Supporting Information

Molecular design towards efficient light-emitting copper(I) halide mononuclear hybrids

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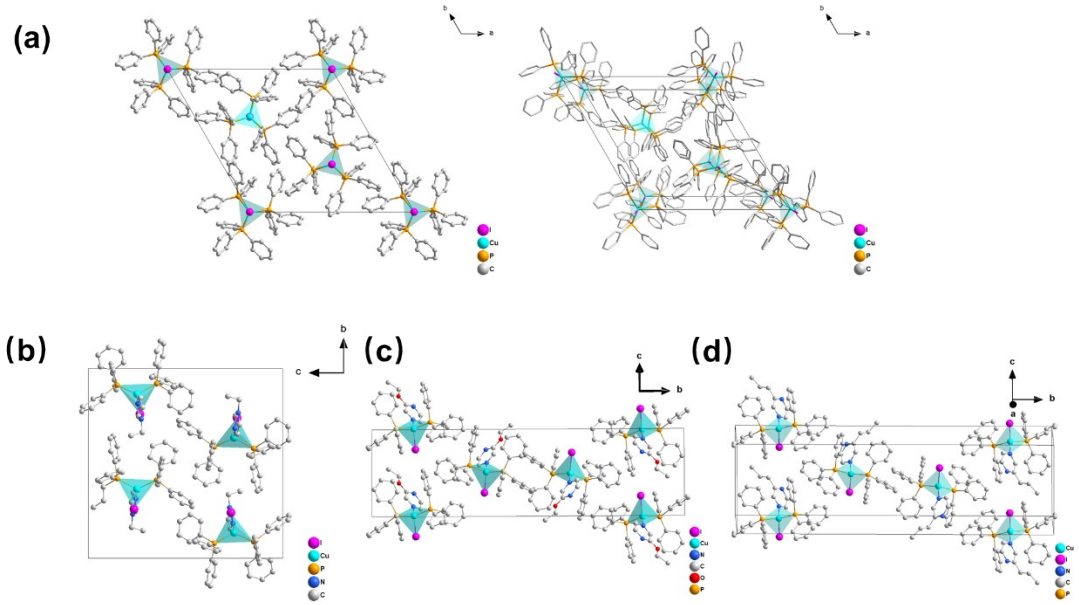

Figure S1. Single-crystal structure of $CuI(PPh_3)_3$ (a) and compound **1-3** (b) (c) (d) .

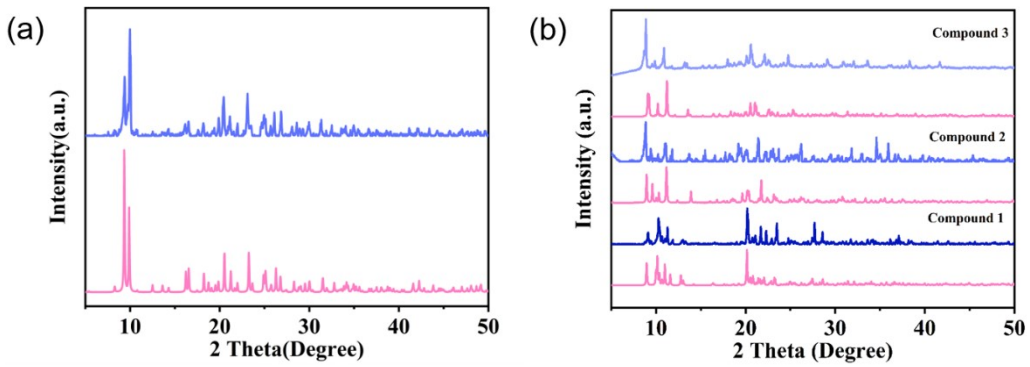

Figure S2. PXRD patterns of simulated (pink lines) and as-made (blue lines) of precursor $CuI(PPh_3)_3$ (a) and compounds **1-3** (b).

