

Supplementary information

Co-Doping of Tellurium with Bismuth Enhances Stability and Photoluminescence Quantum Yield of $\text{Cs}_2\text{AgInCl}_6$ Double Perovskite Nanocrystals

Shixun Wang,^{‡ a} Ran Shi,^{‡ b} Bing Tang,^a Yuan Xiong,^a Arsenii Portniagin,^a Xin Zhao,^a Stephen V. Kershaw,^a Run Long,^{*b} and Andrey L. Rogach^{*a}

* Corresponding authors

^a Department of Materials Science and Engineering, and Centre for Functional Photonics (CFP), City University of Hong Kong, 83 Tat Chee Avenue, Hong Kong S.A.R. 999077, P. R. China

Email: andrey.rogach@cityu.edu.hk

^b College of Chemistry, Key Laboratory of Theoretical & Computational Photochemistry of Ministry of Education, Beijing Normal University, Beijing, 100875 PR China

Email: runlong@bnu.edu.cn

‡ These two authors contributed equally to this research

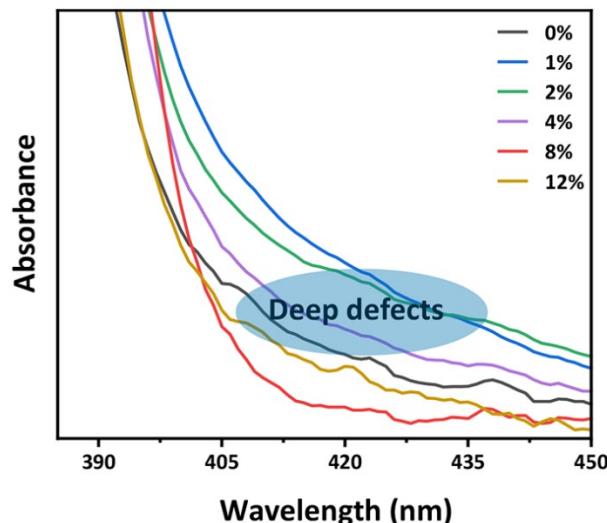


Figure S1. Absorption spectra (enlarged tail region) of $\text{Cs}_2\text{AgInCl}_6$:0% Te, 1% Bi and Te/Bi-co-doped ($\text{Cs}_2\text{AgInCl}_6$:x% Te, 1% Bi) NCs

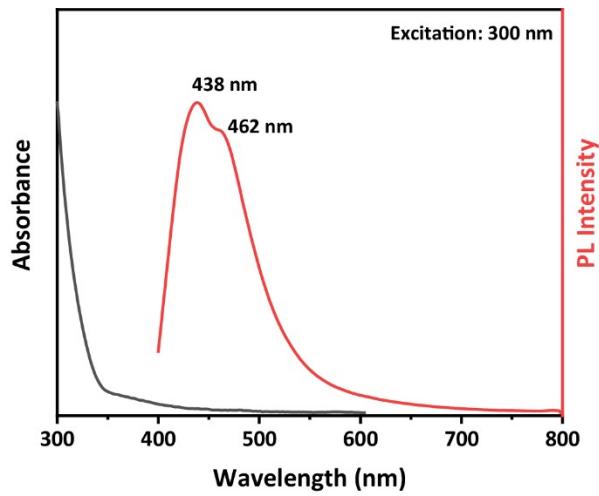


Figure S2. Absorption and PL spectra of $\text{Cs}_2\text{AgInCl}_6$ NCs solely doped by 8% tellurium precursors (without any Bi co-dopant).

