Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Zero-Dimensional Plate-shaped Copper Halide Crystals with Green-yellow Emission

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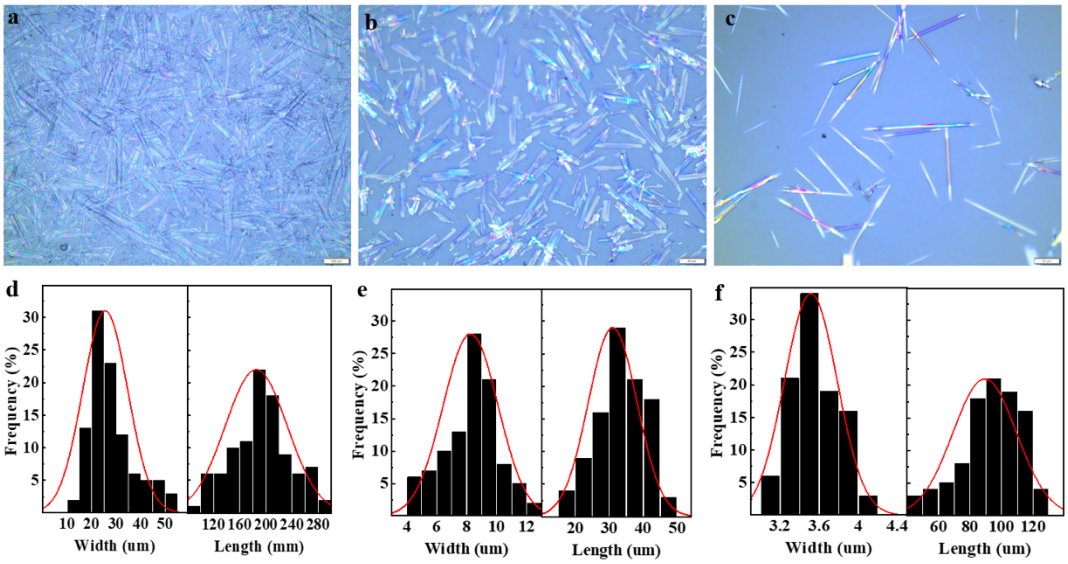

Figure S1. (a, b, c) Optical microscope photograph of as prepared micro-plate crystal at reaction concentrations of 0.167/ 0.083/ 0.08 M CuI (a: the scale bar is 100 μm; b, c: the scale bar is 20 μm) and (d, e, f) corresponding to their size distributions of micro-plates.

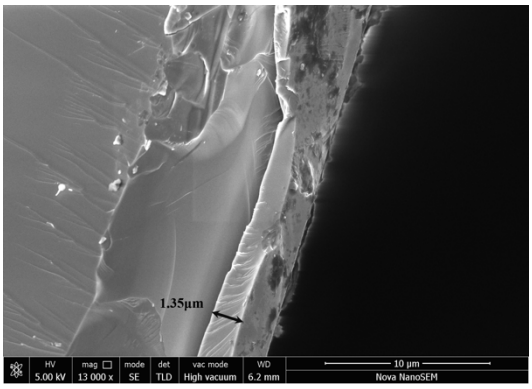

Figure S2. The cross-sectional SEM images of a micro-plate. The thickness of micro-sheet was 1.35 µm.

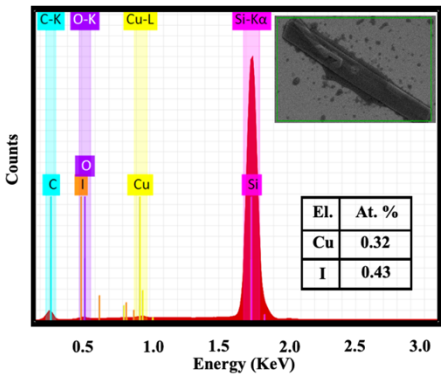

Figure S3. Elemental analysis results of the selected micro-plate crystal.