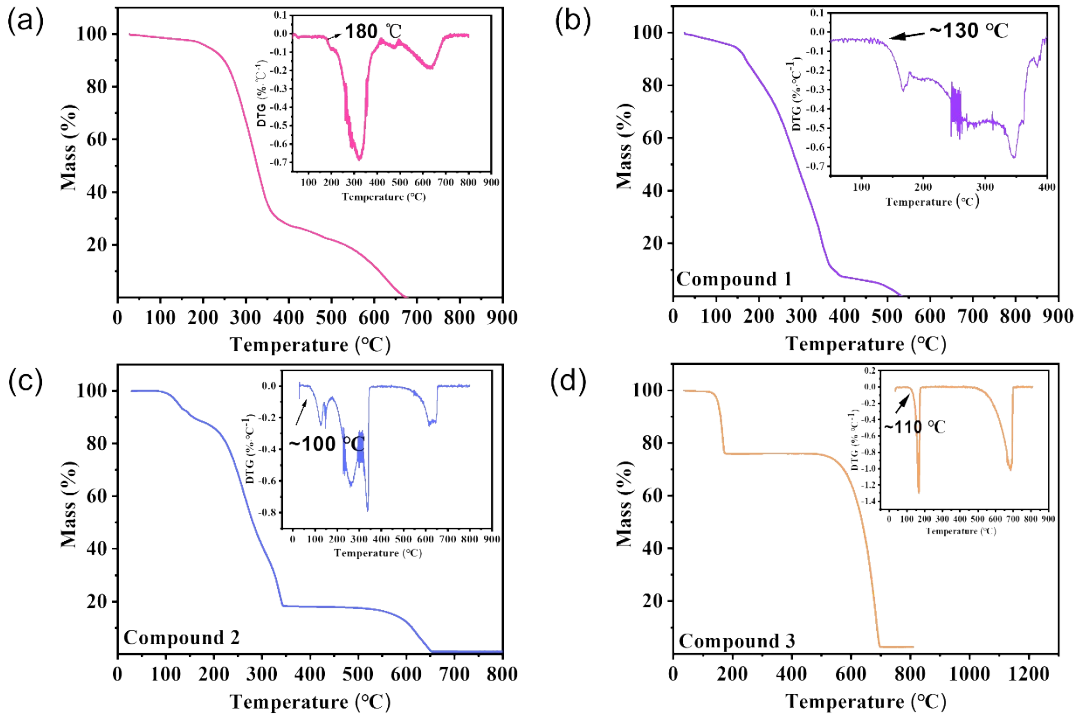

Figure S3. Thermogravimetric analysis curve of $CuI(PPh_3)_3$ (a) and compound **1-3** (b) (c) (d), respectively.

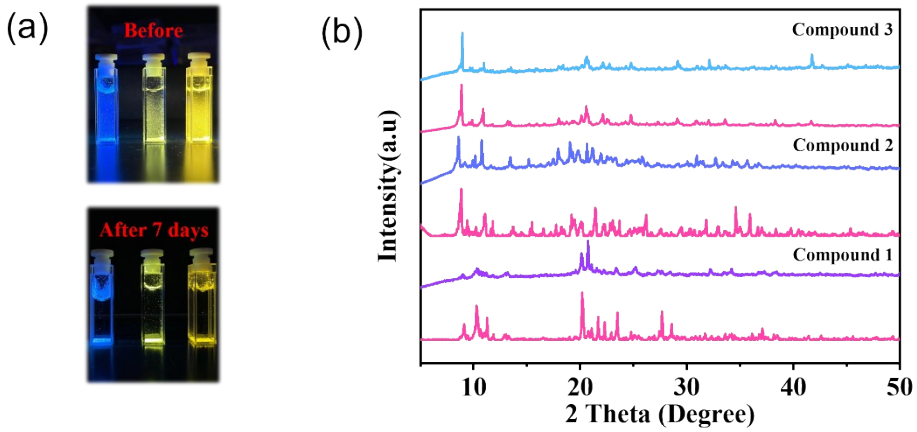

Figure S4. (a) Imagine of compound **1** and **3** before and after soaking in water. (b) PXRD pattern of compound **1-3** before (pink line) and after (blue lines) soaking.

