

2. Supplementary figures

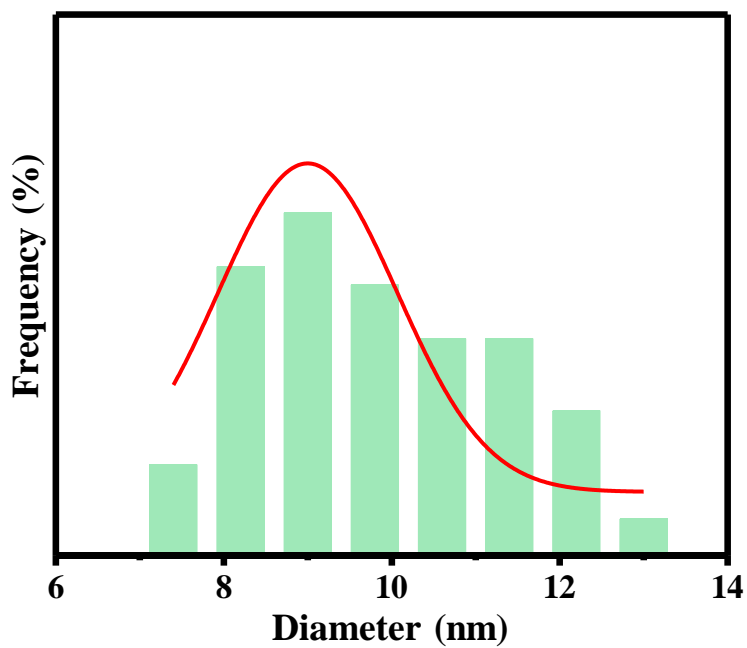


Fig. S1 The particle size distribution map of Cs₃Cu₂I₅ NCs in TEM image.



Fig. S2 Gram-scale $\text{Cs}_3\text{Cu}_2\text{I}_5$ NCs under 254 nm UV light.

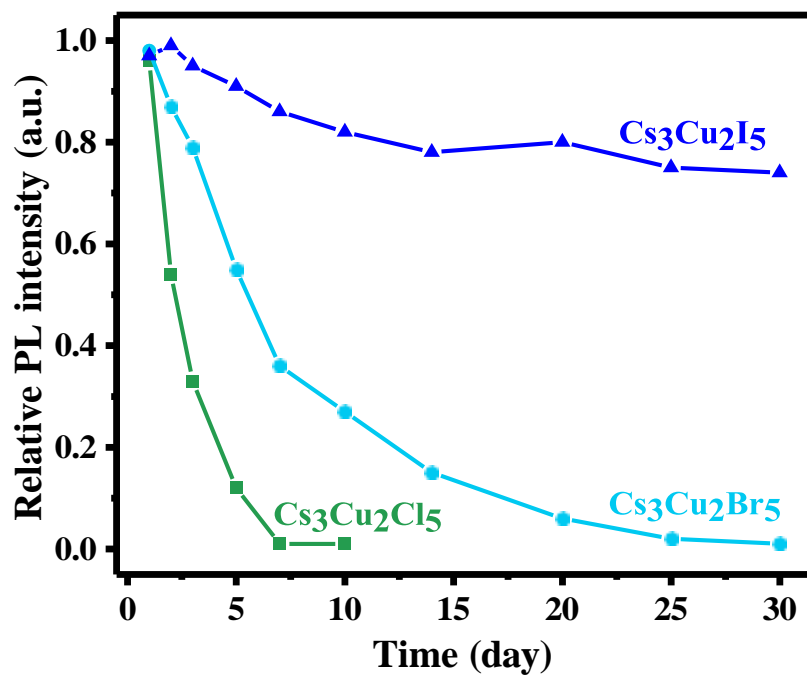


Fig. S3 PL stability evolutions of the NCs with different halide compositions in the ambient atmosphere.

