Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Stabilized photoemission from organic molecules in zero-dimensional hybrid Zn and Cd halides

*Tielyr D. Creason,[1] Hadiah Fattal,[1] Isaiah W. Gilley,[1] Brett N. Evans,[1] Jie Jiang,[2] Ruth Pachter,[2] Daniel T. Glatzhofer,[1] and Bayram Saparov[1]**

[1]Department of Chemistry and Biochemistry, University of Oklahoma, 101 Stephenson Parkway, Norman, OK 73019, United States
[2]Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH, USA

*Corresponding authors: saparov@ou.edu

Table S1. Selected single crystal data and structure refinement parameters for R_2CdCl_4.

Formula	$(C_{13}H_{12}N)_2CdCl_4$
Formula weight (g/mol)	618.67
Temperature (K)	295(2)
Radiation, wavelength (Å)	Mo Kα, 0.71073
Crystal system	Monoclinic
Space group	*C*2/*c*
Z	4
Unit cell parameters	*a* = 14.909(3) Å *b* = 12.1382(17) Å *c* = 15.403(8) Å β = 104.058(4)°
Volume (Å^3)	2704.0(8)
Density (ρ_{calc}) (g/cm^3)	1.520
Absorption coefficient (μ) (mm^{-1})	1.220
$\theta_{min} - \theta_{max}$ (º)	2.190 – 24.711
Reflections collected	24977
Independent reflections	2302
R^a indices ($I > 2\sigma(I)$)	R_1 = 0.0413 wR_2 = 0.0791
Goodness-of-fit on F^2	1.224
Largest diff. peak and hole (e$^-$/Å^3)	0.440 and -0.235

$_aR_1 = \sum||F_0| - |F_c||/\sum|F_0|; WR_2 = |\Sigma|w(F_0^2 - F_c^2)^2/\sum|wF_0^{22}|_{1/2}$

where $w = 1/|\sigma^2F_0^2 + (AP)^2 + BP|$, with $P = (F_0^2 + 2F_c^2)/3$ and weight coefficients *A* and *B*

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (U_{eq}[a]) for R_2CdCl_4.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Cd(1)	0.000000	0.29030(5)	0.250000	0.0934(2)
Cl(1)	0.09694(8)	0.39169(13)	0.17127(9)	0.1058(5)
Cl(2)	0.11555(8)	0.16940(13)	0.34604(11)	0.1256(6)
N(1)	0.2897(3)	0.3416(6)	0.3283(4)	0.136(2)
C(1)	0.3335(4)	0.2750(6)	0.3920(5)	0.161(3)
C(2)	0.4240(4)	0.2909(6)	0.4311(4)	0.131(2)
C(3)	0.4705(3)	0.3769(5)	0.4052(3)	0.0922(15)
C(4)	0.4220(4)	0.4415(5)	0.3388(4)	0.1076(17)
C(5)	0.3319(4)	0.4247(6)	0.2998(4)	0.123(2)
C(6)	0.5683(4)	0.4017(5)	0.4445(4)	0.1087(18)
C(7)	0.6233(4)	0.3556(5)	0.5085(4)	0.1125(18)
C(8)	0.7215(3)	0.3805(5)	0.5484(4)	0.0939(15)
C(9)	0.7653(4)	0.3261(5)	0.6239(4)	0.1171(19)
C(10)	0.8554(4)	0.3452(5)	0.6636(4)	0.130(2)
C(11)	0.9051(4)	0.4194(5)	0.6293(4)	0.1062(17)
C(12)	0.8643(4)	0.4745(5)	0.5549(4)	0.118(2)
C(13)	0.7720(4)	0.4557(5)	0.5133(4)	0.1116(18)

[a]*U*eq is defined as one-third of the trace of the orthogonalized *Uij* tensor.

Table S3. A comparison of bond distances and angles within the $[CdCl_4]^{2-}$ tetrahedra in R_2CdCl_4.

