Electronic Supplementary Information

An electron-transfer photochromic metal–organic framework (MOF) compound with long-lived charge-separated state and high-contrast photoswitchable luminescence

Xiu-Shuang Xing,[a,b] Zi-Wei Chen,[b] Li-Zhen Cai,[b] Cai Sun,[b] Lin-Rong Cai,[b,c] Ming-Sheng Wang,*[b] and Guo-Cong Guo*[b]

[a] *College of Chemistry, Fuzhou University, Fuzhou, Fujian, 350108, P. R. China*

[b] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.*

[c] *College of Materials Science and Engineering, Fujian Normal University, Fuzhou, Fujian 350007, P. R. China.*

** E-mail: gcguo@fjirsm.ac.cn, mswang@fjirsm.ac.cn.*

Table S1. Crystal data and structure refinements for **1**

Empirical formula	$Cd_3C_{30}H_{18}O_{18}N_2$
fw	1031.66
Temperature (K)	100
Crystal system	orthorhombic
Space group	*Ibam*
***a* (Å)**	20.780(1)
***b* (Å)**	7.9154(8)
***c* (Å)**	17.299(2)
***V* (Å^3)**	2845.4(5)
Z	4
D_{calcd} **(g cm^{-3})**	2.408
μ **(mm^{-1})**	18.701
GOF on F^2	1.00
$R_1{}^a$ **[$I > 2\sigma(I)$]**	0.039
$wR_2{}^b$ **[$I > 2\sigma(I)$]**	0.107
$\Delta\rho_{max}/\Delta\rho_{min}$**(e Å^{-3})**	1.34/–1.19

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$; [b] $wR_2 = \sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]^{1/2}$

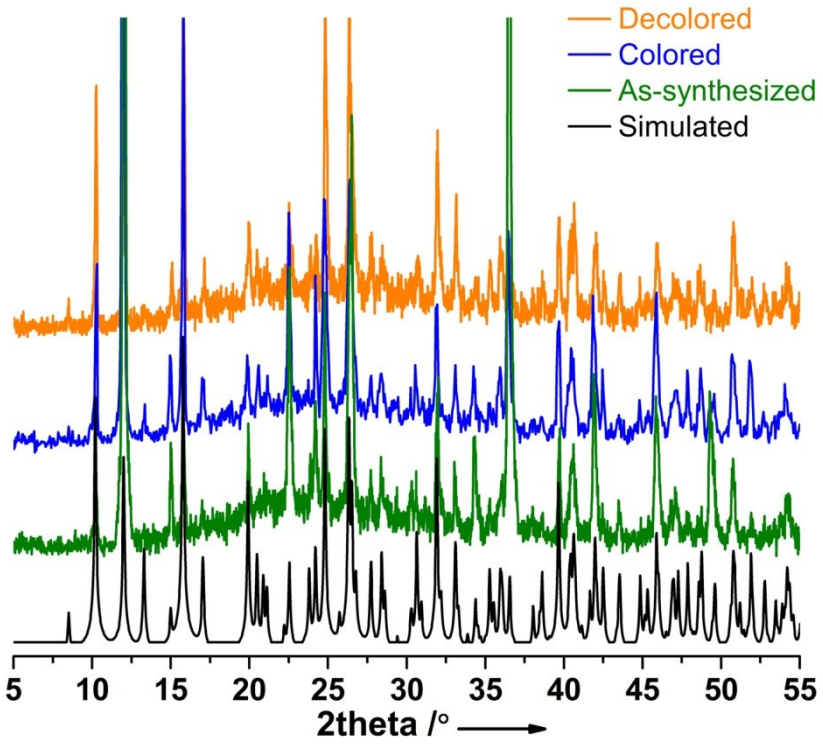

Fig. S1 PXRD patterns of **1** before irradiation (as-synthesized), after irradiation (colored), and after the reverse transformation (decolored).