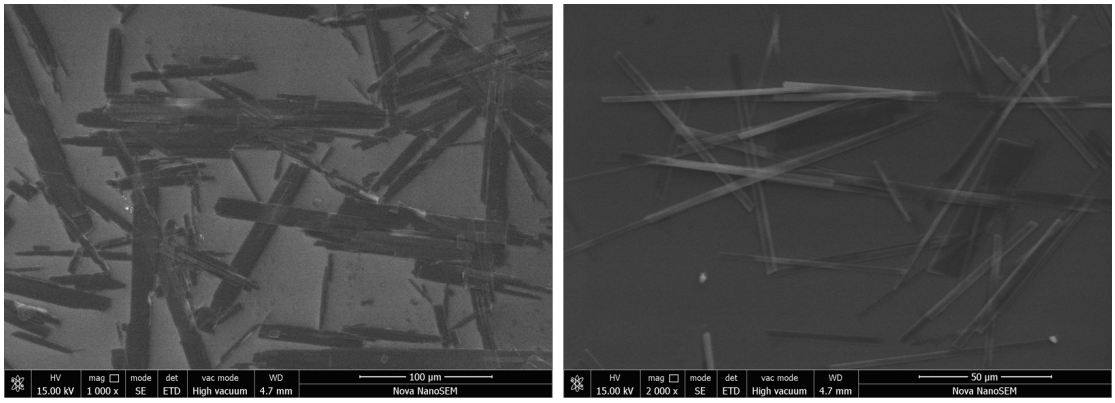

Figure S4. The SEM of two samples with different reaction concentrations (0.167M and 0.08 M)

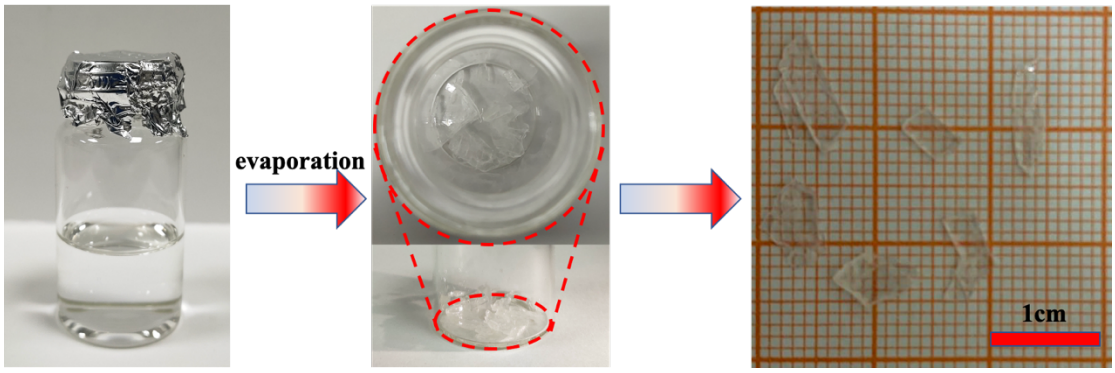

Figure S5. Schematic description of crystal growth pathways of $(DTA)_2Cu_2Cl_4$. The plate-like crystals have sizes on the order of millimeter.

Table S1. Crystal data and structure refinement for **$(DTA)_2Cu_2Cl_4$**

Compound	**$(DTA)_2Cu_2Cl_4$**
Empirical formula	C30H68N2Cu2I4
Formula weight	1091.56
Temperature/K	201K
Crystal system	$P\bar{1}$
a/Å	8.7798
b/Å	10.5044
c/Å	22.9998
α	86.9230°
β	82.8590°
γ	75.8660°
Volume/$Å^3$	2040.42(2)
Z	2
P_{cake} g/cm^3	1.777
μ/mm^{-1}	4.088
F(000)	1064.0
Radiation	Mokα (λ=0.71073)
2θ/°	5.000 to 50.842
Index ranges	-10≤h≤10,-12≤k≤12,-27≤l≤27
Independent reflections	7551
Parameters	351
R1, wR2	0.0153,0.0356
Goodness-of-fit onF^2	1.050

$R1 = \sum||F_o|-|F_c||/\sum|F_o|$. $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S2. Selected bond angles (°) for **$(DTA)_2Cu_2Cl_4$**.

