Supporting Information for

Lead-Free Bright Blue Light-Emitting Cesium Halide Nanocrystals by Zinc Doping

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Materials category	Materials example	PLQY (%)	Emission peak (nm)	CIE	Ref.
Perovskite QDs	$CsPb(Br_{1-x}Cl_x)_3$	80	455	(0.20, 0.04)	1
Carbon QDs	Blue carbon dots	80	433	(0.15, 0.05)	2
Cd-based QDs	CdSe/ZnS	73	475	(0.12, 0.15)	3
Zn based halide NCs	$Cs_2ZnCl_4:Cu^+$	55	477	-	4
Zn based halide NCs	Cs ₂ ZnBr ₄ :Cu ⁺	65	465	-	5
Zn doped halide NCs	CsBr:Zn	79	415 & 438	(0.20, 0.16)	This work
Zn doped halide NCs	CsI:Zn	79	415 & 440	-	This work
Ni doped halide QDs	$CsPb_{0.88}Ni_{0.12}Cl_3$	97	405	-	6
Cu based halide NCs	Cs ₃ Cu ₂ I ₅	67	441	-	7
Sn ⁴⁺ based halide NCs	$Cs_2Sn_{0.97}Bi_{0.03}I_6$	79	455	-	8
Eu doped halide NCs	CsBr:Eu	33	440	-	9
AgBi based halide NCs	Cs ₂ AgBiCl ₆	6.7	395	-	10

Table S1. Properties comparison of differrent blue luminescent materials.



Figure S1. (a) HRTEM image of CsBr:Zn NCs. (b) Calculation of the lattice distance of CsBr:Zn NCs. (c) FFT image of CsBr:Zn NCs.



Figure S2. (a) XPS analysis of CsBr:Zn NCs and the high-resolution spectra of (b) Zn 2*p*, (c) Cs 3*d* and (d) Br 3*d*.



Figure S3. UV-visible absorption spectra of CsBr:Zn NCs. Two weak bands at 381 nm and 404 nm can be seen in the inset.



Figure S4. The PLQY spectra of CsBr:Zn NCs. The reference curve is measured by placing a blank quartz in an integrating sphere.



Figure S5. (a) PL excitation (PLE) spectra of CsBr:Zn NCs for different emission. (b) PL spectra of CsBr:Zn NCs under different excitation wavelength.



Figure S6. Schematic of the photophysical process in CsBr:Zn NCs. Zn doping introduces the intermediate trap states in the original energy level of CsBr to change CsBr into the blue-emitting material. The broad PL spectra and multi peaks of CsBr:Zn NCs can be explained by the multiple intermediate trap states.



Figure S7. PL intensity versus excitation power for CsBr:Zn NCs.



Figure S8. Temperature dependent PL spectra of CsBr:Zn NCs (80-300 K).



Figure S9. XRD patterns of as-prepared CsBr:Zn NCs over stored time.

	0 Day	10 Day	30 Day	45 Day	60 Day
Size (nm)	16.5	18.4	24.8	29.9	49.8
Strain (%)	0.115	0.017	0.010	0.011	0.040

Table S2. Caculation of the size and strain of CsBr:Zn NCs from XRD patterns of different stored days.



Figure S10. Time-resolved PL decay spectra of CsBr:Zn NCs (a) at different temperatures and (b) for different stored days.



Figure S11. Photographs of CsBr:Zn NCs solution after stored for 30 days (left) and 60 days (right) (a) without UV light excitation, (b) with UV light (365 nm) excitation in normal environment, and (c) with UV light (365 nm) excitation in dark environment.



Figure S12. TGA measurement of CsBr:Zn NCs.



Figure S13. The PLQY spectra of CsI:Zn NCs. The reference curve is measured by placing a blank quartz in an integrating sphere.



Figure S14. Elemental characterization of CsI:Zn NCs. (a) SEM image of CsI:Zn NCs. (b) EDS mapping of CsI:Zn NCs. (c-e) Corresponding elemental mapping of Cs, I, and Zn in CsI:Zn NCs. Scale bars are 1 μ m for a-b and 500 nm for c-e.



Figure S15. (a) XPS analysis of CsI:Zn NCs and the high-resolution spectra of (b) Zn 2*p*, (c) Cs 3*d* and (d) I 3*d*.



Figure S16. (a) PLE and PL spectra of CsI:Zn NCs. (b) Time-resolved PL decay and fitting curve of CsI:Zn NCs.



Figure S17. PLQY values of CsI:Zn NCs over storage time at ambient condition.



Figure S18. Photographs of the blue LED fabricated by combining CsBr:Zn NCs with a UV light chip under different operating currents.

References

- [1] S. Hou, M. K. Gangishetty, Q. Quan and D. N. Congreve, *Joule*, 2018, **2**, 2421-2433.
- F. Yuan, Y.-K. Wang, G. Sharma, Y. Dong, X. Zheng, P. Li, A. Johnston, G. Bappi, J. Z. Fan, H. Kung,
 B. Chen, M. I. Saidaminov, K. Singh, O. Voznyy, O. M. Bakr, Z.-H. Lu and E. H. Sargent, *Nature Photonics*, 2019, 14, 171-176.
- [3] H. Shen, Q. Gao, Y. Zhang, Y. Lin, Q. Lin, Z. Li, L. Chen, Z. Zeng, X. Li, Y. Jia, S. Wang, Z. Du, L. S. Li and Z. Zhang, *Nature Photonics*, 2019, **13**, 192-197.
- [4] D. Zhu, M. L. Zaffalon, V. Pinchetti, R. Brescia, F. Moro, M. Fasoli, M. Fanciulli, A. Tang, I. Infante,
 L. De Trizio, S. Brovelli and L. Manna, *Chemistry of Materials*, 2020, **32**, 5897-5903.
- [5] P. Cheng, L. Feng, Y. Liu, D. Zheng, Y. Sang, W. Zhao, Y. Yang, S. Yang, G. Wang and K. Han, Angew Chem Int Ed Engl, 2020, 132, 1-6.
- [6] Z. J. Yong, S. Q. Guo, J. P. Ma, J. Y. Zhang, Z. Y. Li, Y. M. Chen, B. B. Zhang, Y. Zhou, J. Shu, J. L. Gu, L. R. Zheng, O. M. Bakr and H. T. Sun, *J Am Chem Soc*, 2018, **140**, 9942-9951.
- [7] P. Cheng, L. Sun, L. Feng, S. Yang, Y. Yang, D. Zheng, Y. Zhao, Y. Sang, R. Zhang, D. Wei, W. Deng and K. Han, Angew Chem Int Ed Engl, 2019, 58, 16087-16091.
- [8] Z. Tan, J. Li, C. Zhang, Z. Li, Q. Hu, Z. Xiao, T. Kamiya, H. Hosono, G. Niu, E. Lifshitz, Y. Cheng and J. Tang, Advanced Functional Materials, 2018, 28, 1801131.
- [9] Z. Yang, Z. Jiang, X. Liu, X. Zhou, J. Zhang and W. Li, *Advanced Optical Materials*, 2019, **7**, 1900108.
- [10] B. Yang, J. Chen, S. Yang, F. Hong, L. Sun, P. Han, T. Pullerits, W. Deng and K. Han, Angew Chem Int Ed Engl, 2018, 57, 5359-5363.