New Long-Lasting Phosphor Material: A Novel Metal-Organic Framework Showing Intriguing Luminescent Performance

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(1) The synthesis of 1.

A DMF/H_2O solution (6mL, 5:1) of $Zn(NO_3)_2$, L, PhCOOH in a ratio of 1:1:2 was sealed in a Teflon reactor, and heated at 115˚C for 2 days, and then cooled to room temperature at 3˚C/h. Subsequently, block crystals were obtained in 80% yield based on Zn. Element analysis (%) for **1**: calc: C 50.70, H 3.40, N 11.83; found: C 50.65, H 3.44, N 11.79.

(2) The single crystal data of 1.

The structure was solved by direct methods and refined using the shelxl-97 program. Monoclinic, space group *C2/c*, *a* = 24.0674(3) Å, *b*= 5.14990(10) Å, *c*= 15.5647(2)Å, β=97.6260(10) *V*= 1912.10(5)Å^3, *Z* =4, $D_{calcd.}$= 1.646 gcm^{-3}, for all data: R1= 0.0268, *R*w2= 0.0699, GOF = 1.084.

(3) **Materials and Physical Measurements.**

The acylamide ligand of L is synthesized according to literature method.[1] Others were analytically pure from commercial sources and used without further purification. Elemental analyses were performed on a Vario EL-II analyzer. Single crystal X-ray diffraction is carried out on Bruker Smart Breeze. X-ray powder diffraction (XRPD) data were recorded in a Bruker D8 ADVANCE diffractometer. Photoluminescence was performed on an Edinburgh FLS920 luminescence spectrometer. The long-lasting phosphorescence (LLP) emission spectra and afterglow intensity decay curves were measured on the Hitachi F-4500 fluorescence spectrophotometer. Thermoluminescence (TL) measurements were performed on the FJ-427A TL meter (Beijing Nuclear Instrument Factory).Thermal analyses were carried out in air atmosphere using SETARAM LABSYS equipment with a heating rate of 5°C/min.

[1] a) Luo, F.; Zheng, J. -M.; Batten, S. R. *Chem. Comm.* **2007**, 3744. b) Luo, F.; Che, Y. -X.; Zheng, J. M. *Microporous and Mesoporous Materials*, **2009**, *117*, 486.

(4) **Calculation Details.**

TD-DFT calculations were performed by using B3LYP20 functional. The LANL2DZ basis sets were employed for Zn, where C, H, O, N atoms are calculated by 6-31g(d) basis sets . The initial ground-state geometries directly obtained from the

X-ray crystal structures. The calculation is carryout out by the Gaussian 03 software package.[2]

[2] Dennington, R.; Todd, K.; Millam, J.; Eppinnett, K.; Hovell, W. L.; Gilliland, R. GaussView, version 3.09; Semichem, Inc.: Shawnee Mission, KS, **2003**.

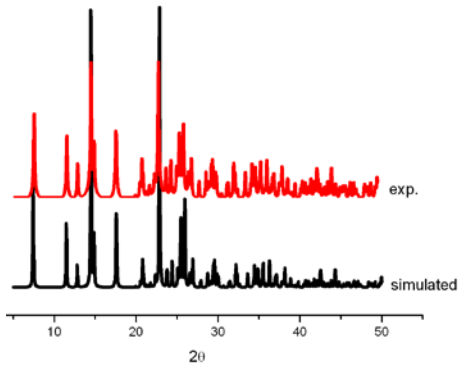

Figure S1. View of the simulated XRD patterns from the single crystal data and the experimental XRD patterns.

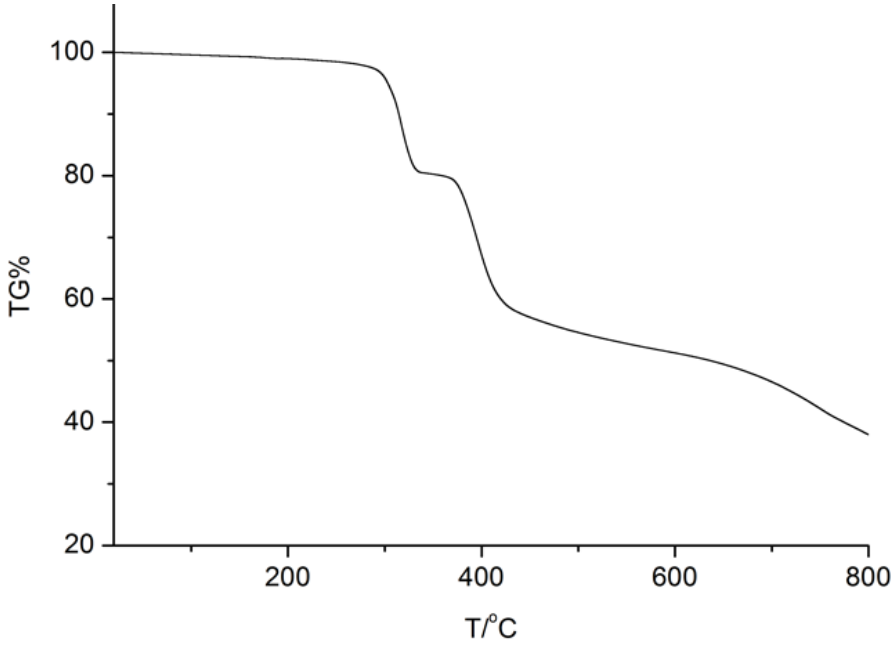

Figure S2. The TG plot of **1**.

