Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Supporting Information

## Unveiling the uncommon blue-excitable broadband yellow emission from self-trapped excitons in a zero-dimensional hybrid tellurium-based double perovskite

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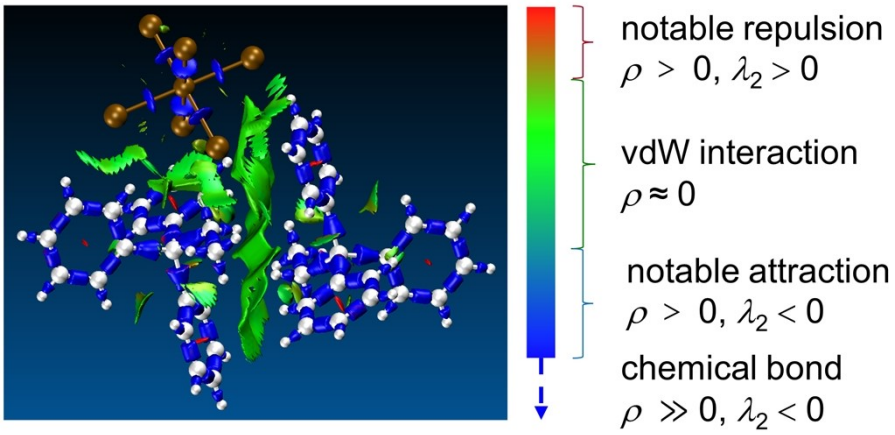


**Figure S1.** Interaction Region Indicator (*IRI*) of compound $(C_{20}H_{20}P)_2TeCl_6$ isosurface diagram of the sign($\lambda_2$)ρ.

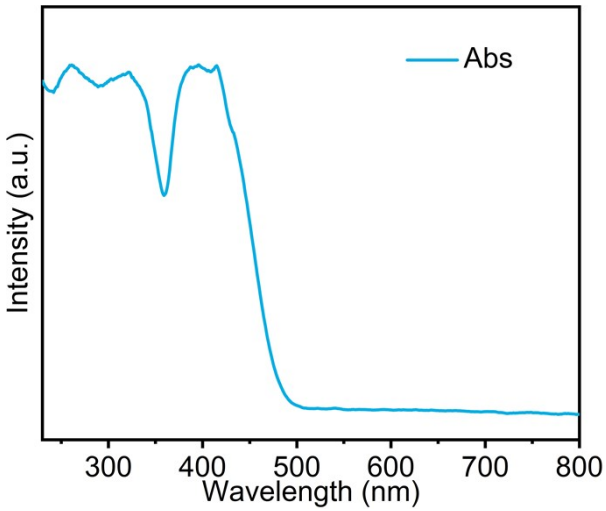


**Figure S2.** The absorption spectrum of $(C_{20}H_{20}P)_2TeCl_6$ at RT.

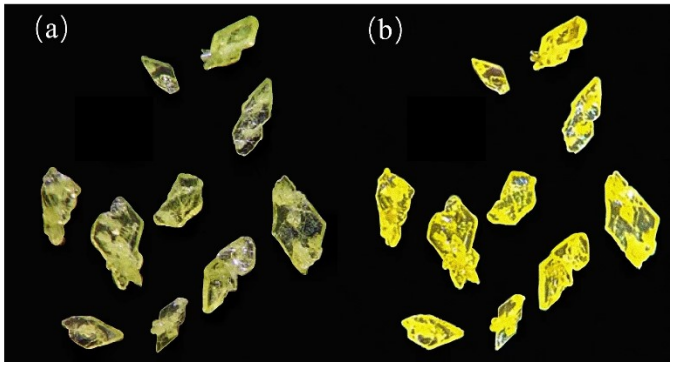


**Figure S3.** Macroscopic appearance of $(C_{20}H_{20}P)_2TeCl_6$: (a) under natural light, (b) under ultraviolet light.

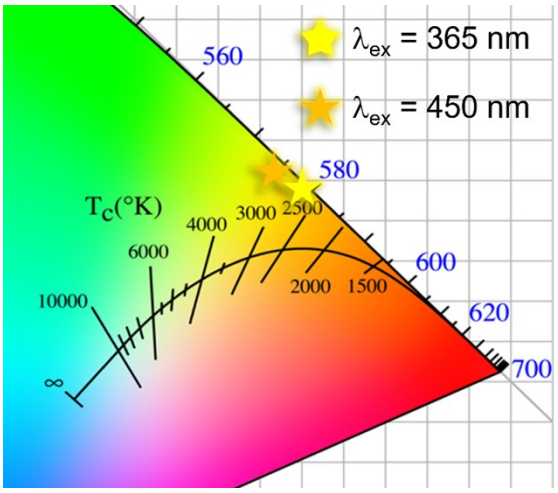


**Figure S4.** CIE coordinates of $(C_{20}H_{20}P)_2TeCl_6$ excited at 365 nm (0.4599,0.5114) and 450 nm (0.464,0.5215) at room temperature. The triangle represents the chromatic coordinate position at 365 nm excitation, and the square represents the chromatic coordinate position at 450 nm excitation.