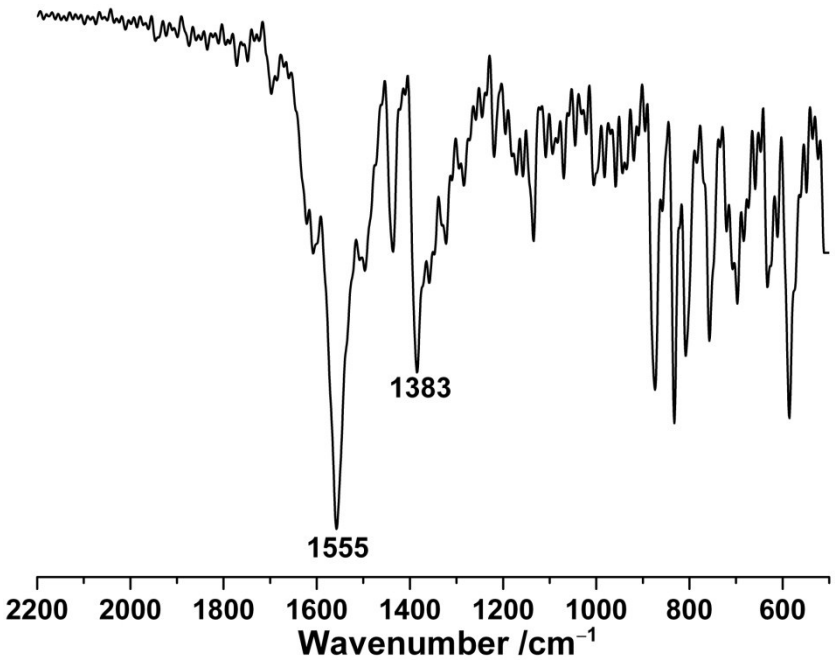

Fig. S2 The FT-IR spectrum of **1** in the KBr matrix.

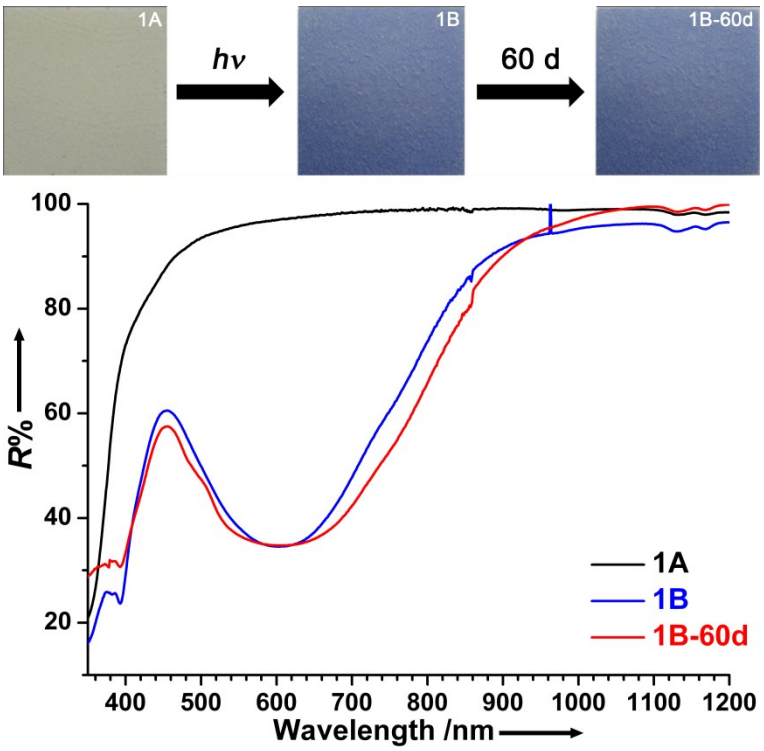

Fig. S3 Photos (top) and DR spectra (bottom) of **1** before irradiation (**1A**), immediately after irradiation (**1B**), and after keeping the irradiated sample in dark under ambient environment for 2 months (**1B-60d**).