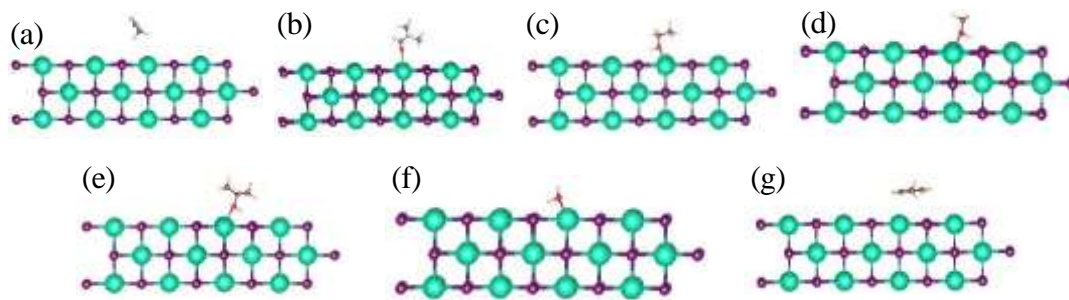


Fig. S4 Schematic illustration of the solvent adsorption process with CsI (a: ACN, b: DMF, c: EtOH, d: MeOH, e: IPA, f: H₂O, g: TOL).

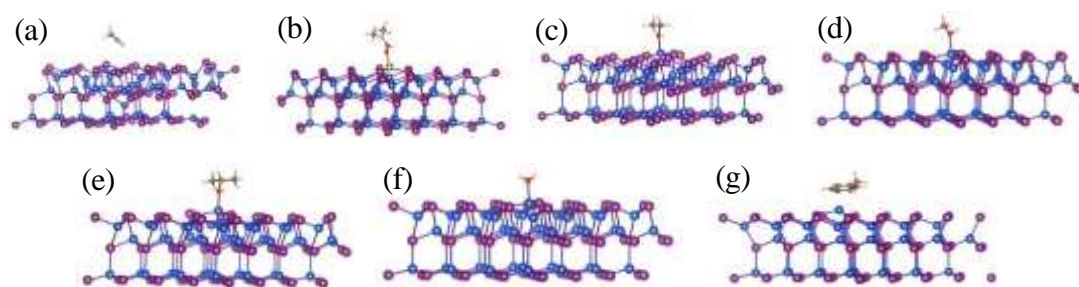


Fig. S5 Schematic illustration of the solvent adsorption process with CuI (a: ACN, b: DMF, c: EtOH, d: MeOH, e: IPA, f: H₂O, g: TOL).