Atom pair	**Distance (Å)**	**Label**	**Angle (°)**
Cd – Cl1	2.4343(14)	Cl1-Cd-Cl1	119.26(7)
Cd – Cl2	2.4641(14)	Cl1-Cd-Cl2 ×2	100.78(5)
		Cl1-Cd-Cl2 ×2	114.53(6)
		Cl2-Cd-Cl2	106.90

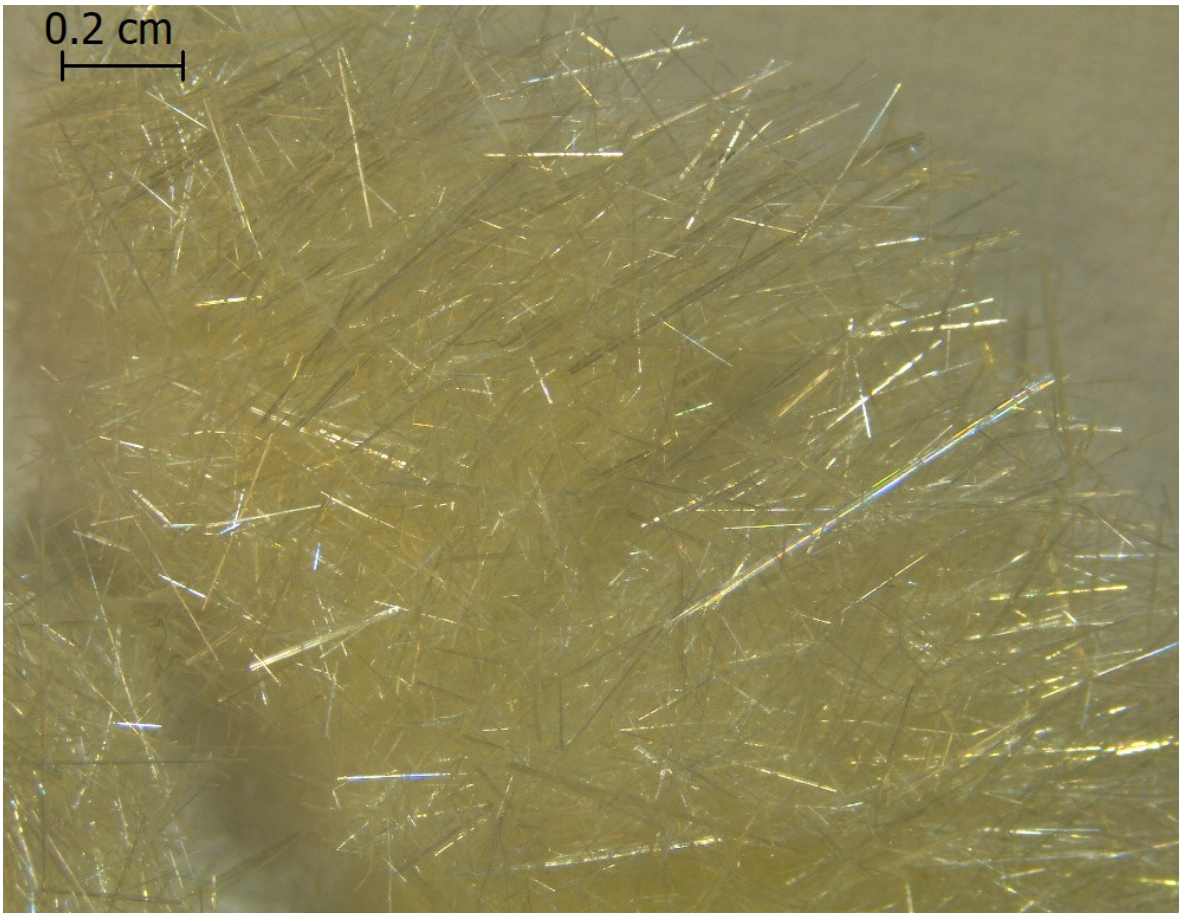

Fig. S1. Picture of RCl single crystals synthesized from slow evaporation.

