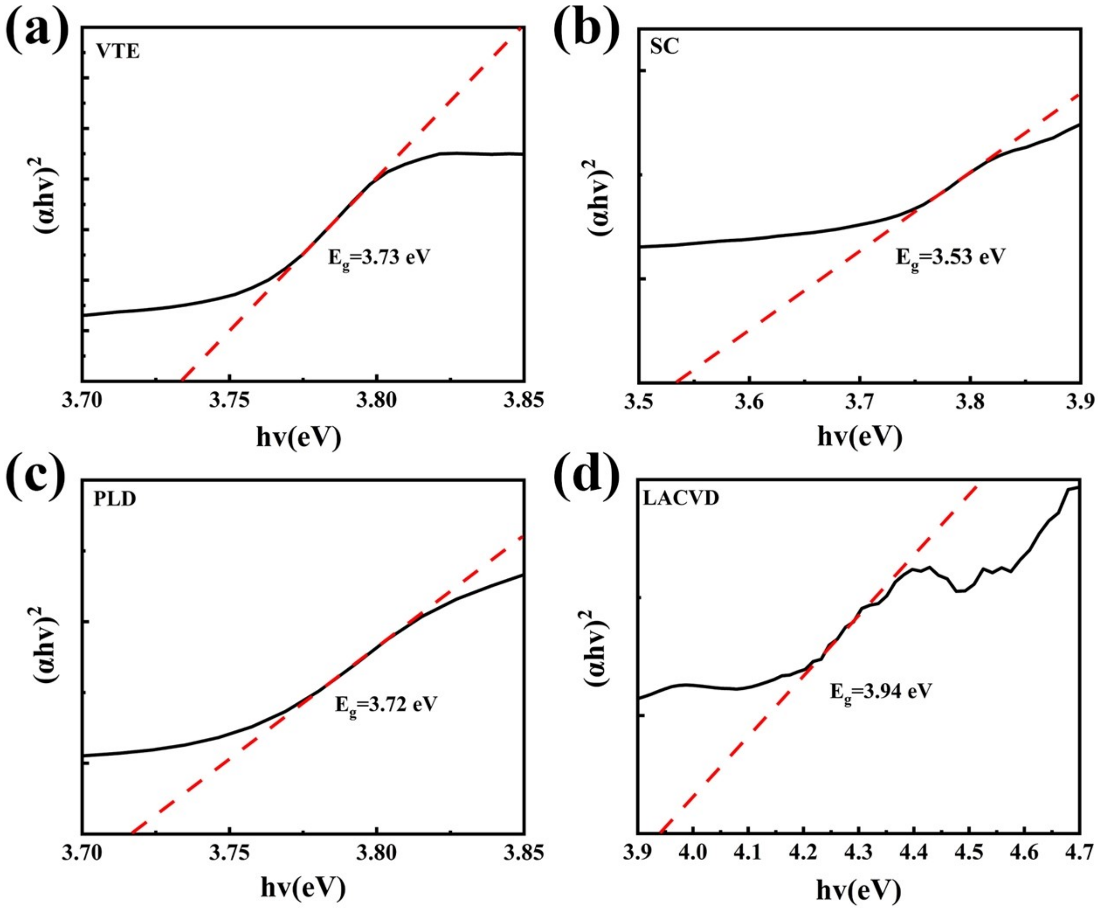

Fig. S10 Optical band gap of $CsCu_2I_3$ films prepared by PLD, VTE, LACVD and SC.

