

Electronic Supplementary Information

Bright tunable luminescence of Sb³⁺ doping in zero-dimensional lead-free halide Cs₃ZnCl₅ perovskite crystals

Xiaoxia Liu, Weibing Zhang,* Rui Xu, Jiayu Tu, Guoyong Fang* Yuexiao Pan*

Key Laboratory of Carbon Materials of Zhejiang Province, College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325035, P.R. China.

E-mail: 00111040@wzu.edu.cn; fanggy@wzu.edu.cn; yxpan@wzu.edu.cn

Fax&Tel: +86-577-8837-3017

Table S1. The experimental mole ratio of Cs, Zn and Sb calculated from starting materials and the actual doping concentration in crystals Cs₃ZnCl₅:Sb measured in the sample by using inductive coupled plasma emission spectrometer (ICP).

Experimental mole ratio	Actual contents	Actual contents	Actual doping
	of Cs	of Zn	concentration of Sb
Cs ₃ Zn _{0.985} Cl ₅ :0.015Sb ³⁺	48.14%	13.60%	0.10%
Cs ₃ Zn _{0.97} Cl ₅ :0.03Sb ³⁺	46.37%	11.67%	0.52%
Cs ₃ Zn _{0.95} Cl ₅ :0.05Sb ³⁺	46.50%	10.55%	1.22%
Cs ₃ Zn _{0.9} Cl ₅ :0.1Sb ³⁺	46.08%	9.88%	2.25%
Cs ₃ Zn _{0.7} Cl ₅ :0.3Sb ³⁺	47.02%	8.88%	4.46%
Cs ₃ Zn _{0.5} Cl ₅ :0.5Sb ³⁺	45.84%	6.91%	5.67%

Table S2. The lattice parameters of Cs_3ZnCl_5 and Sb^{3+} -doped Cs_3ZnCl_5

Crystal	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
Cs_3ZnCl_5 (Exp.)	9.758	9.758	9.758	123.468	123.468	84.091
Cs_3ZnCl_5 (Comput.)	9.931	9.931	9.931	123.498	123.498	84.040
Sb- Cs_3ZnCl_5 (Comput.)	10.448	10.448	10.448	126.985	126.985	78.275

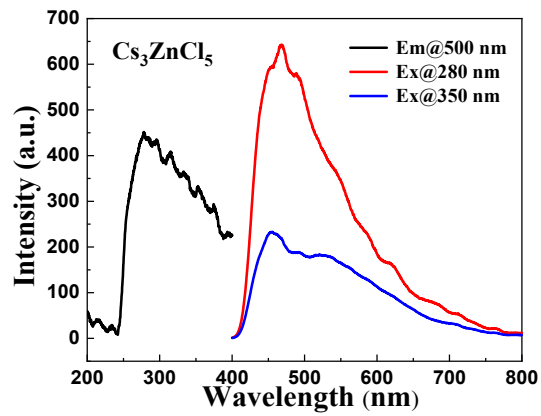


Figure S1. Excitation and emission spectra of undoped Cs_3ZnCl_5 measured at room temperature.

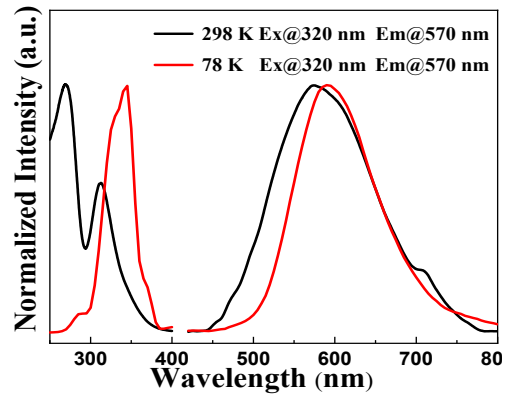


Figure S2. Excitation and emission spectra of $\text{Cs}_3\text{Zn}_{0.5}\text{Cl}_5:0.5\text{Sb}^{3+}$ measured at 78 K and 298 K, respectively.

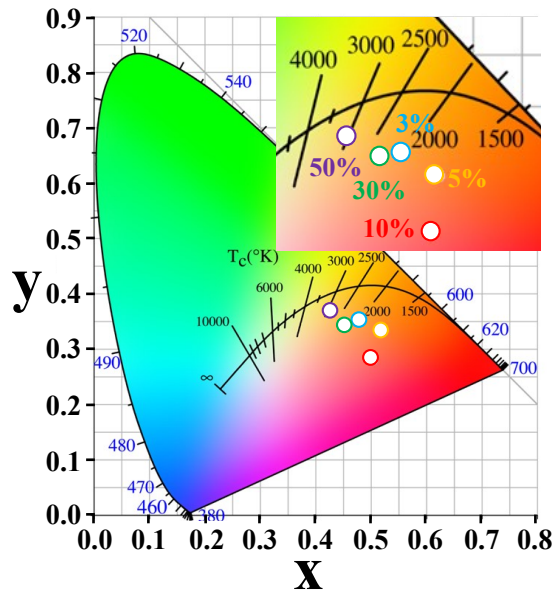


Figure S3. CIE chromaticity coordinates of $\text{Cs}_3\text{Zn}_{1-x}\text{Cl}_5:x\text{Sb}^{3+}$ ($x = 3\text{-}50$ mol%) excited at 320 nm.

