

Uniform nucleation and growth of $\text{Cs}_3\text{Cu}_2\text{I}_5$ nanocrystals with high luminous efficiency and structured stability and their application in white light-emitting diodes

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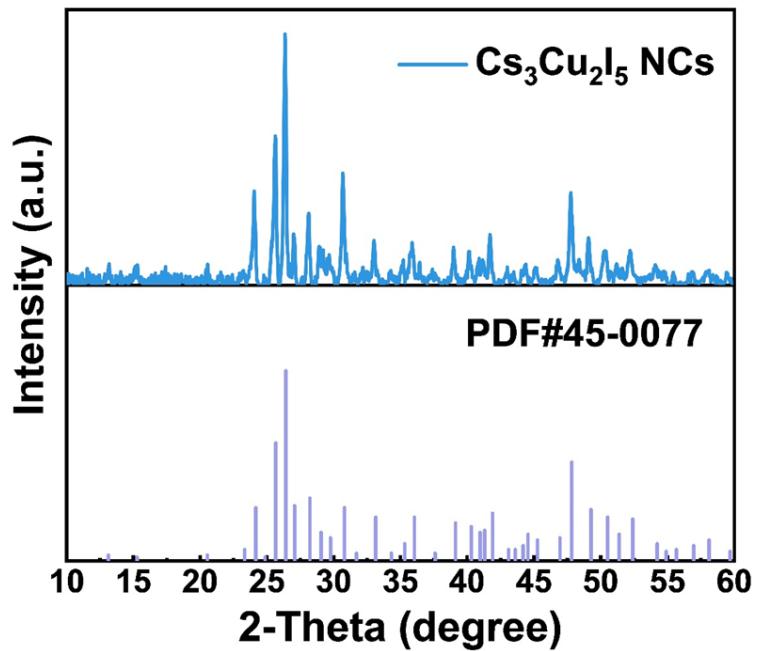


Figure S1. XRD of Cs₃Cu₂I₅ NCs and standard PDF card of Cs₃Cu₂I₅.

Table S1. Summary of elemental contents of Cs, Cu, and I in Cs₃Cu₂I₅ NCs.

Element	Cs	Cu	I
Weight (%)	29.66	24.28	46.06

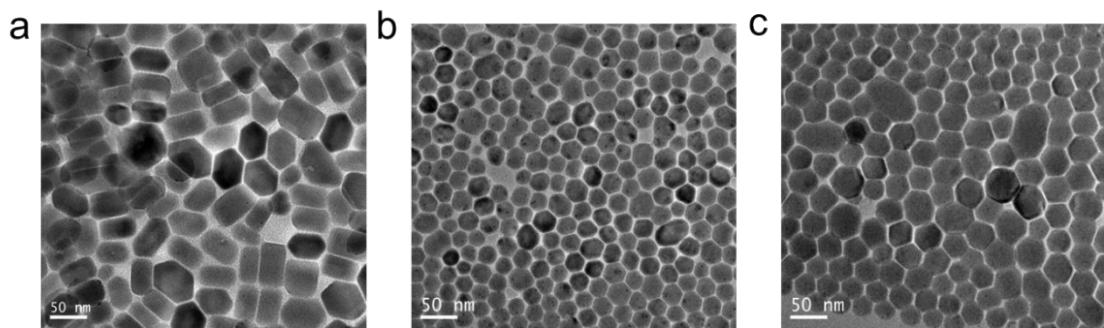


Figure S2. TEM images of Cs₃Cu₂I₅ NCs prepared by high-energy ultrasound method
for (a) 1 min, (b) 2 min and (c) 5 min.

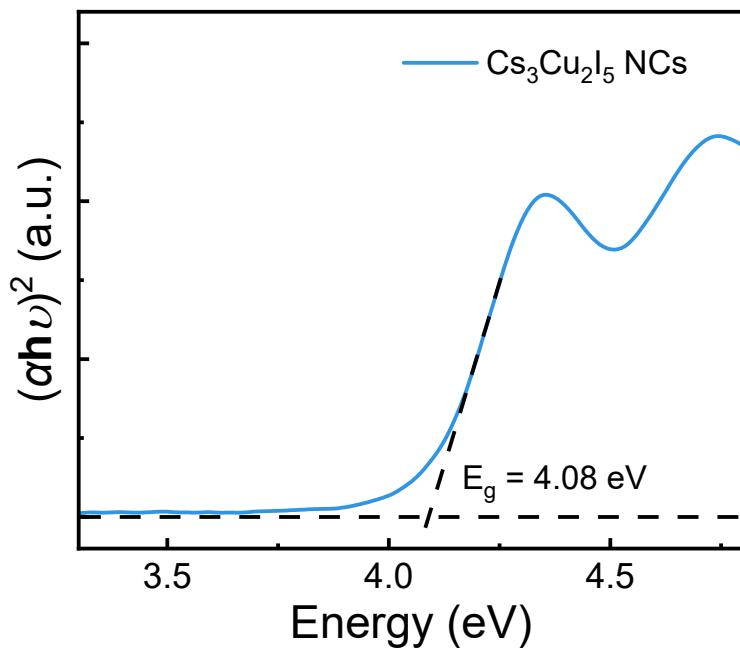


Figure S3. Tauc plot of the $\text{Cs}_3\text{Cu}_2\text{I}_5$ NCs.