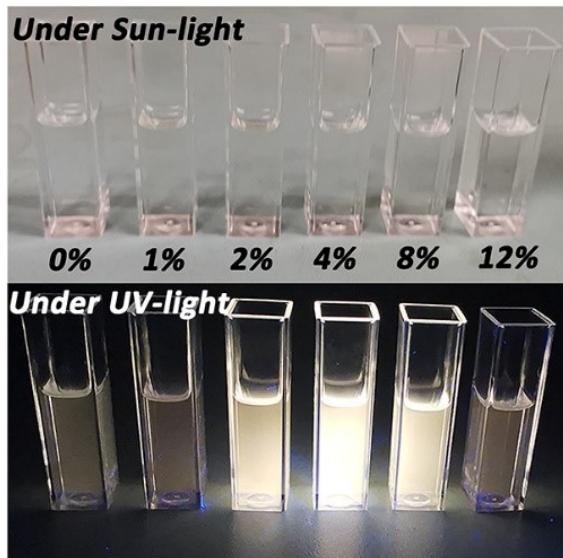


Figure S3. Photographs of $\text{Cs}_2\text{AgInCl}_6:\text{x}\%$ Te, 1% Bi NCs ($\text{x}=0, 1, 2, 4, 8$, and 12) under sun-light and UV-light. Note that in the bottom row the camera lens was focusing on the middle sample ($\text{Cs}_2\text{AgInCl}_6:4\%$ Te, 1% Bi NCs), otherwise the emission of samples with low PL QYs could hardly be observed.

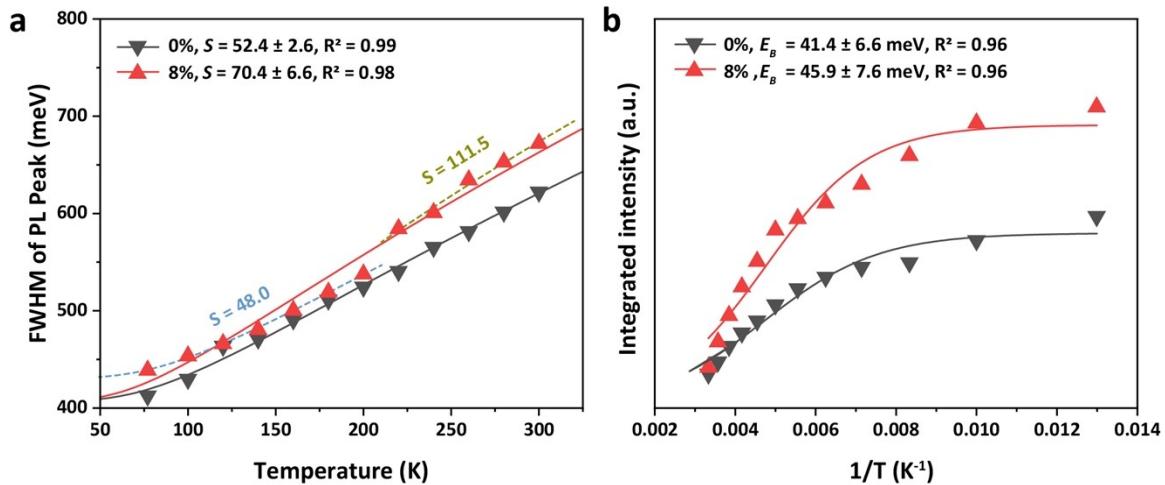


Figure S4. (a) Thermal evolution of the PL FWHM and (b) temperature-dependent integrated PL intensity of $\text{Cs}_2\text{AgInCl}_6$:0% Te, 1% Bi and $\text{Cs}_2\text{AgInCl}_6$:8% Te, 1% Bi NCs.

