Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Compositional Engineering of Doped Zero-dimensional Zinc Halide Blue Emitters for Efficient X-ray Scintillation

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Table S1. Composition of Cu-doped samples measured by ICP-AES.

samples	Cu/Zn precursors ratio	Cu content (at%, ICP)
Cu-doped Cs_2ZnBr_4	2/3	0.67
	3/3	36
	4/3	65
	5/3	103
	6/3	140
Cu-doped Cs_2ZnCl_4	2/3	0.30
Cu-doped Rb_2ZnCl_4	2/3	0.59

$$\text{Cu/Zn precursors ratio} = \frac{molar\ feed\ ratio\ of\ CuBr}{molar\ feed\ ratio\ of\ ZnBr_2}$$

The content of Cu was expressed relative to that Zn, which was assumed to be 1.

$$\text{Cu content} = \frac{Cu\ concentration\ measured\ by\ ICP}{Zn\ concentration\ measured\ by\ ICP} \times 100\%$$

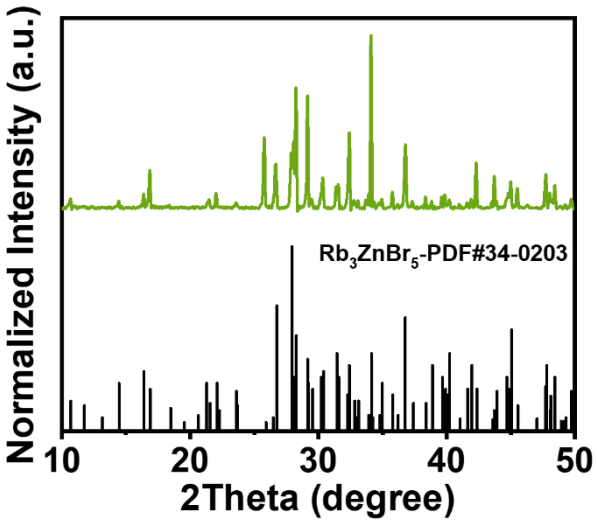

Figure S1. XRD pattern of Rb_3ZnBr_5.

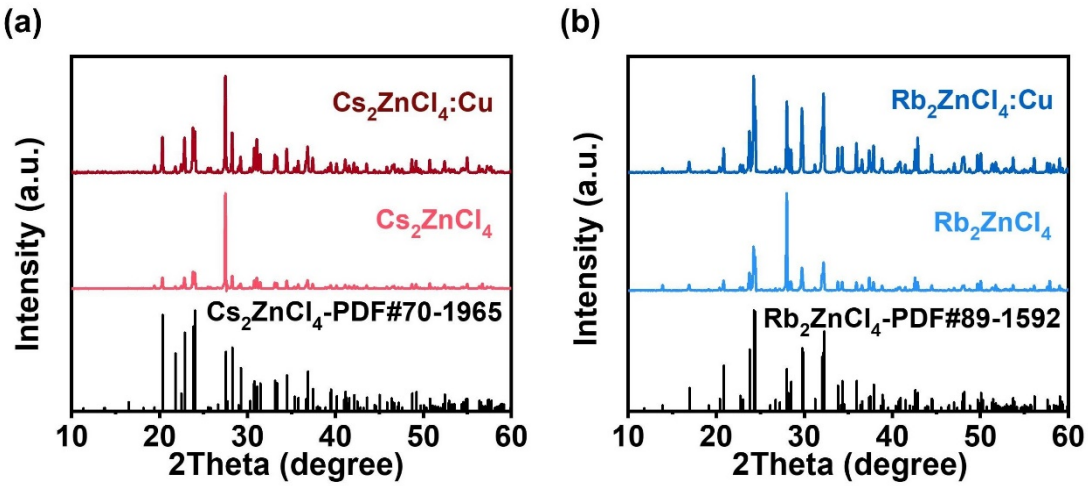

Figure S2. (a) XRD patterns of pristine Cs_2ZnCl_4 and Cs_2ZnCl_4:Cu. (b) XRD patterns of pristine Rb_2ZnCl_4 and Rb_2ZnCl_4:Cu.