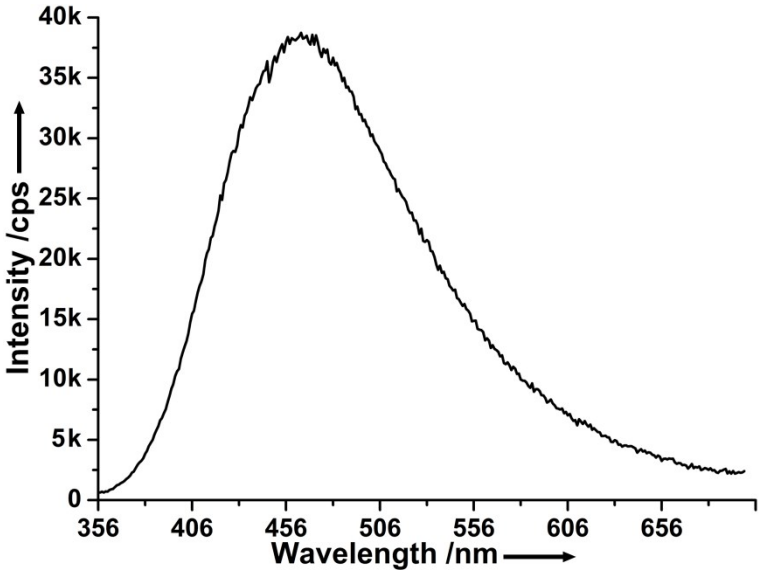

Fig. S4 The photoluminescence spectrum of the known compound $(H_2Bpy)(NO_3)_2$ (λ_{ex} = 306 nm).

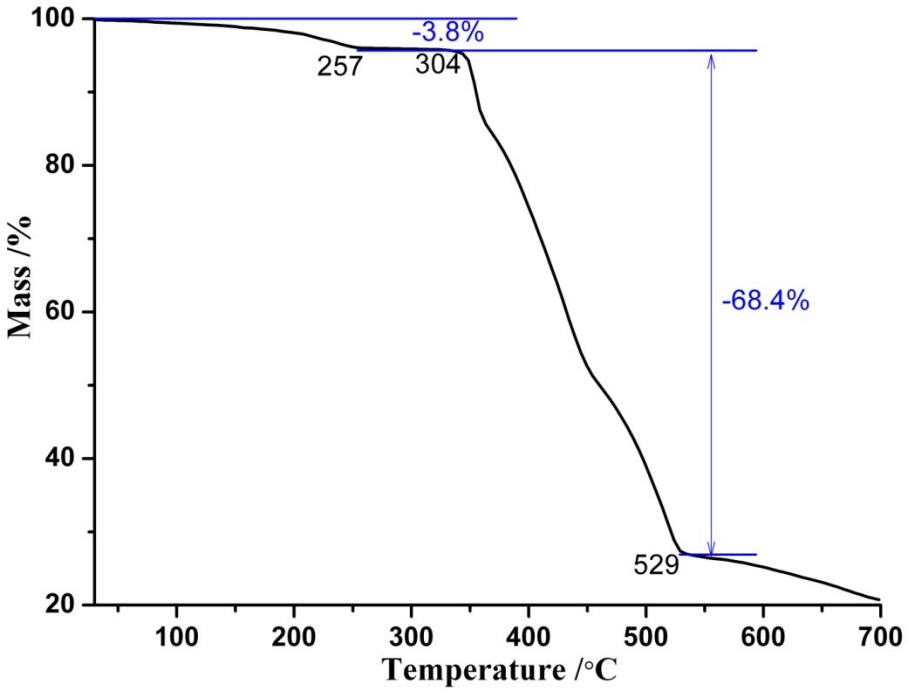

Fig. S5 TGA curve of **1**. The weight loss in the range of 30–257 °C is ~3.8%, corresponding to the content of two lattice water per molecule (3.5%, calculated), and that between 304 and 529 °C is ~68.4%, closing to a calculated weight loss of 66.1% with the residual being Cd.