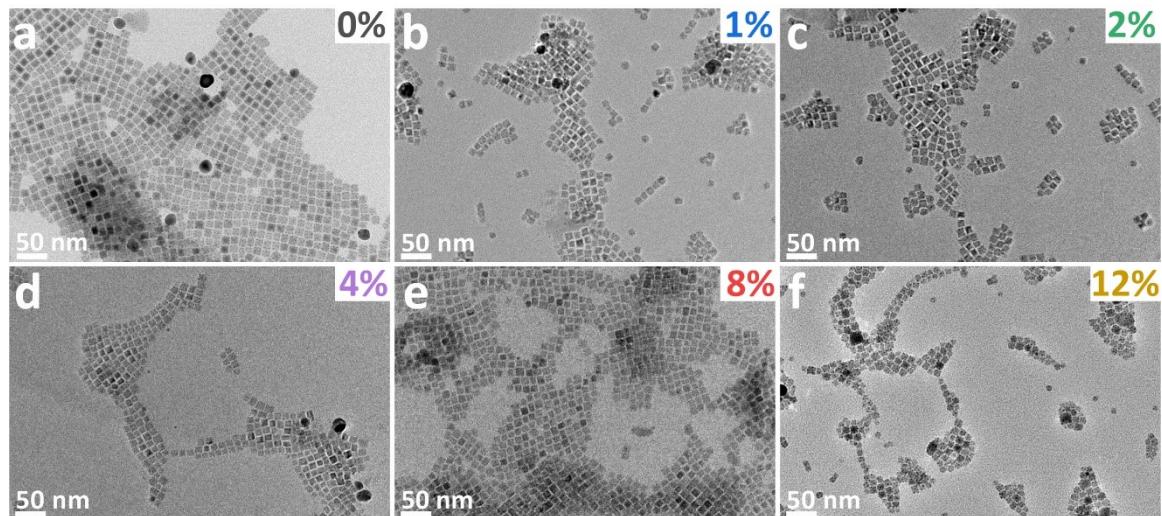


Figure S5. Wide-view TEM images of $\text{Cs}_2\text{AgInCl}_6$:x% Te, 1% Bi NCs (x=0, 1, 2, 4, 8, 12).

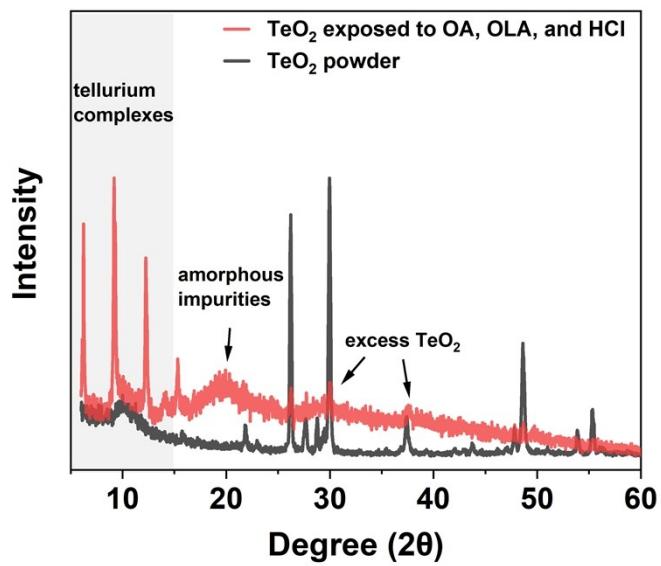


Figure S6. XRD pattern of TeO_2 precursor in the original form and exposed to OA, OLA, and hydrogen chloride. Emerging diffraction peaks below 15° could belong to tellurium complexes such as R_2TeO and/or $\text{Te}_2\text{O}_3\text{Cl}_2$.

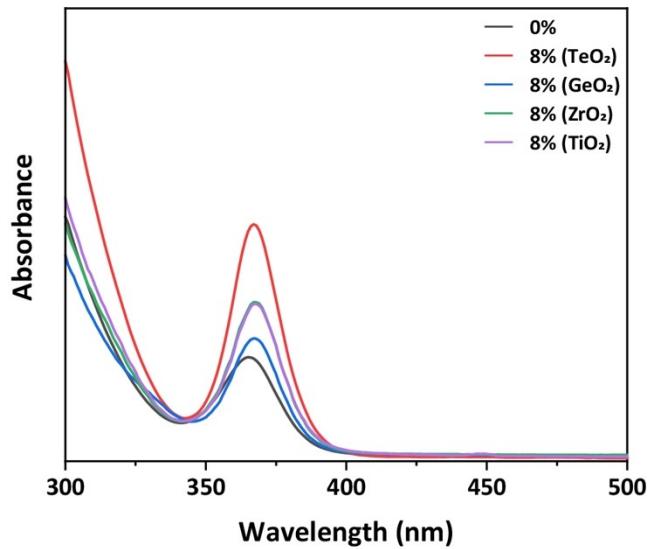


Figure S7. Absorption spectra of $\text{Cs}_2\text{AgInCl}_6$:0% Te, 1% Bi NCs, $\text{Cs}_2\text{AgInCl}_6$:8% Te, 1% Bi NCs (fed by 8% TeO_2), and NCs fed by 1% Bi and 8% of inert dioxides GeO_2 , ZrO_2 , and TiO_2 .