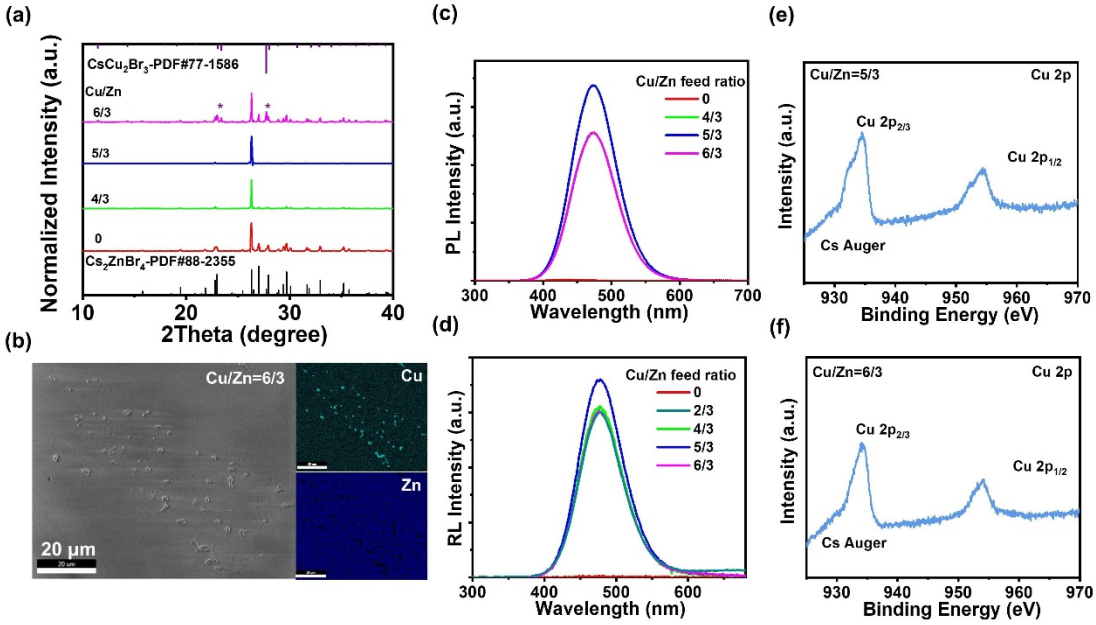

Figure S3. (a) XRD patterns of pristine Cs_2ZnBr_4 and Cu-doped Cs_2ZnBr_4 with different Cu to Zn precursors ratio. (b) SEM image and the element distribution analysis through EDS mapping of the as-prepared Cu-doped Cs_2ZnBr_4 single crystals with Cu/Zn precursors ratio of 6/3 (Scale bar: 20 μm). (c) The PL spectra of pristine Cs_2ZnBr_4 and Cu-doped Cs_2ZnBr_4 with different Cu to Zn precursors ratio. (d) The RL spectra of pristine Cs_2ZnBr_4 and Cu-doped Cs_2ZnBr_4 with different Cu to Zn molar feed ratio. (e) High-resolution XPS spectrum of Cu 2p for Cu-doped Cs_2ZnBr_4 single crystals with Cu/Zn precursors ratio of 5/3 and (f) 6/3.

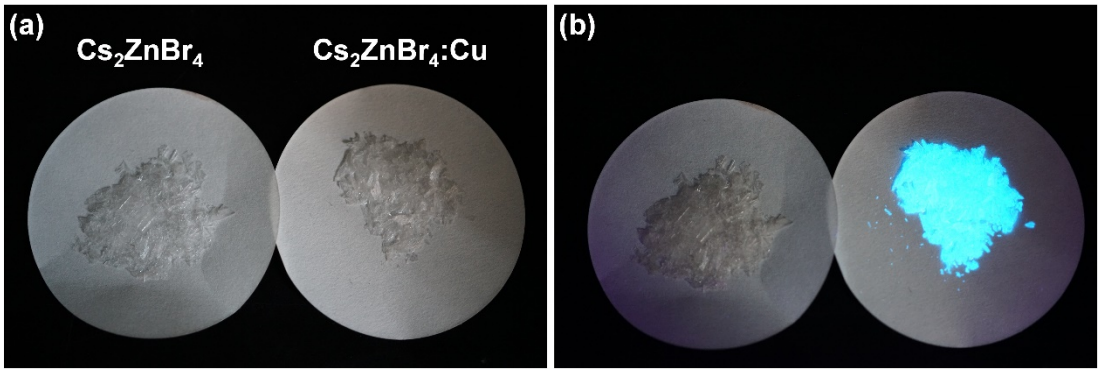

Figure S4. (a) The photographs of Cs_2ZnBr_4 and Cs_2ZnBr_4:Cu under room light. (b) The photographs of Cs_2ZnBr_4 and Cs_2ZnBr_4:Cu under 254 nm UV.