Bonds	Angle/º
I1 Cu1 I2	125.25(2)
I1 Cu1 I3	119.76(2)
I2 Cu1 I3	114.99(1)
I2 Cu2 I4	115.50(1)
I2 Cu2 I3	106.68(1)
I4 Cu2 I4#	102.69(1)
I3 Cu2 I4	117.00(1)
I3 Cu2 I4#	109.76(1)
I2 Cu2 I4#	105.51(1)

Table S3. Selected bond distances (Å) for **$(DTA)_2Cu_2Cl_4$**

Bonds	**bond distances/Å**
Cu1 I1	2.517(5)
Cu1 I2	2.554(3)
Cu1 I3	2.560(3)
Cu2 I2	2.697(6)
Cu2 I3	2.680(3)
Cu2 I4	2.707(4)
Cu2 I4#	2.642(5)

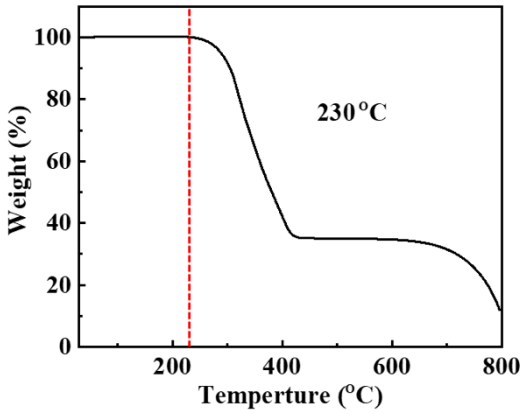

Figure S6. Thermogravimetric analysis of $(DTA)_2Cu_2I_4$ crystal powder.

Table S4. Calculated attachment energies for different crystal faces of the $(DTA)_2Cu_2I_4$ crystal.

hkl	d_{hkl}/Å	E_{att} (Total)/kcal·mol^{-1}	% Total facet area
(0 0 1)	22.81	-32.06	51.38
(0 1 0)	10.18	-83.85	20.50
(1 0 0)	8.46	-76.55	11.81

The growth morphology method was applied to investigate the shapes of organic molecular crystals in this study. In general, the growth rate of one crystal face is assumed to be proportional to its attachment energy (Eatt), that is, the face with lower attachment energy is slower growing and hence has more morphological importance. The attachment energy can be calculated by:

$$E_{att}=E_{lattice}-E_{slice}$$

Where $E_{lattice}$ is the lattice energy of the crystal and E_{slice} is the energy for a growth slice of thickness d_{hkl}, respectively.