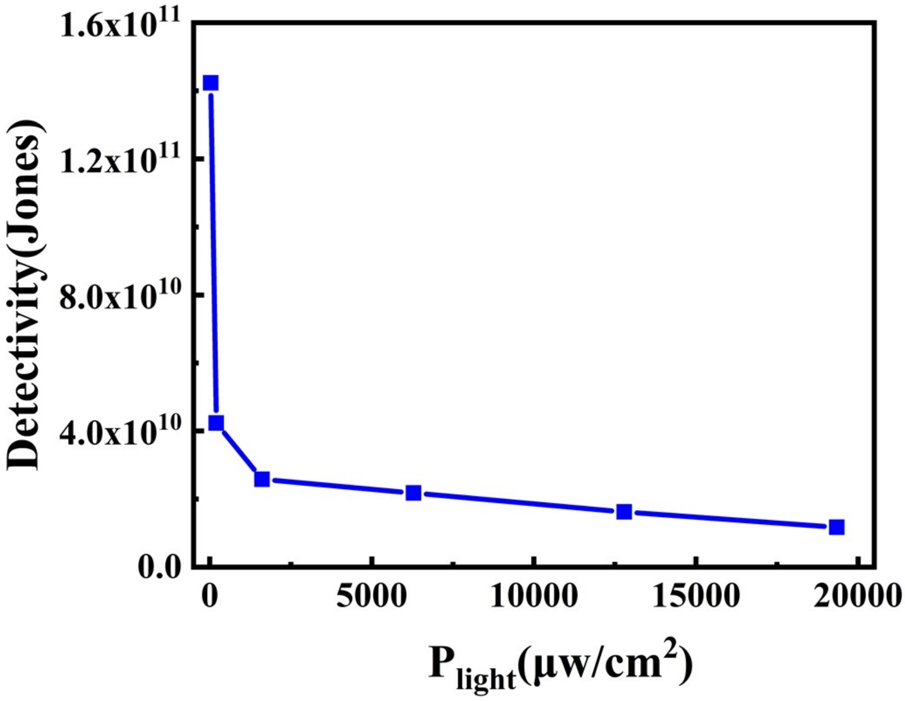

Fig. S11 Detectivity of photodetector under different light intensity prepared by VTE.

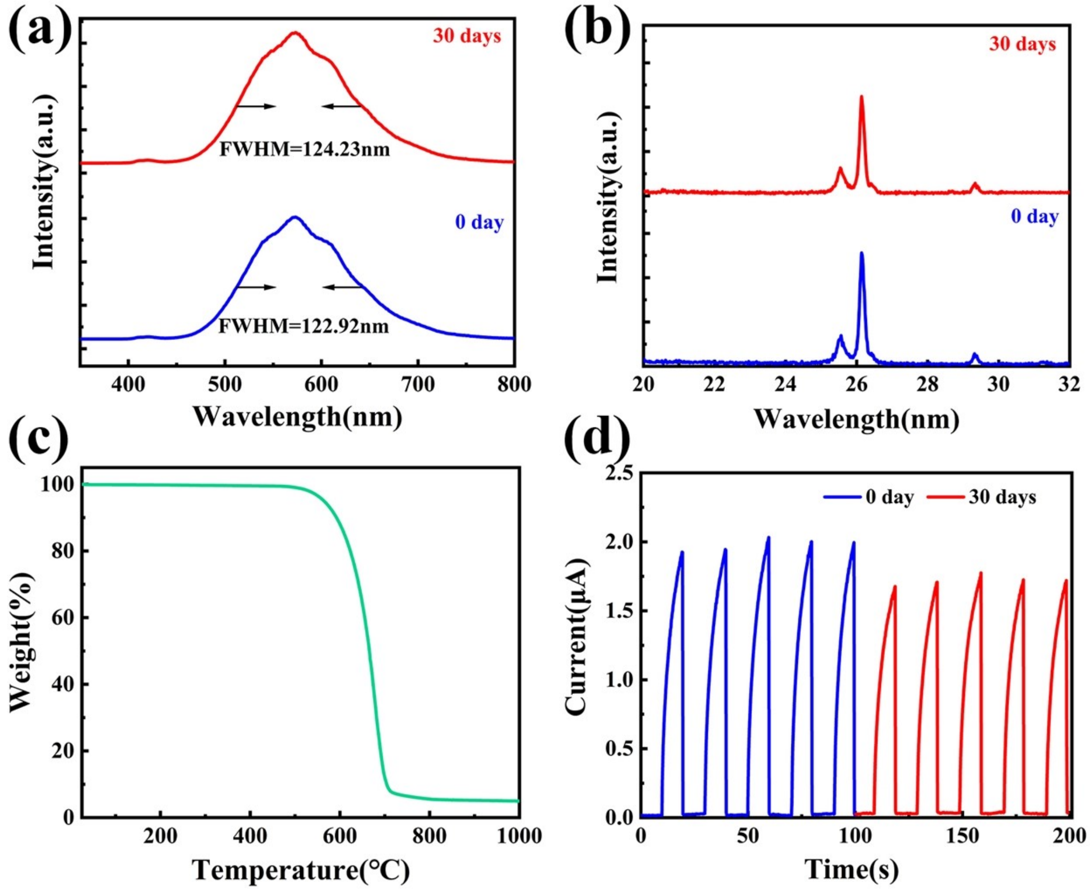

Fig. S12 (a) PL stability and (b) Structural stability of $CsCu_2I_3$ film for 30 days storage in air, (c) Thermal stability of $CsCu_2I_3$ film, (d) long-term storage stability of the $CsCu_2I_3$/GaN heterojunction photodetector.