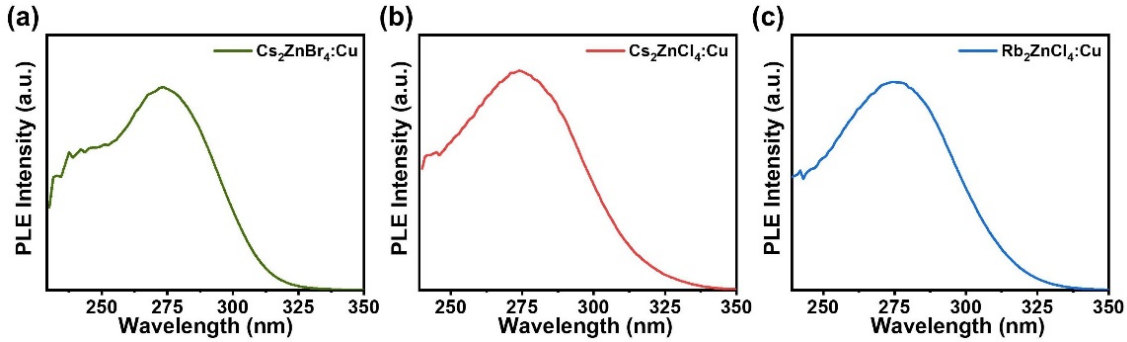

Figure S5. PLE spectra of Cs_2ZnBr_4:Cu, Cs_2ZnCl_4:Cu and Rb_2ZnCl_4:Cu.

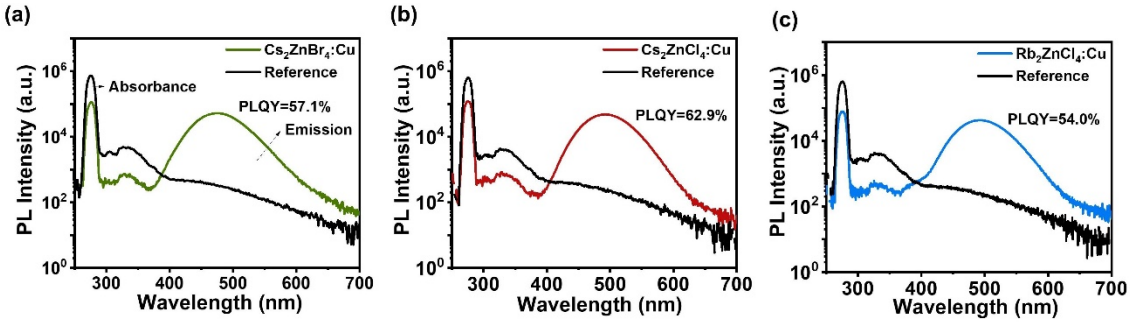

Figure S6. Absolute PL quantum yield (PLQY) measurement results of Cs_2ZnBr_4:Cu, Cs_2ZnCl_4:Cu and Rb_2ZnCl_4:Cu.

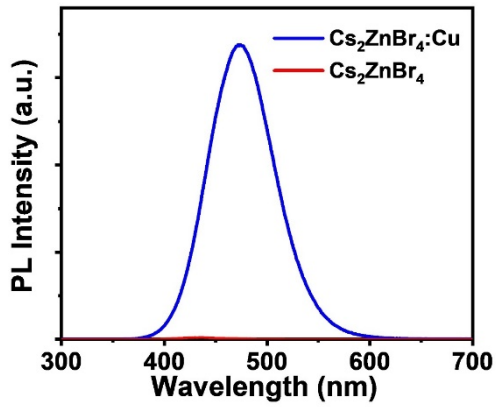

Figure S7. The PL spectra of Cs_2ZnBr_4 and Cs_2ZnBr_4:Cu.