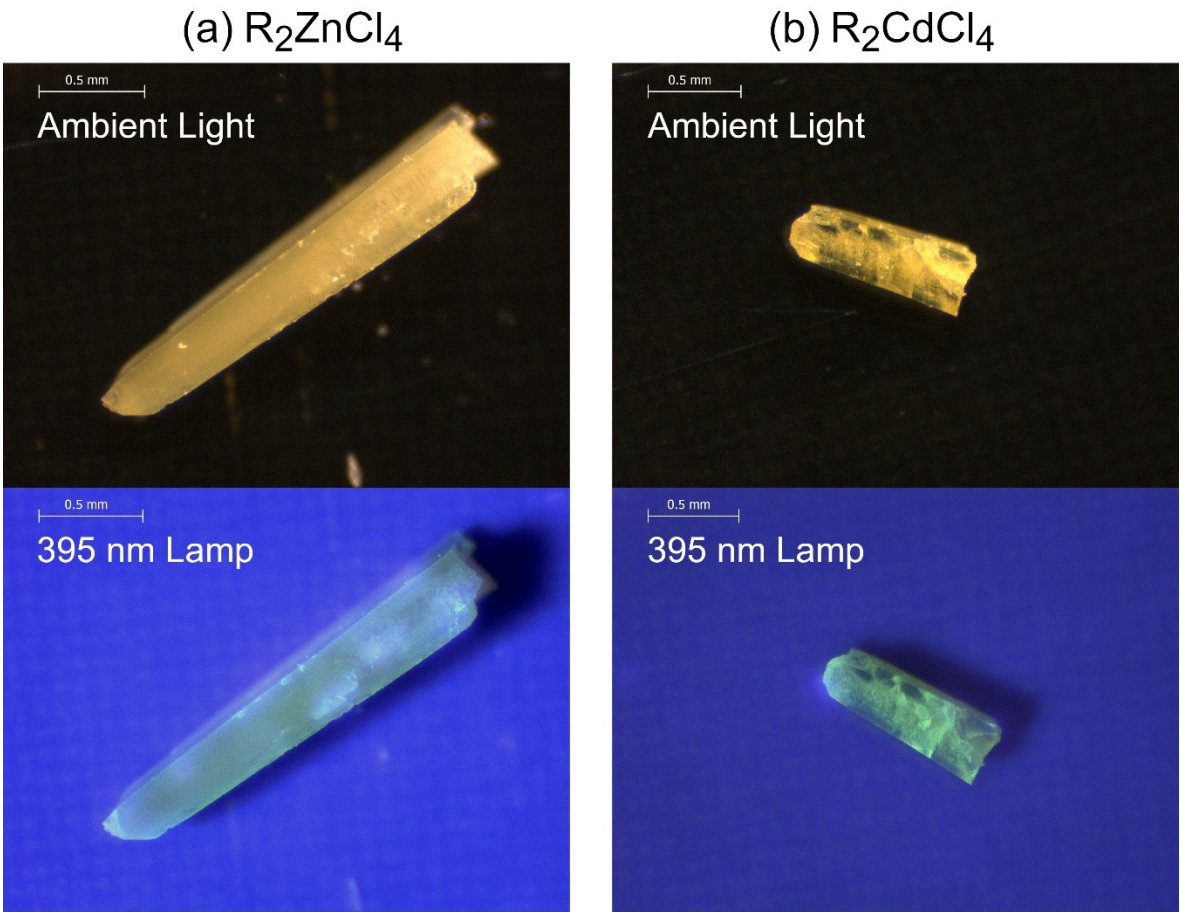

Fig. S2. Pictures of (a) R_2ZnCl_4 and (b) R_2CdCl_4 single crystals under (top) ambient light and (bottom) a 395 nm lamp.