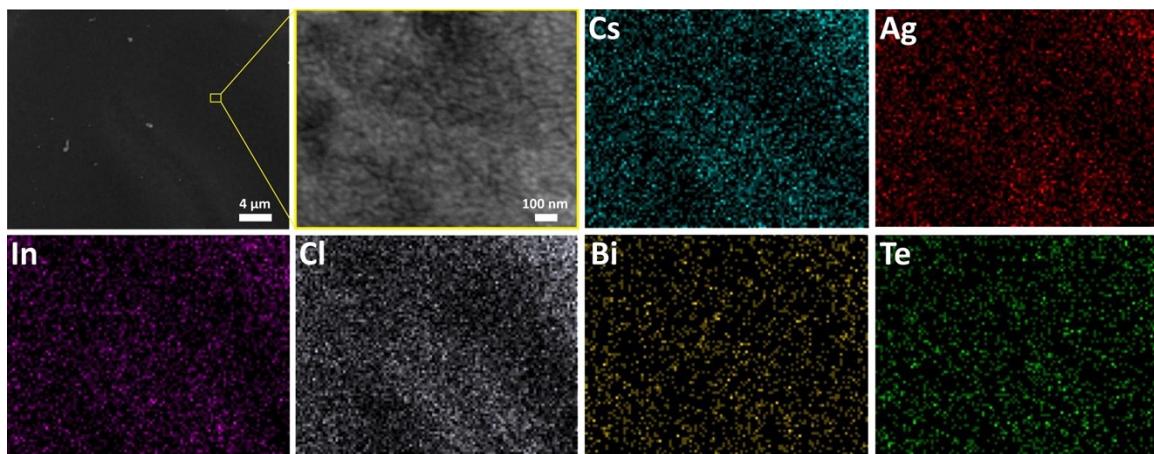


Figure S8. SEM image, and corresponding elemental mapping images for Cs, Ag, In, Cl, Bi and Te elements of thin films based on $\text{Cs}_2\text{AgInCl}_6$:8% Te, 1% Bi NCs that were stored in the refrigerator for around one month.

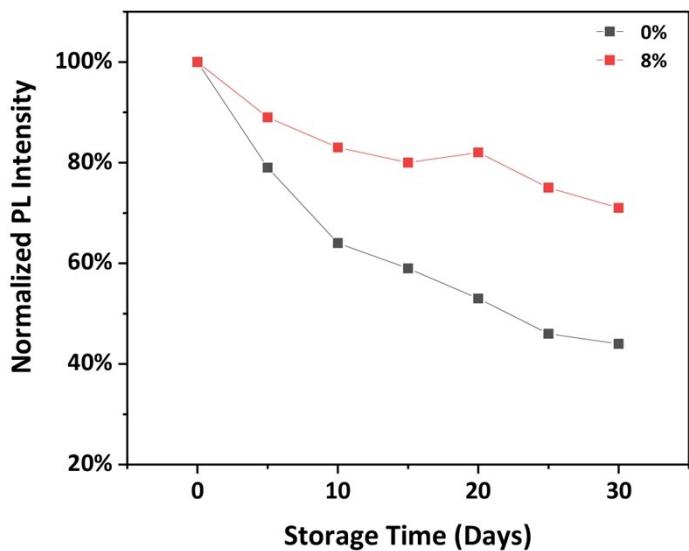


Figure S9. Normalized PL intensity of $\text{Cs}_2\text{AgInCl}_6$:0% Te, 1% Bi and $\text{Cs}_2\text{AgInCl}_6$:8% Te, 1% Bi NCs after storing in the refrigerator for around one month.