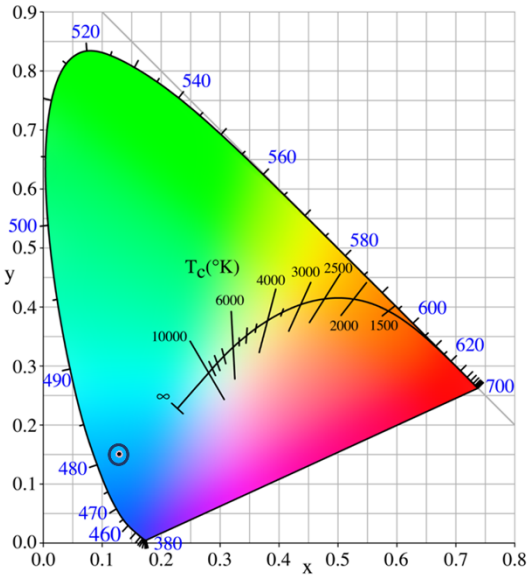

Figure S8. The CIE (International Commission on Illumination) diagram of Cs_2ZnBr_4:Cu. (0.1326,0.1458).

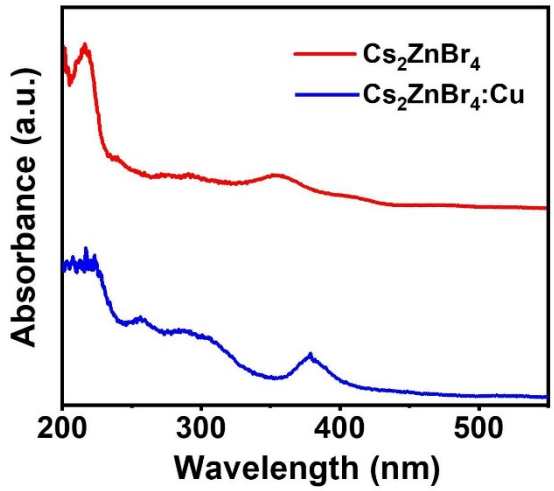

Figure S9. The UV-vis absorption spectra of Cs_2ZnBr_4 and Cs_2ZnBr_4:Cu.

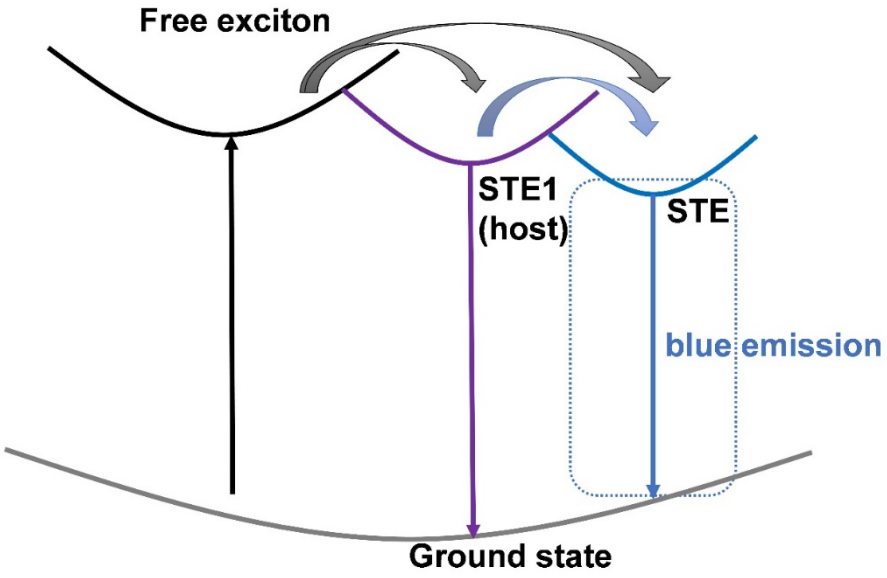

Figure S10. Schematic illustration of photophysical processes of the pure-blue emission in Cs_2ZnBr_4:Cu.

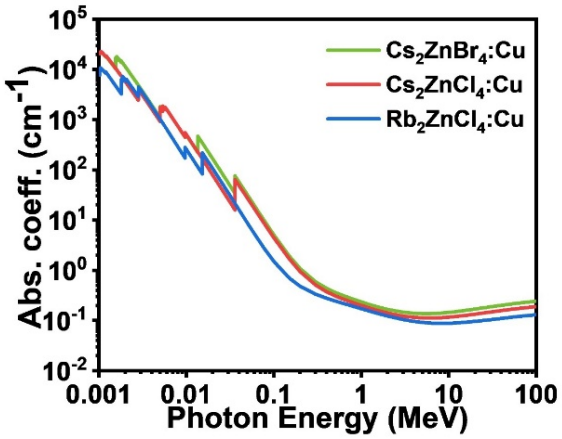

Figure S11. X-ray absorption coefficients of Cs_2ZnBr_4:Cu, Cs_2ZnCl_4:Cu and Rb_2ZnCl_4:Cu as a function of photon energy from 1 keV to 100 MeV.

