Supporting Information

Near-infrared photoluminescence from molecular crystals containing tellurium

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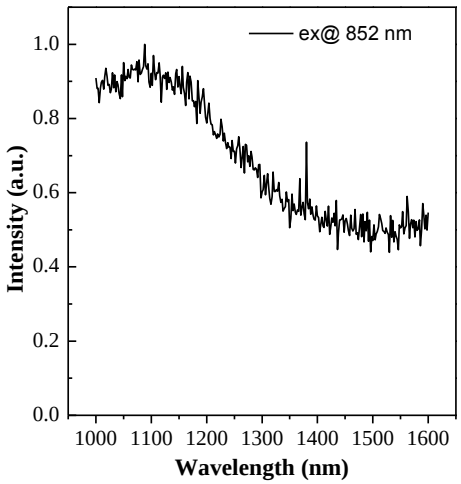

Fig. S1 PL spectrum $Te_4(Ga_2Cl_7)_2$ sample under the excitation of 852 nm.

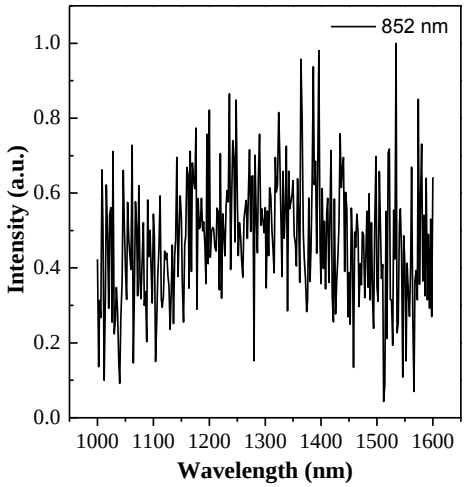

Fig. S2 PL spectrum $Te_4(Al_2Cl_7)_2$ sample under the excitation of 852 nm.

Table S1. The calculated Singlet-Singlet/Triplet excitation energies of Te_4. Spin-restricted density functional theory (DFT) was employed to determine energies and compositions of excited states of this unit, using the Hartree–Fock method. The Slater-type all-electron basis set utilized in the DFT calculation is of triple-ζ-polarized (TZP) quality. The absorption bands were calculated through a Davidson method, and the absorption spectra were fitted with a Gaussian function with a width at half-maximum of 50 nm. The ADF numerical integration parameter was set to 5.0. Scalar relativistic effect was taken into account for the calculation.

No	Wavelength (nm)	Oscillator strength
1	2299	0
2	2195	0
3	1060	1.01E-09
4	1041	6.83E-11
5	747	0
6	551	0
7	487	3.23E-09
8	455	0
9	453	0
10	432	0
11	397	1.05E-02
12	387	0
13	380	3.87E-09
14	330	3.67E-06
15	327	0
16	305	4.28E-09
17	303	0
18	288	2.10E-08
19	267	4.14E-05
20	257	3.87E-08

Table S2. The calculated spin-unrestricted excitation energies of Te_4^{1+}. Spin-unrestricted density functional theory (DFT) was employed to determine energies and compositions of excited states of this unit, using the hybrid Becke three-parameter Lee−Yang−Parr (B3LYP) functional. The Slater-type all-electron basis set utilized in the DFT calculation is of triple-ζ-polarized (TZP) quality. The absorption bands were calculated through a Davidson method, and the absorption spectra were fitted with a Gaussian function with a width at half-maximum of 50 nm. The ADF numerical integration parameter was set to 5.0. Scalar relativistic effect was taken into account for the calculation.

No	Wavelength (nm)	Oscillator strength
1	2349	1.49E-09
2	2272	2.25E-09
3	673	7.64E-09
4	656	2.51E-08
5	641	2.49E-04
6	631	3.78E-05
7	573	4.02E-02
8	572	4.06E-02
9	526	4.50E-08
10	508	1.78E-07

Table S3. The calculated spin-unrestricted excitation energies of Te_4^{3+}. Spin-unrestricted density functional theory (DFT) was employed to determine energies and compositions of excited states of this unit, using the hybrid Becke three-parameter Lee−Yang−Parr (B3LYP) functional. The Slater-type all-electron basis set utilized in the DFT calculation is of triple-ζ-polarized (TZP) quality. The absorption bands were calculated through a Davidson method, and the absorption spectra were fitted with a Gaussian function with a width at half-maximum of 50 nm. The ADF numerical integration parameter was set to 5.0. Scalar relativistic effect was taken into account for the calculation.

No	Wavelength (nm)	Oscillator strength
1	7771	0
2	1314	2.75E-03
3	792	0
4	774	1.50E-03
5	675	3.02E-03
6	645	1.17E-04
7	642	0
8	518	7.37E-04
9	518	0
10	448	5.63E-02