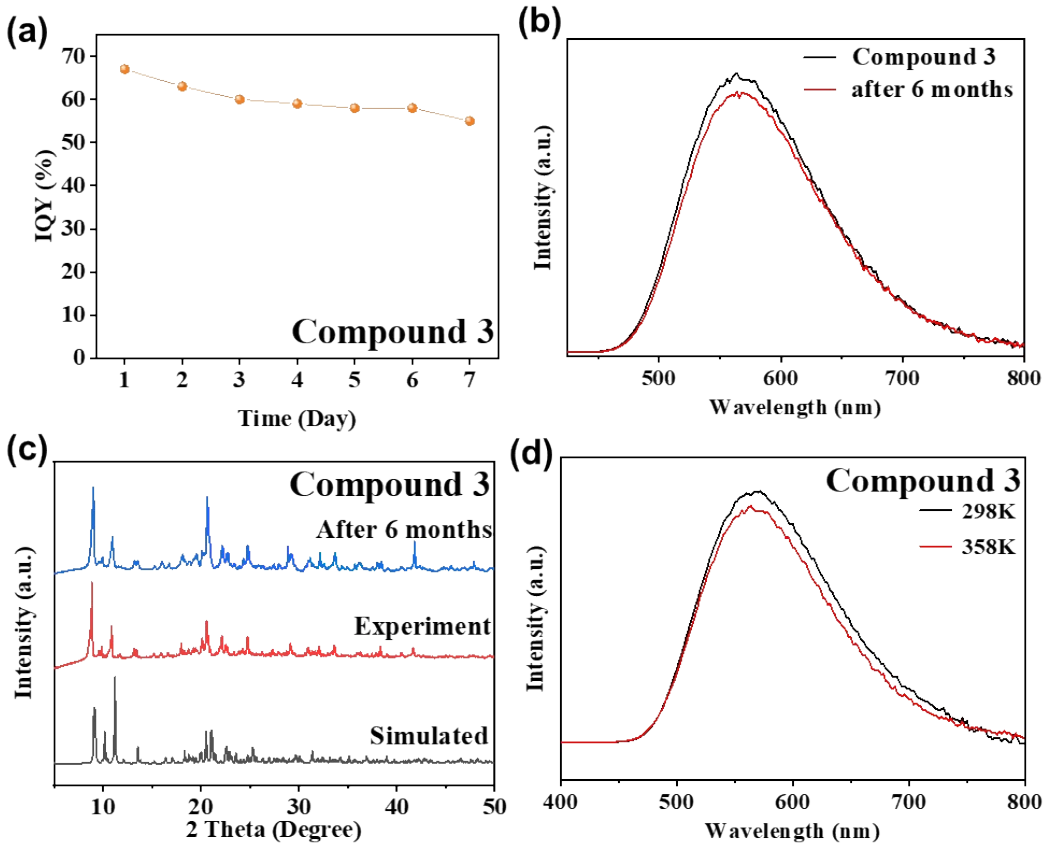

Figure S5. (a) The IQY of the sample compound **3** under UV irradiation. (b) The emission spectra of the fresh-made sample compound **3** and sample stored for 6 months. (c) The PXRD patterns of fresh-made sample and sample compound **3** stored for 6 months. (d) The emission spectra of fresh-made sample compound **3** and sample stored for 6 months

Table S1. The quantum efficiency and stability of reported copper halide hybrids with pyridine and pyrazine derivatives

Compound	λ_{em} [nm]	IQY [%]	Decomposition temperature [°C]
0D-CuBr(3-pc)$_3$[1]	535	98	Room temperature
1D-CuI(4-pc)[2]	433	35.8	100
1D-CuI(3,5-dm-py)[2]	490	35.3	100
1D-CuI(2,6-dm-pz)[2]	525	15.4	90
2D-CuI(pz)$_{0.5}$[3]	12.7	12.7	170
2D-CuI(*bpee*)$_{0.5}$[3]	695	1.0	300

Reference:

[1] C. Xu, L. Lu, L. Lv, Y. Li, F. Lin, Y. Yang, F. Lin, C. Luo, D. Luo and W. Liu, *Molecular Crystals and Liquid Crystals* **2020**, *709*, 54-60.

[2] X. Zhang, W. Liu, G. Z. Wei, D. Banerjee, Z. Hu and J. Li, *Journal of the American Chemical Society* **2014**, *136*, 14230-14236.
[3] W. Ki, X. Hei, H. T. Yi, W. Liu, S. J. Teat, M. Li, Y. Fang, V. Podzorov, E. Garfunkel and J. Li, *Chemistry of Materials* **2021**, *33*, 5317-5325.