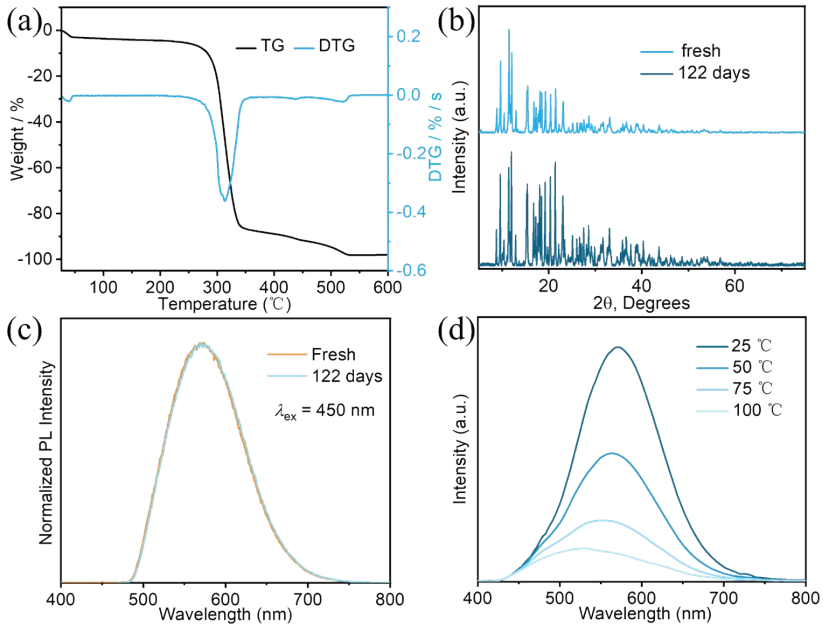


**Figure 5.** TG and DTG diagrams of $(C_{20}H_{20}P)_2TeCl_6$. **(b)** PXRD of fresh $(C_{20}H_{20}P)_2TeCl_6$ powder and the powder after being exposed in air for 122 days. **(c)** PL spectra of fresh $(C_{20}H_{20}P)_2TeCl_6$ and after exposure to air for 122 days under excitation at 450 nm. **(d)** High temperature-dependent spectroscopy.