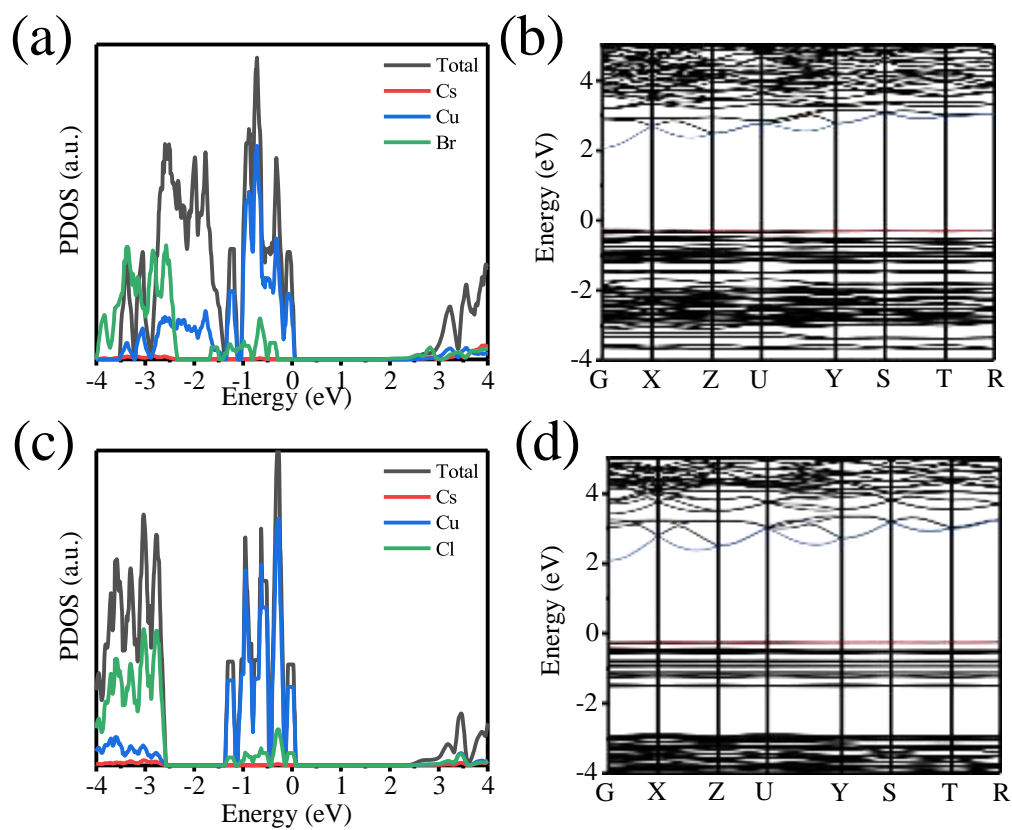


Fig. S6 The calculated density of states (a and c) and band structures (b and d) of $\text{Cs}_3\text{Cu}_2\text{Br}_5$ (a and b) and $\text{Cs}_3\text{Cu}_2\text{Cl}_5$ (c and d).

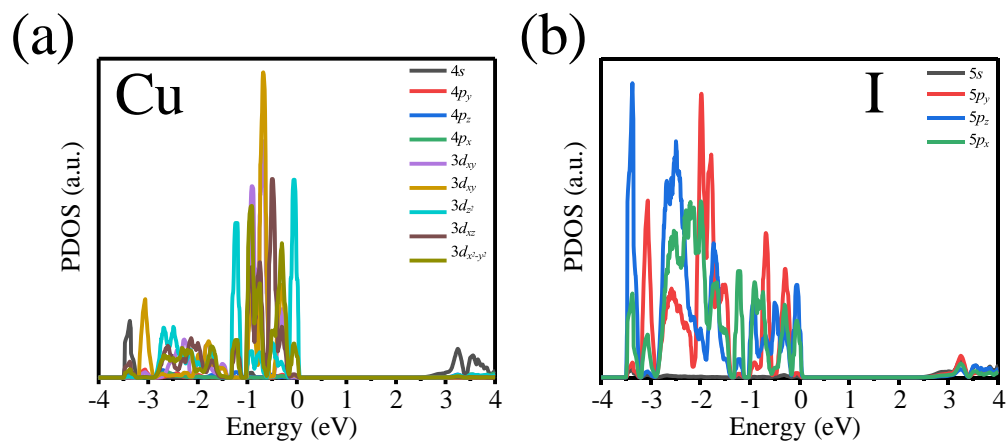


Fig. S7 Density of states of for Cu and I.