Table S1. Preparation parameters for different methods.

Preparation Methods	Substrate	Substrate Temperature (°C)	Annealing Treatment (°C, min)	Laser Parameters (mJ, Hz)	Base Pressure (Pa)
PLD	n-GaN	200	—	200, 5	1×10^{-6}
VTE	n-GaN	200	—	—	3×10^{-4}
LACVD	n-GaN	200	—	200, 5	0
SC	n-GaN	—	200°C, 60	—	1×10^{5}

Table S2. Performance comparisons of perovskites ultraviolet photodetector.

Preparation Technology	Device Structure	Wavelength (nm)	R (A W^{-1})	D^* ($\times 10^{12}$ Jones)	Bias (V)	On/off ratio	Ref.
Antisolvent	Ni/$CsCu_2I_3$/Ni	340	—	—	-5	—	28
Antisolvent	Ag/$CsCu_2I_3$/Ag	350	0.052	0.093	3	188	29
VTE	Au/$CsCu_2I_3$	340	0.049	2.49	2	3150	32
PLD	$Cs_3Cu_2I_5$/n-Si	280	0.0708	0.944	-1.3	130	33
SC	$Cs_3Cu_2I_5$/n-Si	200-1200	0.13	3.1	0	~1×10^5	34
Solution	Au/$CsCu_2I_3$/Au	325	32.3	1.89	5	2600	35
Antisolvent	Au/$CsCu_2I_3$/Au	265	22.1	0.12	3	22	38
Antisolvent	$CsCu_2I_3$	365	0.27	6.38×10^{-4}	2	—	39
Antisolvent	Ga_2O_3/$CsCu_2I_3$	254	0.02	1×10^{-5}	0	1×10^5	40
SC	$Cs_3Cu_2I_5$/Au	200-325	17.8	1.12	5	—	41
SC	GaN-$Cs_3Cu_2I_5$	300-370	0.28	1.4	-6	1.2×10^5	42
Antisolvent	$Cs_3Cu_2I_5$/ITO	265	0.0649	0.69	0	142	43
SC	$Cs_3Cu_2I_5$/n-Si	200-1200	0.0836	2.1	0	3720	44
VTE	Ga_2O_3/$Cs_3Cu_2I_5$	248	—	2.4×10^{-4}	0	5.1×10^4	45
PLD	$CsCu_2I_3$/n-Si	330	0.0071	0.26	0	2150	46
VTE	$CsCu_2I_3$/$Ca_2Nb_{3-x}Ta_xO_{10}$	250	81.3	—	-5	—	47
Antisolvent	$CsCu_2I_3$/CuI	350	0.253	0.31	3	280	48
SC	$CsCu_2I_3$/GaN	300-350	0.37	18.3	0	325	49

Preparation Technology	Device Structure	Wavelength (nm)	R (A W^{-1})	D^* ($\times 10^{12}$ Jones)	Bias (V)	On/off ratio	Ref.
VTE	$CsCu_2I_3$/GaN	330-360	0.042	0.142	0	640	This work
PLD	$CsCu_2I_3$/GaN	330-360	0.0064	0.0548	0	1.3	
LACVD	$CsCu_2I_3$/GaN	330-360	0.012	0.0497	0	1	
SC	$CsCu_2I_3$/GaN	330-360	0.014	0.0591	0	61	

Table S3. Hall parameters of $CsCu_2I_3$ and GaN.

Material	Conduction Type	Carrier Concentration (cm^{-3})	Mobility ($cm^2\ Vs^{-1}$)
GaN	n	1.01×10^{18}	200
$CsCu_2I_3$	p	7.87×10^{14}	9