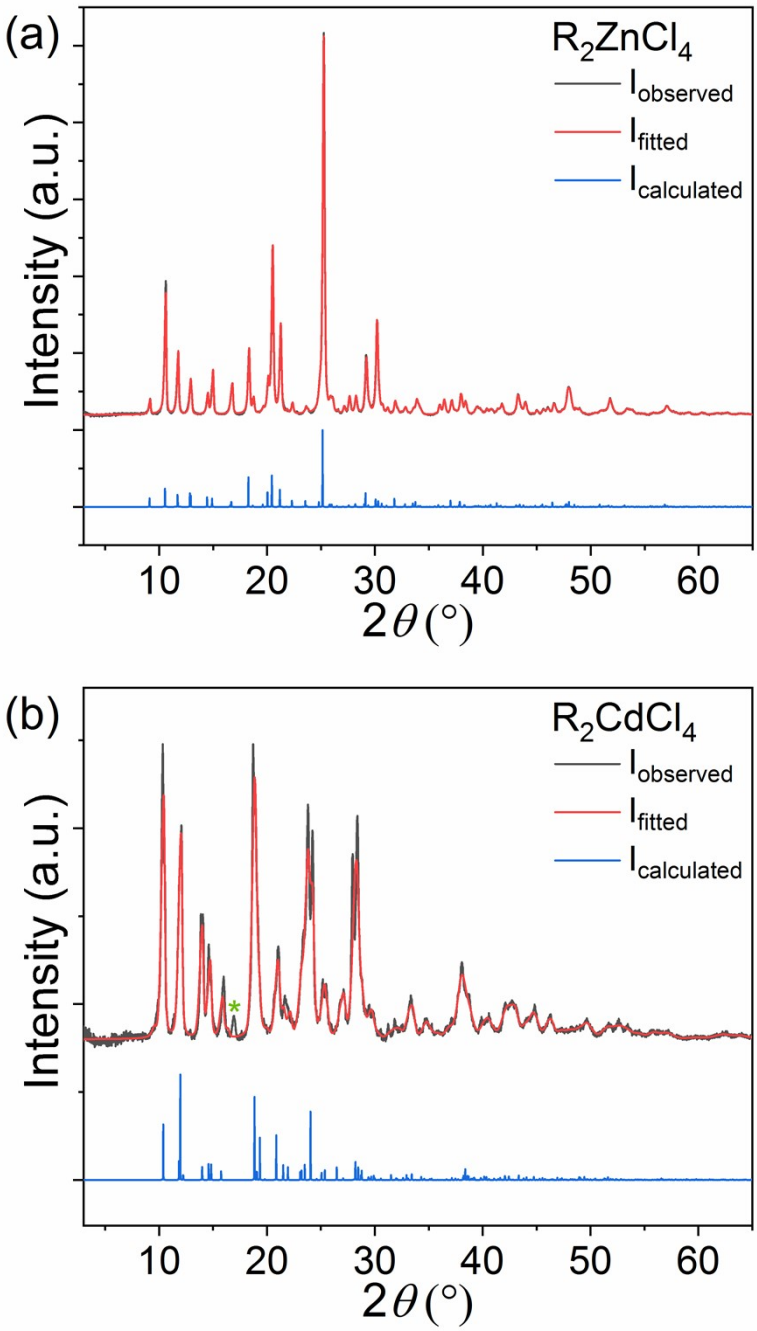

Fig. S3. Room temperature powder X-ray diffraction (PXRD) patterns of (a) R_2ZnCl_4 and (b) R_2CdCl_4. The green asterisk represents a small impurity of RCl that forms when grinding R_2CdCl_4.