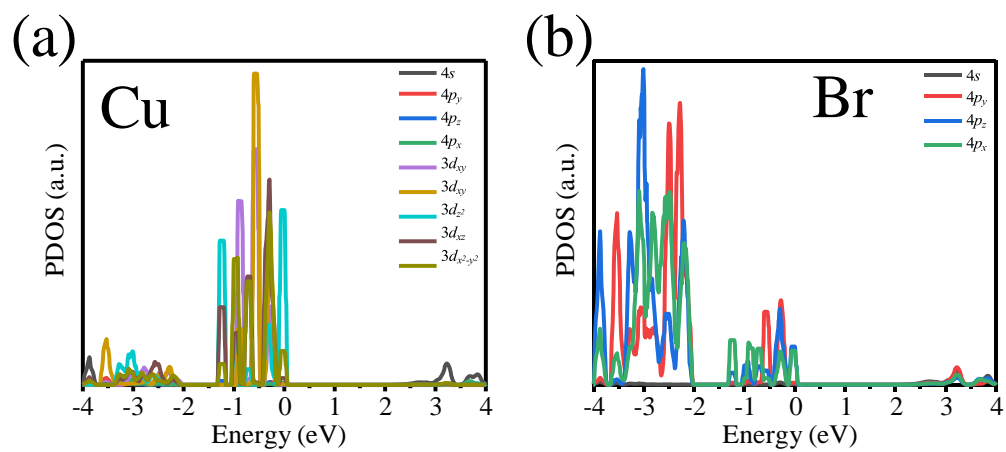


Fig. S8 Density of states of for Cu and Br.

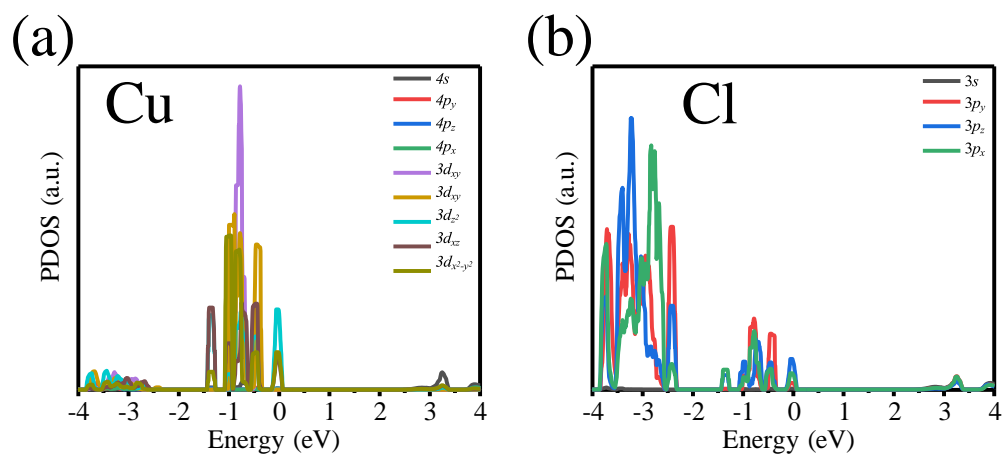


Fig. S9 Density of states of for Cu and Cl.

Table S1. The binding energies between the solvent and precursors.

Compounds	Binding Energy(eV)
CsI-ACN	-0.026
CsI-DMF	-1.353
CsI-EtOH	-0.469
CsI-MeOH	-0.490
CsI-IPA	-0.495
CsI-H₂O	-0.488
CsI-TOL	-0.083
CuI-ACN	-0.098
CuI-DMF	-0.201
CuI-EtOH	0.002
CuI-MeOH	-0.018
CuI-IPA	-0.136
CuI-H₂O	0.019
CuI-TOL	0.152

Reference

- [1] Kresse, G.; Hafner, J. Ab-Initio Molecular-Dynamics for Open-Shell Transition-Metals. *Phys. Rev.* **1993**, *48*, 13115-13118.
- [2] Kresse, G.; Furthmüller, J. Efficiency of Ab-initio Total Energy Calculations for Metals and Semiconductors Using a Plane-wave Basis Set. *Comput. Mater. Sci.* **1996**, *6*, 15-50.
- [3] Kresse, G.; Furthmüller, J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys. Rev. B* **1996**, *54*, 11169-11186.
- [4] Blöchl PE, Projector Augmented-wave Method. *Phys. Rev. B* **1994**, *50*, 17953-17979.
- [5] Perdew JP, Burke K, Ernzerhof M, Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.