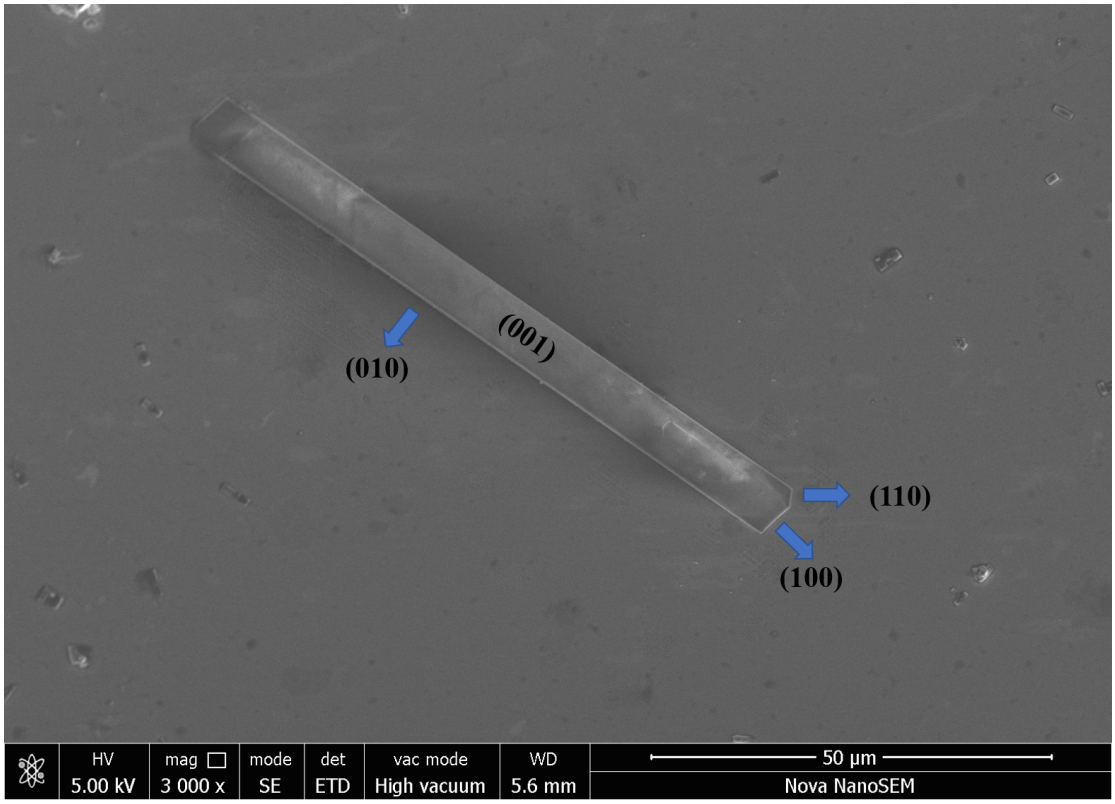

Figure S7. The high magnification SEM images of a micro-plate crystal with typical lattice planes.

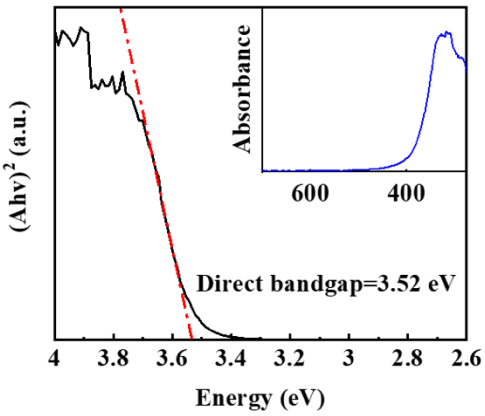

Figure S8. Tauc plots and corresponding optical diffuse reflection spectra (inset) of $(DTA)_2Cu_2I_4$.

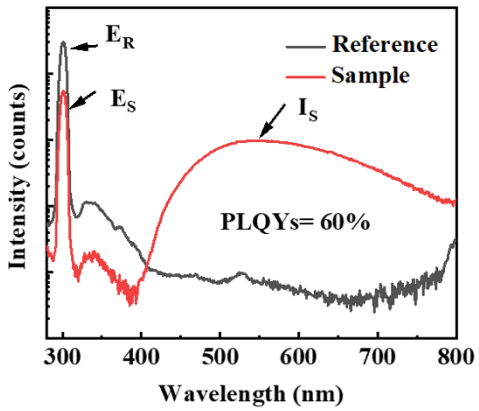

Figure S9. Excitation line of reference (300 nm) and emission spectrum of $(DTA)_2Cu_2I_4$ crystal powder collected by an integrating sphere system. The PLQYs was calculated based on the equation: $\eta_{QE} = I_S / (E_R - E_S)$, which I_S represents the luminescence emission spectrum of the sample, E_R is the spectrum of the excitation light from the empty integrated and E_S is the excitation spectrum for exciting the sample.

