Electronic Supplementary Information

Te^{4+}-Doped Zero-Dimensional Cs_2ZnCl_4 Single Crystals for Broadband Yellow Light Emission

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Tables:

Table S1. Crystal data and structure refinement for Cs_2ZnCl_4 and $Cs_2ZnCl_4:Te^{4+}$.

	Cs_2ZnCl_4	$Cs_2ZnCl_4:Te^{4+}$
Temperature, K	296(2)	296(2)
Crystal system	Orthorhombic	Orthorhombic
space group	*Pnma*	*Pnma*
Unit cell dimensions	a = 9.7749(11) Å b = 7.4136(8) Å c = 12.9810(14) Å β = 90.00 deg	a = 9.867(10) Å b = 7.458(8) Å c = 12.959(13) Å β = 90.00 deg
Volume/ $Å^3$, Z	940.70(18), 2	953.6(17), 2
ρ_{calc} /g cm^{-3}	3.340	3.294
μ / mm^{-1}	11.282	11.129
F(000)	832	832
θ range /deg	3.77 to 25.0	3.77 to 28.31
Limiting indices	-11 < = h < = 10 -8 < = k < = 5 -15 < = l < = 15	-12 < = h < = 13 -9 < = k < = 9 -17 < = l < = 12
Reflections collected	3629	6342
Independent reflections	869[R(int) = 0.0413]	850[R(int) = 0.0282]
Absorption coefficient / mm^{-1}	0.022	0.015
Data / restraints / parameters	888 / 0 / 41	996 / 0 / 41
Goodness-of-fit on F^2	1.349	1.176
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0387	R1 = 0.0757, wR2 = 0.1073
R indices (all data)	R1 = 0.1137, wR2 = 0.1239	R1 = 0.2248, wR2 = 0.2941

$R1=\sum(||F_o|-|F_c||) / \sum|F_o|$; $wR2=\{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)]^2\}^{1/2}$

Table S2. The experimental mole ratio of Te^{4+} calculated from starting materials and the actual doping concentration of Te^{4+} in crystals Cs_2ZnCl_4 measured in the sample by using inductive coupled plasma emission spectrometer (ICP).

Experimental mole ratio of Te	Conc. (mg/L)	Actual doping concentration of Te
1%	0.312	0.21%
2%	0.651	0.43%
4%	1.796	1.19%
6%	3.688	2.46%
8%	4.397	2.93%
10%	4.564	3.04%
12%	6.043	4.02%

Table S3. Second order fitting parameters of decay at 0, 1, 2, 4, 6, 8, 10 and 12 mol% Te^{4+} doped Cs_2ZnCl_4.

Te%	1	2	4	6	8	10
τ (ns)	62.94	55.42	54.01	53.22	53.22	50.87

Figures:

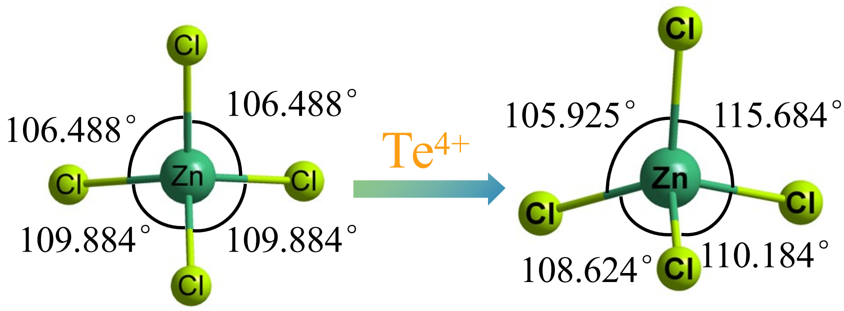

Fig. S1 The change of bond Angle during Te^{4+} substitution.