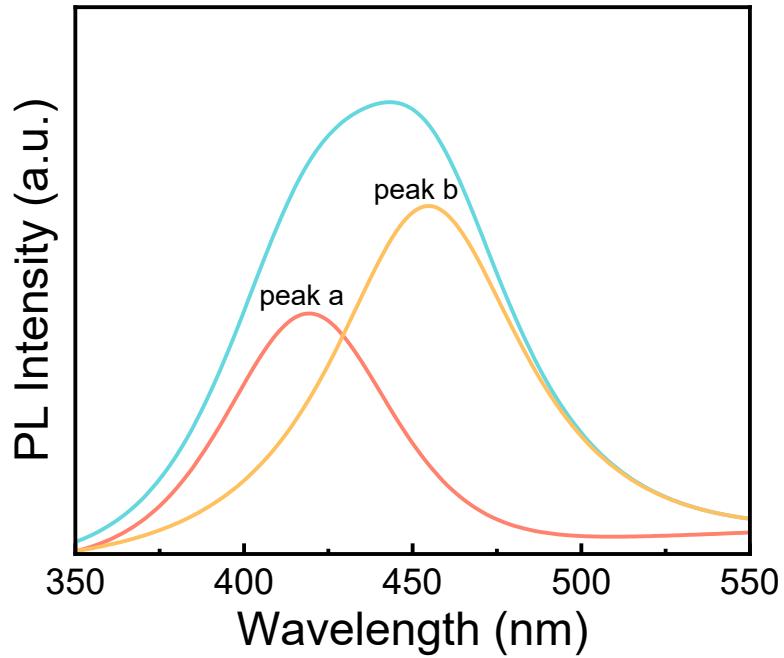


Figure S4. The PL spectra and the fitting results of $\text{Cs}_3\text{Cu}_2\text{I}_5$ NCs.

Table S2. Summary of fitting data of PL decay curve.

Samples	τ_1 (ns)	A ₁ (%)	τ_2 (ns)	A ₂ (%)	τ_{avg} (ns)
Cs ₃ Cu ₂ I ₅ -NCs	124	0.16	1072	0.84	1051

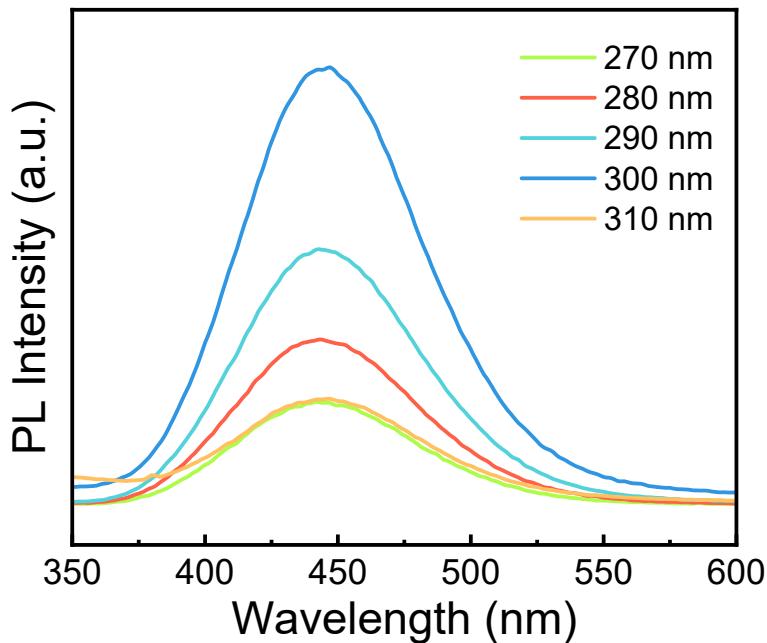


Figure S5. PL spectra of Cs₃Cu₂I₅ NCs under different excitation wavelengths from 270 to 310 nm.

Table S3. Summary of the properties Cs₃Cu₂I₅ NCs in literatures.