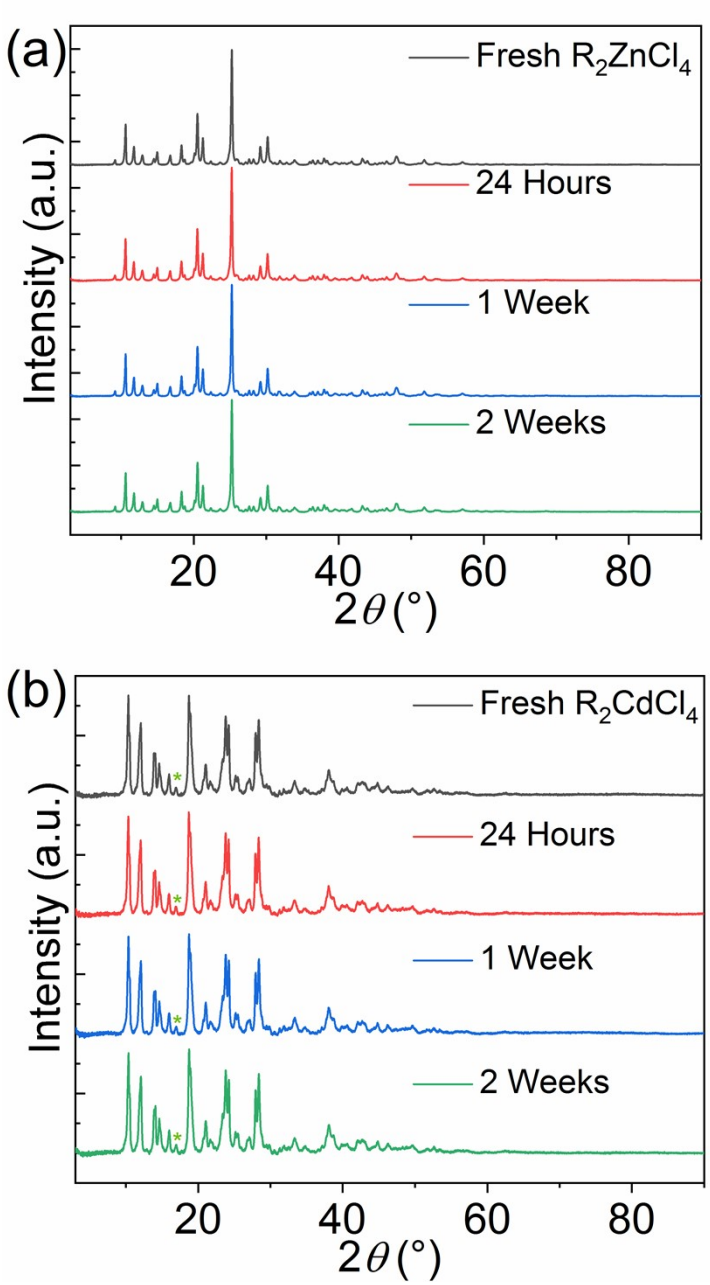

Fig. S4. PXRD measured over a 2-week period for (a) R_2ZnCl_4 and (b) R_2CdCl_4. When left in ambient air, neither sample demonstrates noticeable degradation. The green asterisk indicates the presence of RCl impurity formed during the PXRD sample preparation.