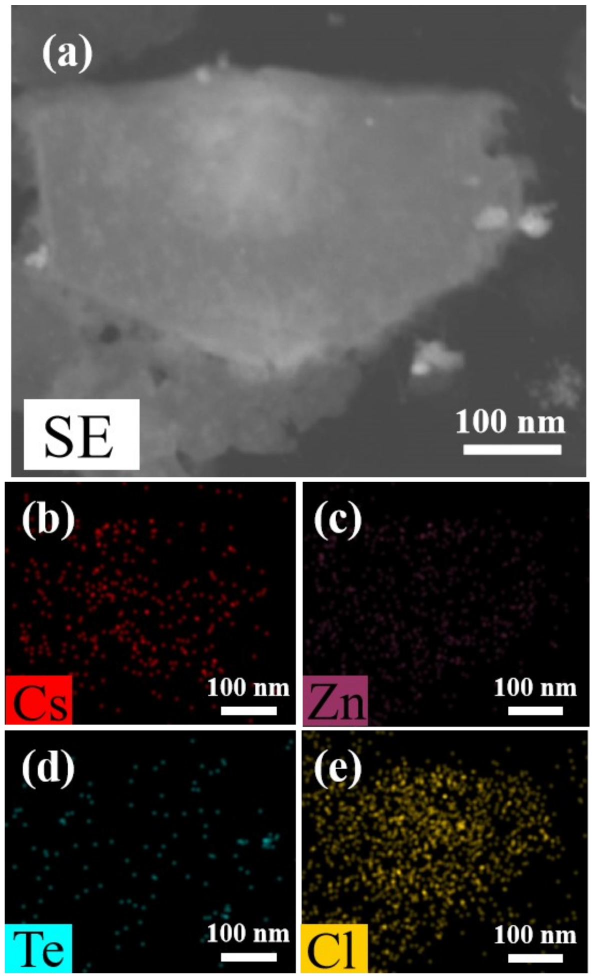

Fig. S2 (a) Elemental mapping of the Cs_2ZnCl_4:Te^{4+} showing the presence of (b) caesium, (c) zinc, (d) tellurium, and (e) chlorine.

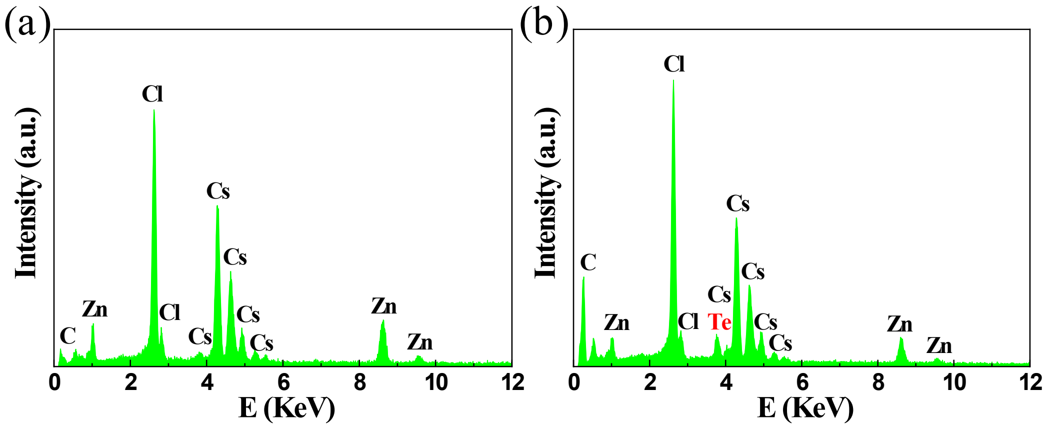

Fig. S3 The corresponding energy dispersive spectroscopy (EDS) of the as-prepared (a) undoped Cs_2ZnCl_4 and (b) Cs_2ZnCl_4:Te^{4+} sample collected on FEI Nova 200 NanoSEM instrument.

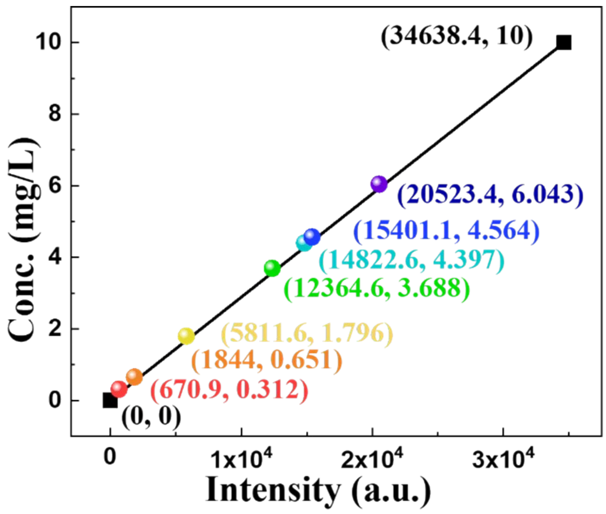

Fig. S4 The actual doping amount of Te^{4+} at different concentrations was measured by inductive coupled plasma optical emission spectrometer (ICP-OES) is performed on PerkinElmer ICP-OES OPTIMA8000.