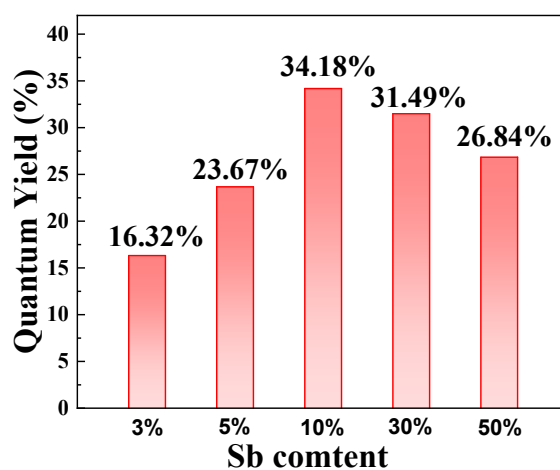


Figure S4. PLQY of $\text{Cs}_3\text{Zn}_{1-x}\text{Cl}_5:x\text{Sb}^{3+}$ ($x = 3\text{-}50$ mol%) excited at 320 nm.

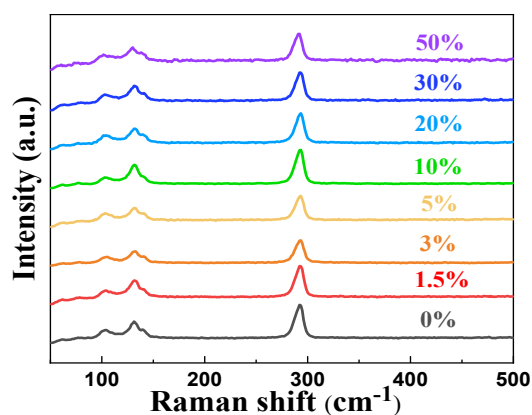


Figure S5. The Raman spectra of Cs_3ZnCl_5 and $\text{Cs}_3\text{ZnCl}_5:\text{Sb}^{3+}$ doped with different concentration of Sb^{3+} (performed using Horiba Jobin Yvon LabRAM HR80 equipped with a microscope and a CCD camera as the detector and a 532 nm diode laser as the excitation source).

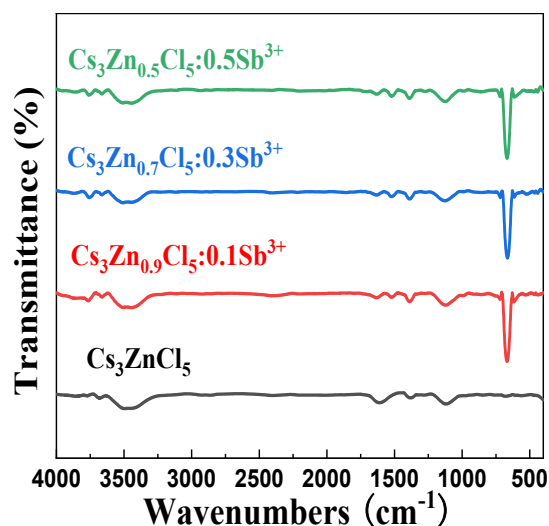


Figure S6. The infrared (IR) spectra of the Cs_3ZnCl_5 , $\text{Cs}_3\text{Zn}_{0.9}\text{Cl}_5:0.1\text{Sb}^{3+}$, $\text{Cs}_3\text{Zn}_{0.7}\text{Cl}_5:0.3\text{Sb}^{3+}$, and $\text{Cs}_3\text{Zn}_{0.5}\text{Cl}_5:0.5\text{Sb}^{3+}$ performed on Perkin-Elmer 580 B infrared spectrophotometer using the KBr pellet technique.

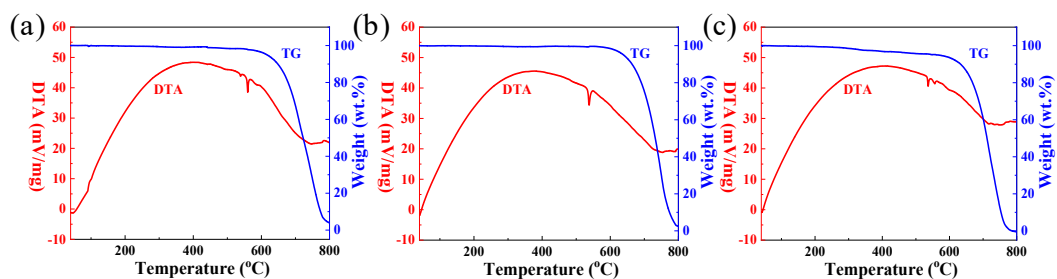


Figure S7. The thermogravimetrics (TG) analysis and differential thermal analysis (DTA) of (a) Cs_3ZnCl_5 , (b) $\text{Cs}_3\text{Zn}_{0.9}\text{Cl}_5:0.1\text{Sb}^{3+}$, and (c) $\text{Cs}_3\text{Zn}_{0.5}\text{Cl}_5:0.5\text{Sb}^{3+}$ performed on a PerkinElmer Diamond TG-DTA at $10\text{ }^\circ\text{C}/\text{min}$ in an argon flow from room temperature to $800\text{ }^\circ\text{C}$ under N_2 atmosphere.