Table S1. Comparison of the PL characteristics of the B^{III} site doped Cs₂AgInCl₆ NCs. RT: room temperature.

Composition (NCs)	Reaction temperature	Excitation	PL peak	PL QY	Year	Refs
Cs ₂ AgInCl ₆	105 °C	300 nm	560 nm	1.6%	2018	¹
Cs ₂ AgInCl ₆ :1.6% Mn	105 °C	290 nm	620 nm	16%	2018	¹
Cs ₂ AgIn _{0.9} Bi _{0.1} Cl ₆	RT	-	570 nm	2%	2018	²
Cs ₂ AgInCl ₆	100 °C	300 nm	> 550 nm	0.6%	2019	³
Cs ₂ AgInCl ₆ :1% Bi	260 °C	368 nm	580 nm	11.4%	2019	⁴
Cs ₂ AgInCl ₆ : Cu ²⁺	220 °C	350 nm	460 nm	-	2020	⁵
Cs ₂ AgInCl ₆ : 1% Bi-2% Ce	260 °C	375 nm	580 nm	26%	2021	⁶
Cs₂AgInCl₆:8% Te, 1% Bi	280 °C	370 nm	591 nm	34%	This work	

Table S2. Optical parameters of Cs₂AgInCl₆:x% Te, 1% Bi NCs (x=0, 1, 2, 4, 8, 12), including PL QY, average lifetime of excitons τ_{avg} and the radiative recombination rate K_r.

Samples	PL QY (%)	$\tau_{\text{avg}} (\mu\text{s})$	K _r ($\times 10^5 \text{ s}^{-1}$)
Cs ₂ AgInCl ₆ : 0% Te, 1% Bi	12	1.06	1.13
Cs ₂ AgInCl ₆ : 1% Te, 1% Bi	5	0.63	0.79
Cs ₂ AgInCl ₆ : 2% Te, 1% Bi	13	0.94	1.38
Cs ₂ AgInCl ₆ : 4% Te, 1% Bi	22	1.11	1.98
Cs ₂ AgInCl ₆ : 8% Te, 1% Bi	34	0.96	3.54
Cs ₂ AgInCl ₆ : 12% Te, 1% Bi	10	1.05	0.95

Table S3. XPS analysis of elemental ratios in Cs₂AgInCl₆ NCs doped by 1% Bi and different amounts of Te.

Samples	Cl:In	In:Ag	Cl:Ag
Cs ₂ AgInCl ₆ :0% Te, 1% Bi	6.4	1.2	7.5
Cs ₂ AgInCl ₆ :1% Te, 1% Bi	6.5	1.2	7.7
Cs ₂ AgInCl ₆ :8% Te, 1% Bi	5.9	1.1	6.7
Cs ₂ AgInCl ₆ :12% Te, 1% Bi	6.5	1.2	7.5

References

1. F. Locardi, M. Cirignano, D. Baranov, Z. Dang, M. Prato, F. Drago, M. Ferretti, V. Pinchetti, M. Fanciulli, S. Brovelli, et al., *J. Am. Chem. Soc.*, 2018, **140**, 12989-12995.
2. B. Yang, X. Mao, F. Hong, W. Meng, Y. Tang, X. Xia, S. Yang, W. Deng and K. Han, *J. Am. Chem. Soc.*, 2018, **140**, 17001-17006.
3. J. C. Dahl, W. T. Osowiecki, Y. Cai, J. K. Swabeck, Y. Bekenstein, M. Asta, E. M. Chan and A. P. Alivisatos, *Chem. Mater.*, 2019, **31**, 3134-3143.
4. Y. Liu, Y. Jing, J. Zhao, Q. Liu and Z. Xia, *Chem. Mater.*, 2019, **31**, 3333-3339.
5. Q. Liao, J. Chen, L. Zhou, T. Wei, L. Zhang, D. Chen, F. Huang, Q. Pang and J. Z. Zhang, *J. Phys. Chem. Lett.*, 2020, **11**, 8392-8398.
6. S. Wang, J. Qi, S. V. Kershaw and A. L. Rogach, *ACS Nanosci. Au*, 2021, **2**, 93-101.