## The growth of Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub> and CsCu<sub>2</sub>Br<sub>3</sub> single crystals by

## cooling crystallization for scintillator application

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## **Supporting Information**

Fig. S1 Tyndall effect in solution



Fig. S2 XPS analysis of (a) Cs 3d, (b) Cu 2p, and (c) Br 3d of  $Cs_3Cu_2Br_5$  crystal powder.



Fig. S3 TG and DTG curves of Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5.</sub>

	Preparation method	Crystal picture	Excitation (nm)	Emission (FWHM) (nm)	TRPL (us)	Light yield (photon·MeV <sup>-1</sup> )	Energy resolution	Afterglow	Reference
Cs <sub>3</sub> Cu <sub>2</sub> Br <sub>5</sub>	AVC		298	458(80)	15.77	/	/	/	1
	EC	C.	301	464(78)	20.03	/	/	/	2
	VB		311	453(69)	13.6	4000	/	Comparable to BGO	3
	LTC		310	456(83)	15.6	6384	17.50%	6%@10ms	Our work
CsCu <sub>2</sub> Br <sub>3</sub>	LTC		266	580(68)	/	5800	/	0.07 %@3ms	Our work

Table S1 Current research on  $Cs_3Cu_2Br_5$  single crystals

Cooling crystallization method: LTC; Evaporation crystallization method: EC; Bridgman method: VB; Antisolvent method: AVC

	Sample state	Excitation (nm)	Emission (FWHM) (nm)	TRPL (us)	E <sub>b</sub> (meV)	PLQY(%)	Reference
		300	460(78)	16.88	/	27.38	4
		298	460(83)	/	630	23	5
	powder	298	455(75)	/	400	50.1	6
	-	290	461(82)	29	720	17.3	7
Cs <sub>3</sub> Cu <sub>2</sub> Br <sub>5</sub>		290	451(93)	/	/	/	8
	-	290	458(79)	21.69	/	11.6	9
	nanocrystals	268	459(85)	18.4	/	6.3	10
	-	290	451(93)	/	/	/	11
	film	270	463	/	/	/	12
CsCu <sub>2</sub> Br <sub>3</sub>	polycrystalline ingots	325	533(106)	0.018	155	18.3	13

Table S2 the reported research work on Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub> and CsCu<sub>2</sub>Br<sub>3</sub> (non-single crystal)

## References

- 1 X. Zheng, J. Huang, Y. Liu, T. Wang, S. Han, Z. Wang, B. Teng and S. Ji, *Adv. Photonics Res.*, 2022, **3**(4), 2100289.
- 2 D. Liang, L. Tan, S. Lu, Z. Sun, H. Wang, W. Cai and Z. Zang, ACS Appl. Mater. Inter., 2023, 15, 24622-24628.
- 3 Q. Wang, J. Kang, S. Cheng, G.Ren, X. Zhu and Y. Wu, J. Synth. Cryst., 2021, 50, 1919-1924.
- 4 Y. Zhou, Z. Wang, G. Pan, M. Xu, C. Wang, Y. Chen, X. Yang, Z. Xu, J. Zhao, Q. Li and H Feng, *Cryst. Growth Des.*, 2023, **23**, 8024-8033.
- 5 X. Huang, S. Wang, B. Devakumar and N. Ma, Mater. Today Chem., 2022, 23, 100678.
- 6 R. Roccanova, A. Yangui, H. Nhalil, H. Shi, M. Du and B. Saparov, ACS Appl. Electron. Mater., 2019, 1(3), 269-274.
- 7 L. Lian, M. Zheng, P. Zhang, Z. Zheng, K. Du, W. Lei, J. Gao, G. Niu, D. Zhang, T. Zhai, S. Jin, J. Tang,
  X. Zhang and J. Zhang, *Chem. Mater.*, 2020, **32**(8), 3462-3468.
- 8 T. Le, M. Kim, H. Lee, J. Lee, C. Kim, W. Nie and H. Yoon, Chem. Eng. J., 2023, 467, 143523.
- 9 Y. Zhou, S. Wu, G. Huang, J. Zeng, B. Meteku, X. Tan, H. Lu, F. Li, Z. Cai, X. Wang and M. Zhang, J. Alloys Compd., 2022, 918, 165565.
- 10 M. Ng, P. Geng, S. Shivarudraiah, L. Guo and J. Halpert, Adv. Opt. Mater., 2022, 10(21), 2201031.
- 11 T. Le, S. Lee, H. Jo, M. Kim, J. Lee, M. Chang and H. Yoon, ACS Appl. Nano Mater., 2021, 4(8), 7621-7627.
- 12 S. He, L. Zhang, D. Tian, Z. Zhou, A. Guo, B. Xia, Y. Zhu and F. Zhao, J. Alloys Compd., 2023, 937, 168538.
- 13 R. Roccanova, A. Yangui, H. Nhalil, H. Shi, M. Du and B. Saparov, ACS Appl. Electron. Mater., 2019, 1(3), 269-274.