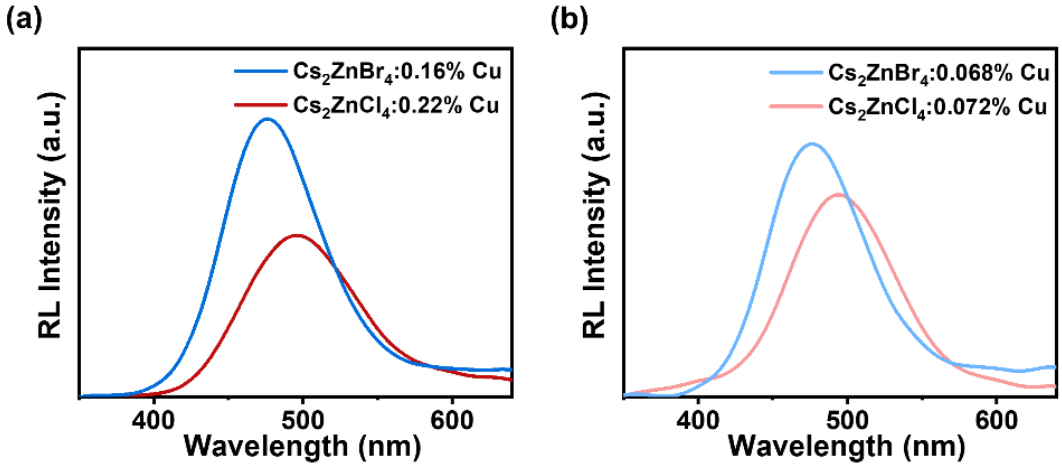

Figure S12. RL spectra of Cu-doped Cs_2ZnBr_4 and Cu-doped Cs_2ZnCl_4 samples with similar Cu content. RL spectra of Cu-doped Cs_2ZnBr_4 and Cu-doped Cs_2ZnCl_4 samples with (a) the relatively higher and (b) the relatively higher Cu content.

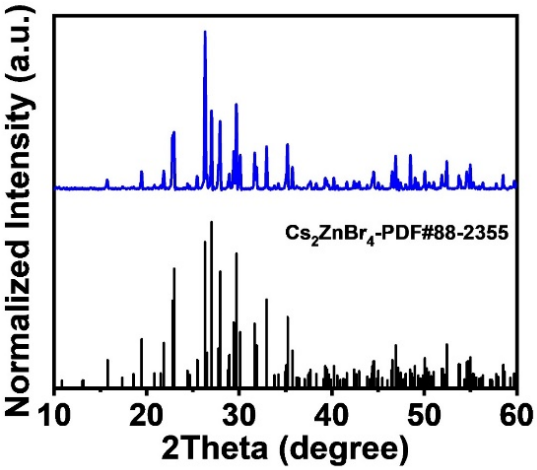

Figure S13. XRD pattern Cs_2ZnBr_4:Cu after storing in ambient atmosphere for four months.

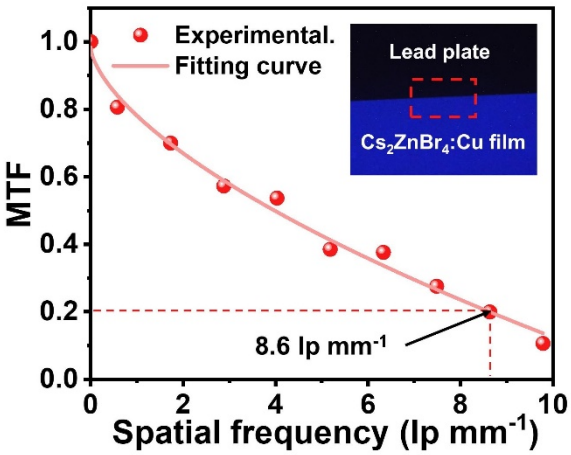

Figure S14. Modulation transfer function (MTF) curve of Cs_2ZnBr_4:Cu film.