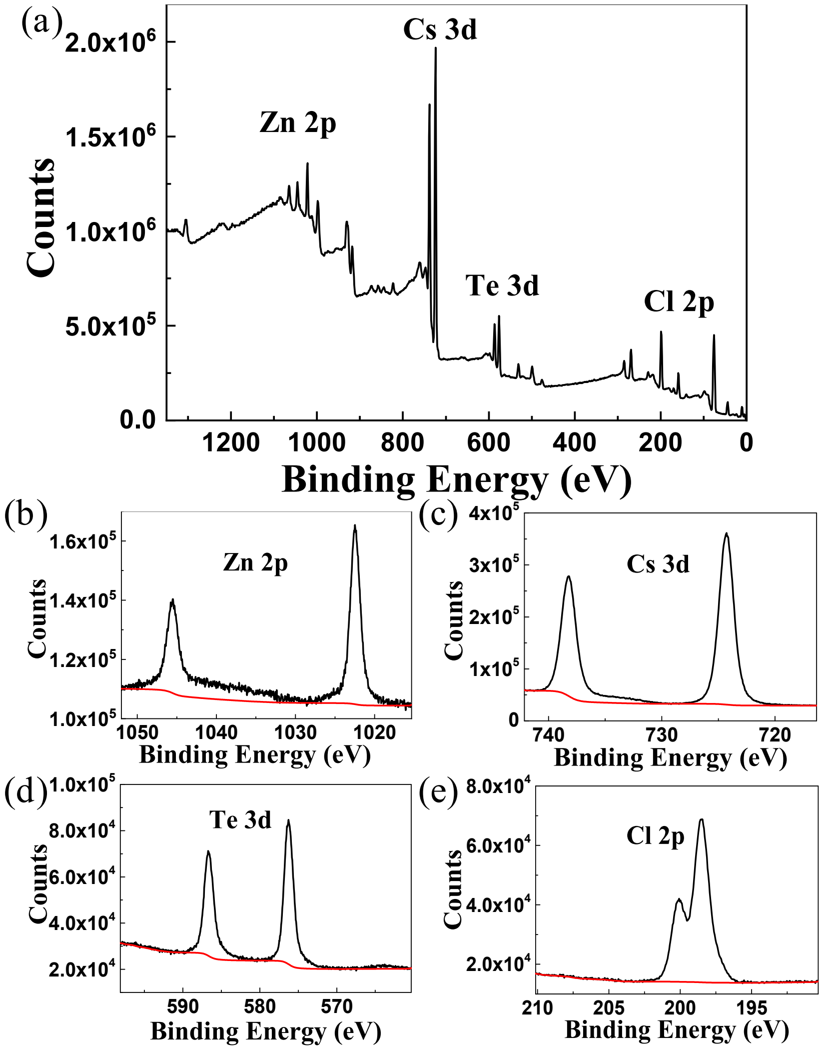

Fig. S5 (a) The high-resolution XPS analysis of $Cs_2ZnCl_4:Te^{4+}$ corresponding to (b) Zn 2p, (c) Cs 3d, (d) Te 3d and (e) Cl 2p, respectively, which was done with a Thermo Scientific Escalab 250 Xi instrument using monochromatic Al *K*α radiation (h*v* = 1486.7 eV).

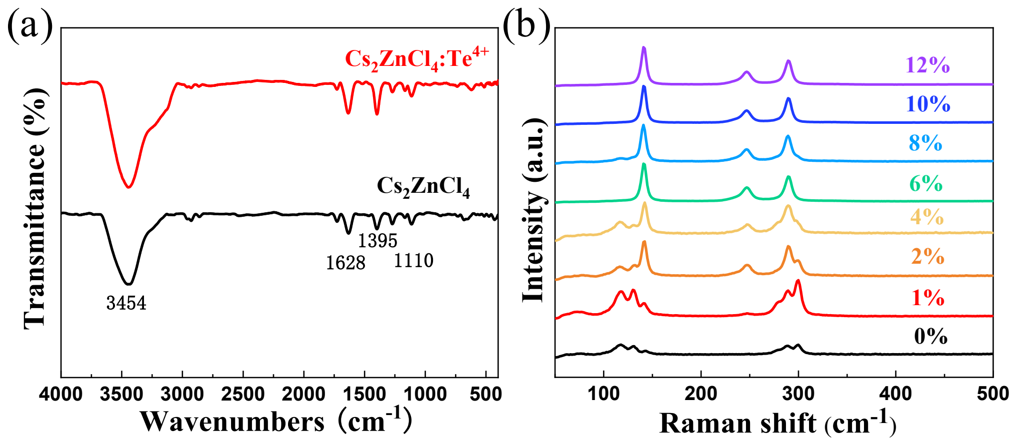

Fig. S6 (a) FT-IR spectra of the Cs_2ZnCl_4 and Cs_2ZnCl_4:Te^{4+} were recorded on a Nicolet iS20 Fourier-transform infrared spectrometer using the KBr method. Raman was performed by Renishaw inVia, and (b) the Raman spectra for Cs_2ZnCl_4:Te^{4+} doped with different concentration of Te^{4+}.