NCs	PL peak (nm)	PLQY (%)	Ref
Cs ₃ Cu ₂ I ₅	445	73.7	1
Cs ₃ Cu ₂ I ₅	445	72.6	2
Cs ₃ Cu ₂ I ₅	445	78.42	3
Cs ₃ Cu ₂ I ₅	447	72.4	4
Cs ₃ Cu ₂ I ₅	445	59	5
Cs ₃ Cu ₂ I ₅	445	39.8	6

$\text{Cs}_3\text{Cu}_2\text{I}_5$	395	10	7
$\text{Cs}_3\text{Cu}_2\text{I}_5$	441	85	Our work

References

1. L. Lian, M. Zheng, W. Zhang, L. Yin, *Adv. Sci.*, 2020, **7**, 2000195.
2. X. Hu, Y. Li, Y. Wu, W. Chen, H. Zeng, and X. Li, *Mater. Chem. Front.*, 2021, **5**, 6152–6159
3. X. Hu, P. Yan, P. Ran, L. Lu, *J. Phys. Chem. Lett.*, 2022, **13**, 2862–2870.
4. C. Li, S. Cho, D. Kim, and I. Park, *Chem. Mater.*, 2022, **34**, **15**, 6921–6932.
5. J. Zhou, K. An, P. He, J. Yang, et al, *Adv. Optical Mater.*, 2021, **9**, 2002144.
6. F. Zhang, W. Liang, L. Wang, Z. Ma, et al, *Adv. Funct. Mater.*, 2021, **31**, 2105771.
7. A. L. M. Freitas, A. Tofanello, F. P. Sabino, et al, *ACS Appl. Nano Mater.*, 2023, **6**, 7196–7205.

Table S4. Summary of the lead-free device performances of the prepared WLEDs.

Emitter	CRI	CCT (K)	LE (lm/W)	Ref
$(\text{CH}_6\text{N}_3)_2\text{MnCl}_4$	93.7	3984	90.41	1
$(\text{NH}_4)_2\text{Sn}_{1-x}\text{Te}_x\text{Cl}_6$	83	3855	—	2
$\text{Cs}_2\text{AgIn}_{0.9}\text{Bi}_{0.1}\text{Cl}_6$	94.5	6432	—	3
$(\text{C}_{13}\text{H}_{30}\text{N})_2\text{SnCl}_6$	96.7	—	—	4
Cs_2SnCl_6 : $\text{Bi}^{3+}/\text{Te}^{4+}$	94	6386-3668	—	5
Cs_2TeCl_6 : Cr^{3+}	81.3	5826	—	6
$\text{Cs}_2\text{Zr}_{1-x}\text{Te}_x\text{Cl}_6$	74.8	4959	91.16	7
$\text{OTA}_{2+x}\text{SnI}_{4+x}$	92	2654	—	8
CsCu_2I_3	83	6718	—	9

$\text{Cs}_2\text{NaInCl}_6:\text{Sb}^{3+}/\text{Sm}^{3+}/\text{Eu}^{3+}/\text{Tb}^{3+}/\text{Dy}^{3+}$	80	8035	37.5	10
$(\text{OCTAm})_2\text{SnBr}_4$	89	6530	—	11
$(\text{Cs}_4\text{N}_2\text{H}_{14}\text{Br})_4\text{SnBr}_x\text{I}_{6-x}$	84	5632	32.2	12
$(\text{C}_4\text{N}_2\text{H}_{14}\text{Br})_4\text{SnBr}_6$	70	4946	—	13
$\text{Cs}_3\text{Cu}_2\text{I}_5/\text{CsCu}_2\text{I}_3$	89.5	5877	54.6	14
$\text{Cs}_3\text{Cu}_2\text{I}_5$	95.3	5489	41.5	This work

References

1. S. Wang, X. Han, T. Kou, et al, *J. Mater. Chem. C.*, 2021, **9**, 4895-4902.
2. Z. Li, C. Zhang, B. Li, C. Lin, Y. Li, L. Wang, R. Xie, *Chemical Engineering Journal.*, 2021, **420**, 129740.
3. Y. Zhang, Z. Zhang, W. Yu, et al, *Adv. Sci.*, 2022, **9**, 2102895.
4. W. Lin, Q. Wei, T. Huang, et al, *J. Mater. Chem. C*, 2023, Advance Article.
5. Z. Liu, X. Ji, Z. Ma, *Laser Photonics Rev.*, 2023, 2300094.
6. L. Zi, W. Xu, Z. Song, R. Sun, *J. Mater. Chem. C.*, 2023, **11**, 2695-2702.
7. Z. Li, Z. Rao, Q. Li, L. Zhou, X. Zhao, X. Gong, *Adv. Optical Mater.*, 2021, **9**, 2100804.
8. Z. Li, Z. Deng, A. Johnston, *Adv. Funct. Mater.*, 2022, **32**, 2111346.
9. W. Liu, K. W. Ng, H. Lin, Z. Dai, *J. Phys. Chem. C.*, 2021, **125**, 13076–13083.
10. X. Li, D. Wang, Y. Zhong, F. Jiang, *Adv. Sci.*, 2023, 2207571.
11. J. Sun, J. Yang, J. I. Lee, J. H. Cho, and M. S. Kang, *J. Phys. Chem. Lett.*, 2018, **9**, 1573–1583.
12. C. Zhou, Y. Tian, Z. Yuan, et al, *ACS Appl. Mater. Interfaces.*, 2017, **9**, 44579–44583.
13. C. Zhou, H. Lin, Y. Tian, Z. Yuan, *Chem. Sci.*, 2018, **9**, 586-593.
14. L. Wang, Z. Ma, F. Zhang, et al, *J. Mater. Chem. C.*, 2021, **9**, 6151-6159.