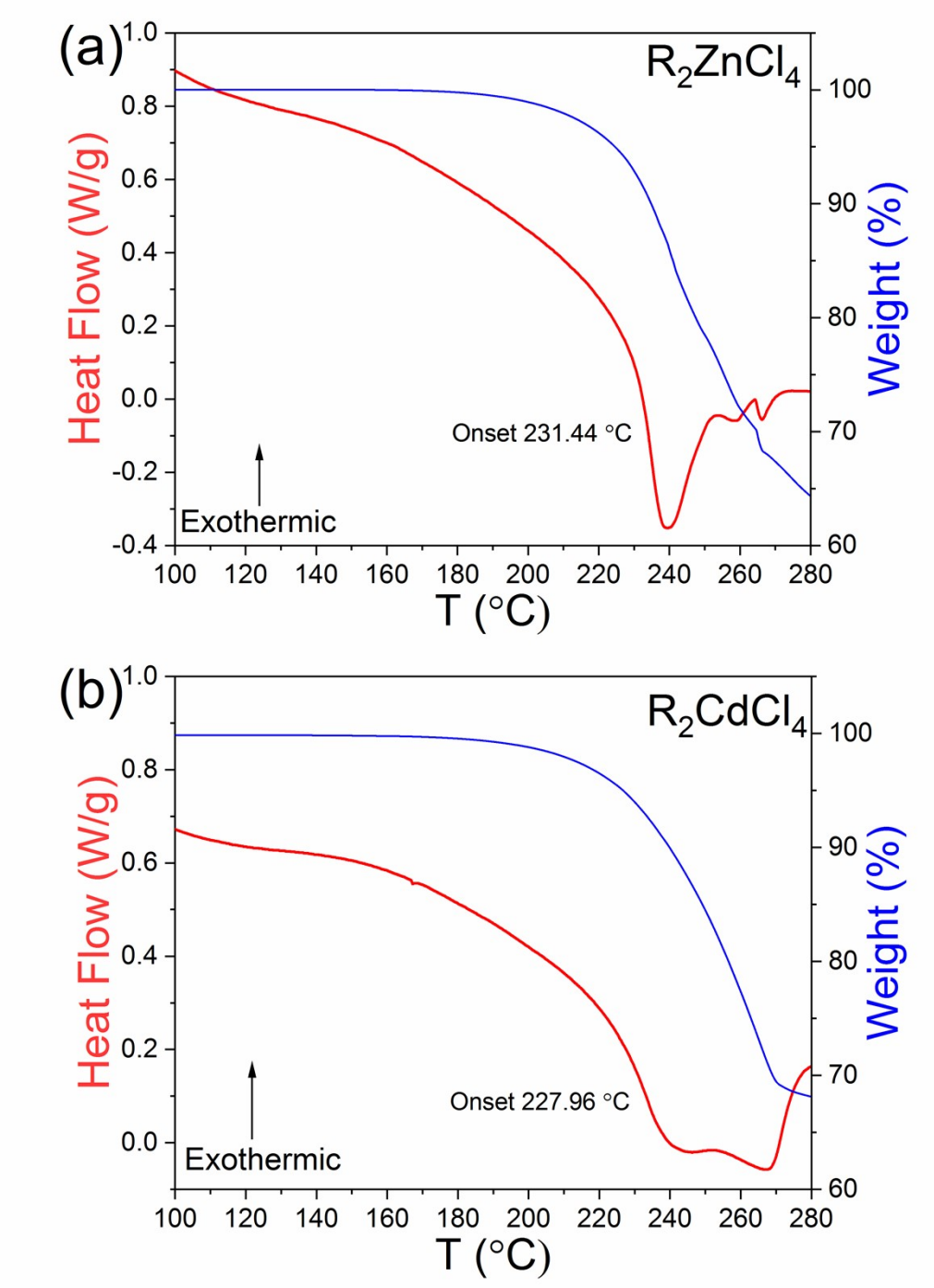

Fig. S5. Thermogravimetric analysis (TGA, in blue) and differential scanning calorimetry (DSC, in red) plots for (a) R_2ZnCl_4 and (b) R_2CdCl_4.

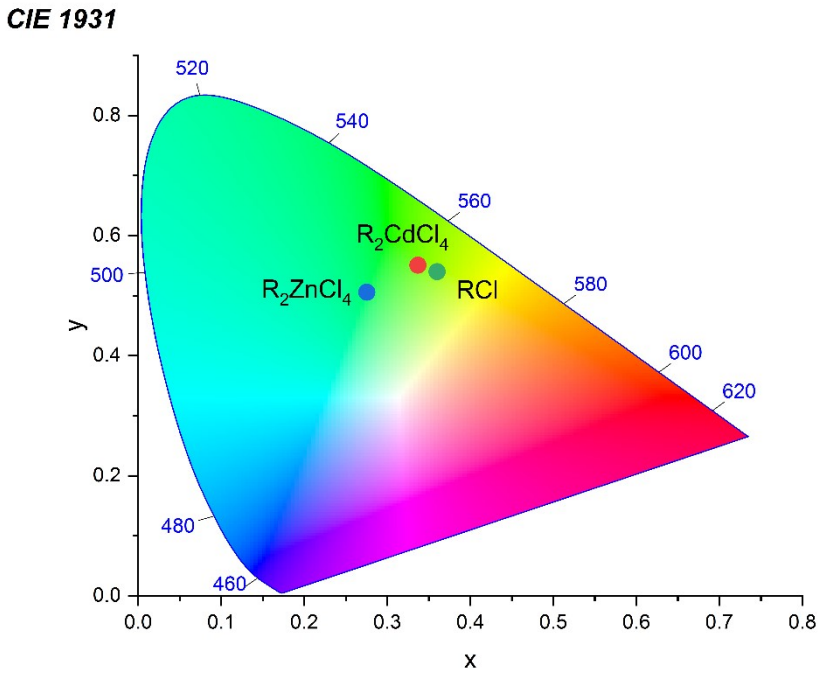

Fig. S6. The Commission Internationale de l'Eclairage (CIE) emission color coordinates for R_2ZnCl_4 (blue dot) , R_2CdCl_4 (red dot), and RCl (green dot).