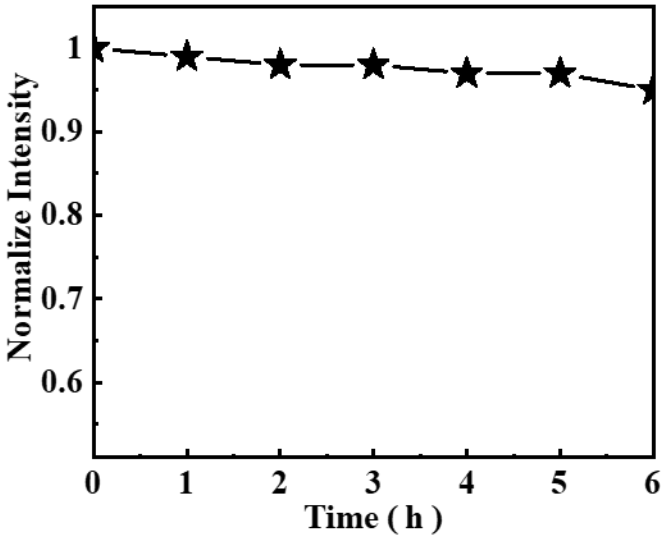

Figure S10. The PL intensities of cold-white phosphor exposing to UV light (302 nm) for 12 hours.

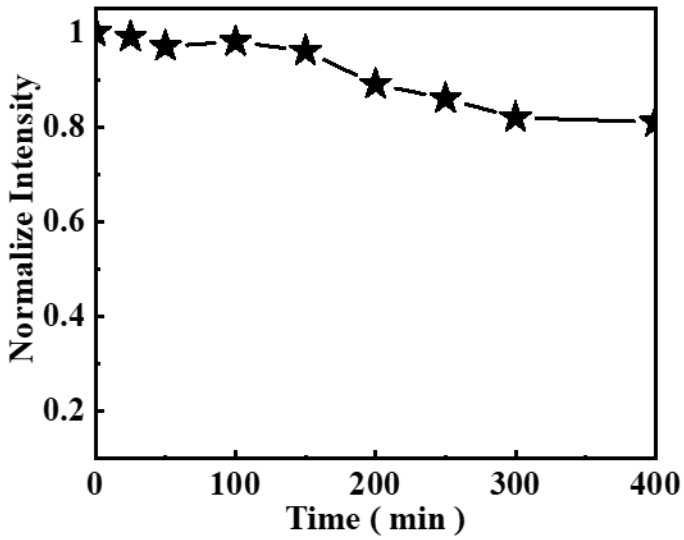

Figure S11. PL intensity of the WLED measured at different working time.

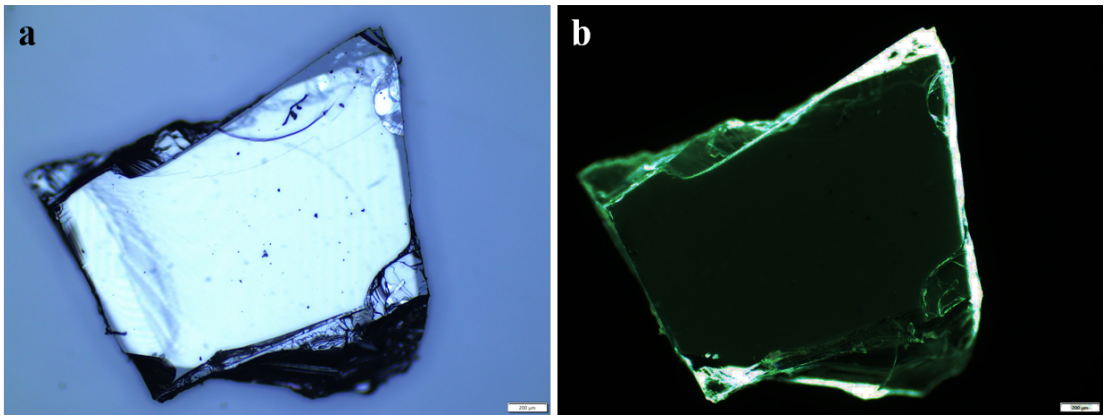

Figure S12. (a,b) The microscope and PL images of plate-like crystal (the scale bar is 200 μm).