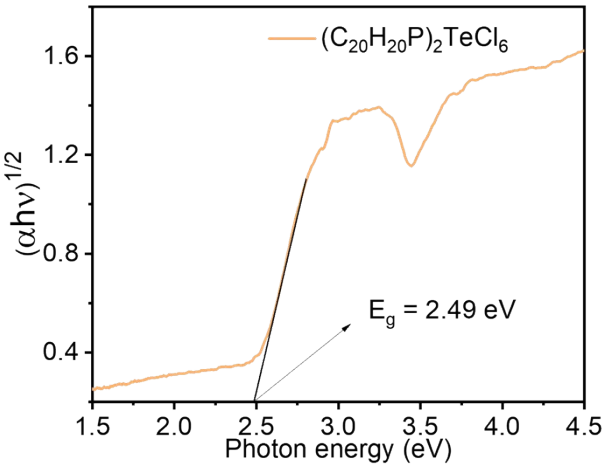


**Figure S6.** The extrapolations of band gap energy of $(C_{20}H_{20}P)_2TeCl_6$.

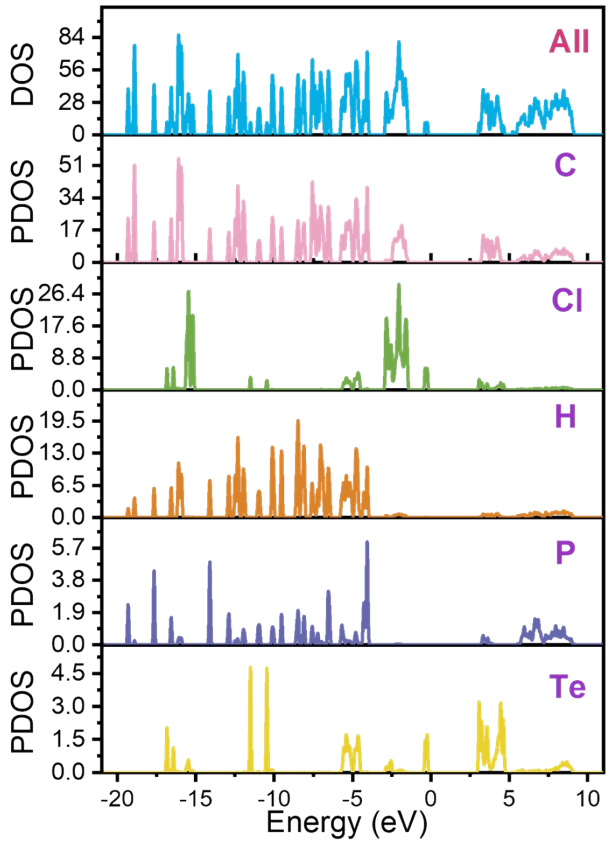


**Figure S7.** The total and orbital-projected partial density of states of $(C_{20}H_{20}P)_2TeCl_6$.

**Table S1.** Main parameters of processing and refinement of the $(C_{20}H_{20}P)_2TeCl_6$ sample.

| | |
|---|---|
| Chemical formula | $C_{20}H_{20}Cl_3PTe_{0.50}$ |
| Molecular weight | 461.48 |
| Temperature (K) | 301(2) |
| Space Group, *Z* | *P*-1, 2 |
| *a* (Å) | 10.2961(3) |
| *b* (Å) | 10.4440(3) |
| *c* (Å) | 10.8938(3) |
| *α* (°) | 80.080(3) |
| *β* (°) | 66.809(3) |
| *γ* (°) | 73.849(3) |
| *V* (Å$^3$) | 1031.67(6) |
| $\rho_{calc}$(g/cm$^3$) | 1.486 |
| μ (mm$^{-1}$) | 10.209 |
| Reflections measured | 19334 |
| Reflections independent | 4211 |
| Reflections with $F > 4\sigma(F)$ | 4057 |
| $2\theta_{max}$ (°) | 152.788 |
| *h*, *k*, *l* - limits | $-12 \le h \le 12$; $-13 \le k \le 13$; $-13 \le l \le 13$ |
| $R_{int}$ | 0.0541 |
| *Refinement results* | |
| The weighed refinement of $F^2$ | $w=1/[\sigma^2(F_o^2)+(0.0855P)^2+0.1317P]$ where $P=\max(F_o^2+2F_c^2)/3$ |
| Number of refinement parameters | 223 |
| $R1[F_o > 4\sigma(F_o)]$ | 0.0420 |
| *wR2* | 0.1164 |
| *Goof* | 1.075 |
| $\Delta\rho_{max}$(e/Å$^3$) | 1.190 |
| $\Delta\rho_{min}$(e/Å$^3$) | -1.139 |
| $(\Delta/\sigma)_{max}$ | <0.001 |
| Extinction coefficient (SHELXL 2014/7) | none |

**Table S2.** The main bond lengths (Å) of compound $(C_{20}H_{20}P)_2TeCl_6$

| | | | |
|---|---|---|---|
| Te—Cl1 | 2.5344(9) | Te—Cl1$^i$ | 2.5344(9) |
| Te—Cl3$^i$ | 2.5366(9) | Te—Cl3 | 2.5366(9) |
| Te—Cl2 | 2.5418(9) | Te—Cl2$^i$ | 2.5418(9) |
| P—C7 | 1.795(3) | P—C1 | 1.796(3) |
| P—C13 | 1.796(3) | P—C19 | 1.799(4) |
| C1—C6 | 1.382(5) | C1—C2 | 1.389(6) |
| C2—C3 | 1.377(6) | C3—C4 | 1.372(7) |
| C4—C5 | 1.359(7) | C5—C6 | 1.393(5) |
| C7—C12 | 1.385(5) | C7—C8 | 1.395(5) |
| C8—C9 | 1.381(6) | C9—C10 | 1.372(6) |
| C10—C11 | 1.368(6) | C11—C12 | 1.399(5) |
| C13—C14 | 1.384(5) | C13—C18 | 1.395(5) |
| C14—C15 | 1.377(6) | C15—C16 | 1.373(8) |