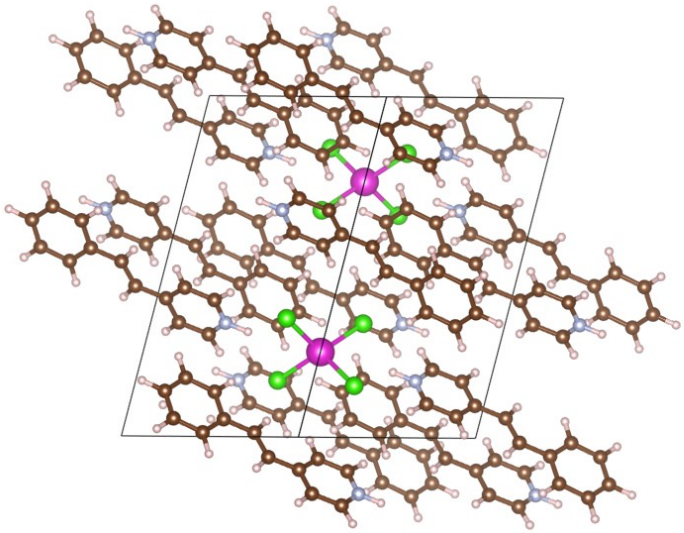

Fig. S7. DFT-optimized (PBE functional) primitive unit cell for R_2CdCl_4

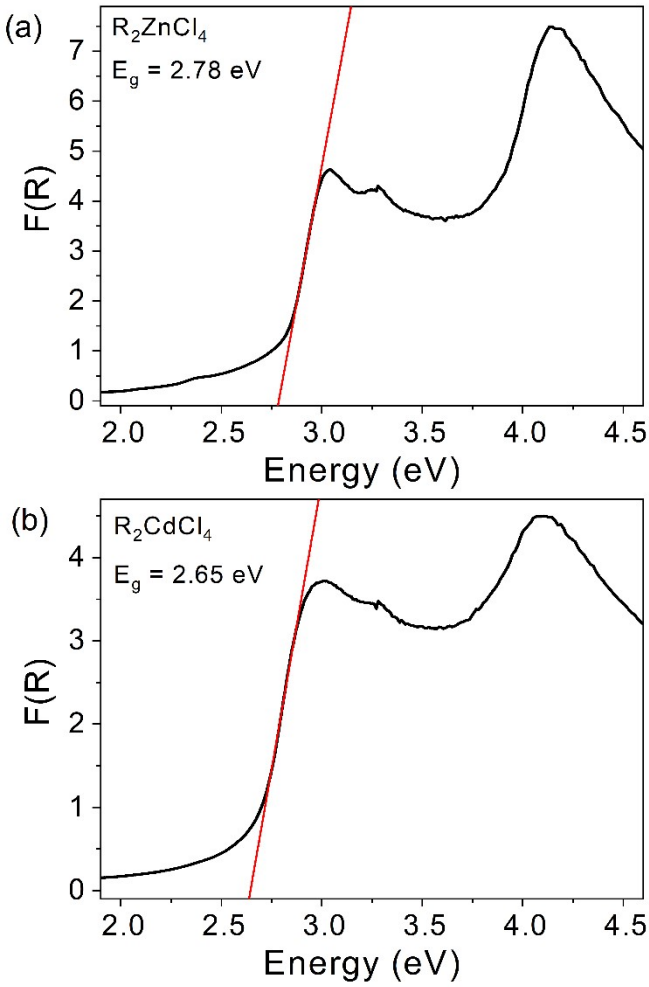

Fig. S8. The Kubelka-Munk pseudoabsorbance plots for (a) R_2ZnCl_4 and (b) R_2CdCl_4.

.