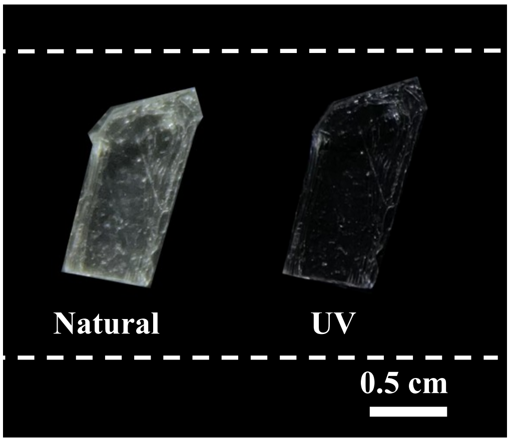

Fig. S7 Optical microscopic images of undoped Cs_2ZnCl_4 single crystal taken under natural light (left) and UV light (right).

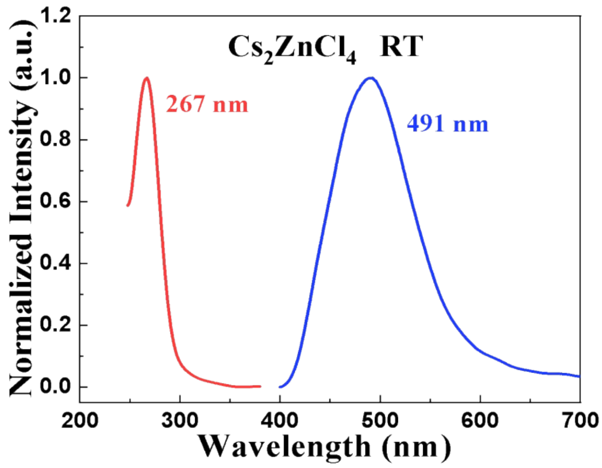

Fig. S8 Normalized PL and PLE of Cs_2ZnCl_4 at room temperature (λ_{ex} = 267 nm, λ_{em} = 491 nm).

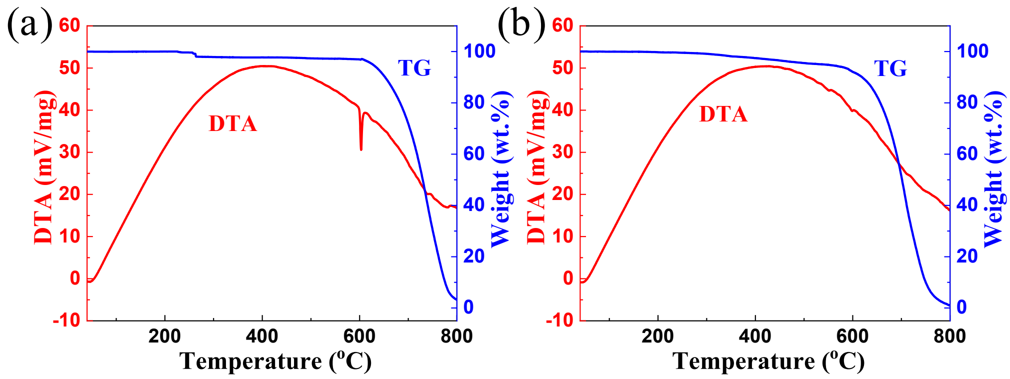

Fig. S9 Thermogravimetrics (TG) and differential thermal analysis (DTA) graphs of as the synthesized (a) Cs_2ZnCl_4 and (b) Cs_2ZnCl_4:Te^{4+} performed on a PerkinElmer Diamond TG-DTA at 10 °C/min in an argon flow from room temperature to 800 °C. under N_2 atmosphere.

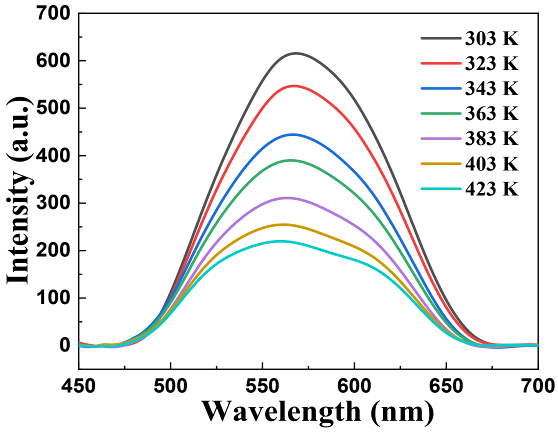

Fig. S10 The emission intensities of Cs_2ZnCl_4:Te^{4+} dependent on the temperatures.