| | | | |
|---|---|---|---|
| C16—C17 | 1.377(8) | C17—C18 | 1.385(6) |
| C19—C20 | 1.511(6) | | |

Symmetry codes: (i) -x+1, -y+2, -z

**Table S3.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | *Occ.* |
|---|---|---|---|---|---|
| Te | 0.5000 | 1.0000 | 0.0000 | 0.05161(12) | 1 |
| Cl1 | 0.63887(10) | 0.77377(9) | 0.06248(9) | 0.0700(2) | 1 |
| Cl2 | 0.65991(11) | 0.97777(10) | -0.24573(9) | 0.0763(2) | 1 |
| Cl3 | 0.32680(12) | 0.88877(11) | -0.03207(12) | 0.0818(3) | 1 |
| P | 0.70951(8) | 0.65199(8) | 0.42375(8) | 0.05425(19) | 1 |
| C1 | 0.8128(3) | 0.7768(3) | 0.3823(3) | 0.0578(7) | 1 |
| C2 | 0.8143(5) | 0.8641(5) | 0.2704(4) | 0.0761(10) | 1 |
| H2 | 0.7580 | 0.8604 | 0.2226 | 0.091* | 1 |
| C3 | 0.8989(6) | 0.9562(5) | 0.2301(5) | 0.0883(12) | 1 |
| H3 | 0.9003 | 1.0143 | 0.1548 | 0.106* | 1 |
| C4 | 0.9811(5) | 0.9620(4) | 0.3012(5) | 0.0821(11) | 1 |
| H4 | 1.0382 | 1.0243 | 0.2738 | 0.099* | 1 |
| C5 | 0.9797(5) | 0.8774(4) | 0.4113(5) | 0.0786(11) | 1 |
| H5 | 1.0362 | 0.8822 | 0.4584 | 0.094* | 1 |
| C6 | 0.8948(4) | 0.7836(4) | 0.4544(4) | 0.0676(8) | 1 |
| H6 | 0.8933 | 0.7266 | 0.5303 | 0.081* | 1 |
| C7 | 0.6984(3) | 0.5676(3) | 0.5845(3) | 0.0562(7) | 1 |
| C8 | 0.6483(4) | 0.6408(4) | 0.6965(4) | 0.0695(9) | 1 |
| H8 | 0.6273 | 0.7337 | 0.6871 | 0.083* | 1 |
| C9 | 0.6300(5) | 0.5750(5) | 0.8213(4) | 0.0773(10) | 1 |
| H9 | 0.5980 | 0.6236 | 0.8960 | 0.093* | 1 |
| C10 | 0.6590(5) | 0.4381(5) | 0.8355(4) | 0.0763(10) | 1 |
| H10 | 0.6451 | 0.3948 | 0.9202 | 0.092* | 1 |
| C11 | 0.7078(4) | 0.3639(4) | 0.7274(4) | 0.0711(9) | 1 |
| H11 | 0.7268 | 0.2711 | 0.7384 | 0.085* | 1 |
| C12 | 0.7290(4) | 0.4293(4) | 0.6000(3) | 0.0601(7) | 1 |
| H12 | 0.7637 | 0.3798 | 0.5257 | 0.072* | 1 |
| C13 | 0.7990(4) | 0.5303(3) | 0.3007(3) | 0.0580(7) | 1 |
| C14 | 0.9482(5) | 0.4842(5) | 0.2606(4) | 0.0831(12) | 1 |
| H14 | 1.0004 | 0.5205 | 0.2929 | 0.100* | 1 |
| C15 | 1.0194(6) | 0.3847(6) | 0.1729(6) | 0.1027(16) | 1 |
| H15 | 1.1196 | 0.3535 | 0.1467 | 0.123* | 1 |
| C16 | 0.9433(6) | 0.3313(5) | 0.1239(5) | 0.0952(14) | 1 |
| H16 | 0.9920 | 0.2646 | 0.0641 | 0.114* | 1 |
| C17 | 0.7947(6) | 0.3766(5) | 0.1630(5) | 0.0870(13) | 1 |
| H17 | 0.7436 | 0.3400 | 0.1297 | 0.104* | 1 |
| C18 | 0.7209(5) | 0.4761(4) | 0.2517(4) | 0.0713(9) | 1 |
| H18 | 0.6206 | 0.5064 | 0.2782 | 0.086* | 1 |

| | | | | | |
|---|---|---|---|---|---|
| C19 | 0.5288(4) | 0.7276(4) | 0.4263(4) | 0.0684(8) | 1 |
| H19A | 0.5361 | 0.7711 | 0.3384 | 0.082* | 1 |
| H19B | 0.4782 | 0.6572 | 0.4421 | 0.082* | 1 |
| C20 | 0.4376(5) | 0.8288(5) | 0.5293(5) | 0.0898(13) | 1 |
| H20A | 0.3437 | 0.8631 | 0.5226 | 0.108* | 1 |
| H20B | 0.4265 | 0.7867 | 0.6173 | 0.108* | 1 |
| H20C | 0.4845 | 0.9008 | 0.5134 | 0.108* | 1 |

**Table S4.** Hydrogen-bond geometry in the $(C_{20}H_{20}P)_2TeCl_6$ structure (Å, °)

| D—H | d(D—H) | d(H···A) | < D—H···A | D···A | A | Transformation for A atom |
|---|---|---|---|---|---|---|
| C(9) —H(9) | 0.93 | 2.81 | 153 | 3.660(5) | Cl(1) | x,y,1+z |
| C(15) —H(15) | 0.93 | 2.81 | 141 | 3.579(6) | Cl(1) | 2-x,1-y,-z |
| C(19) —H(19A) | 0.97 | 2.76 | 152 | 3.652(4) | Cl(1) | x,y,z |