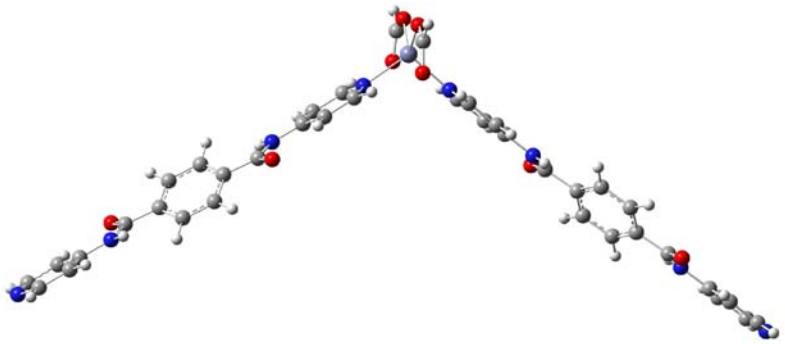

Figure S5. The molecular model used here for DFT studies.

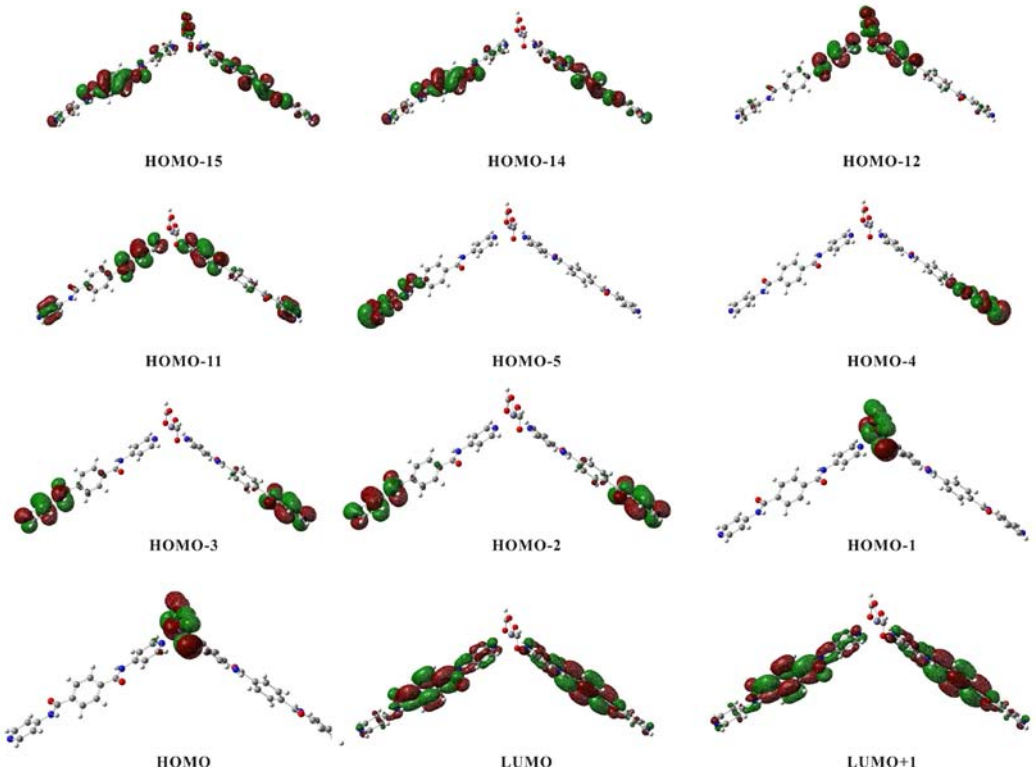

Figure S3. The electron-density distribution of various orbit involved in **1**.

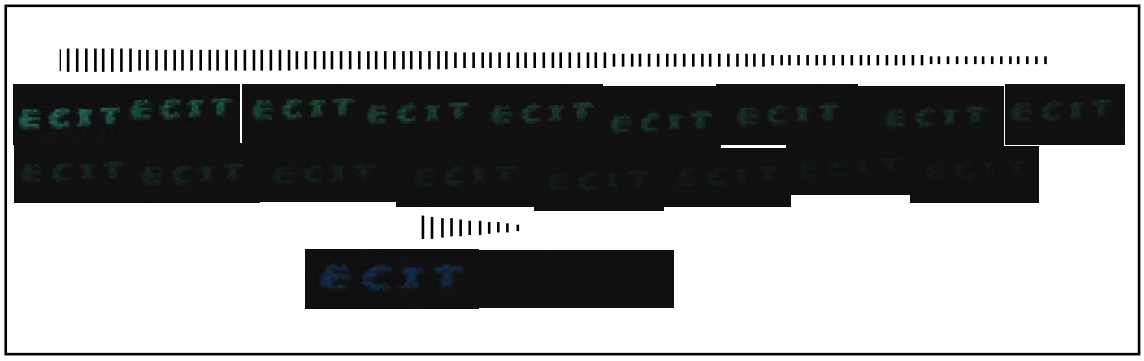

Figure S4. The photograph of compound **1**, excited at 340 nm (green) and 351 nm (blue), and the photograph of compound **1** after the removal of UV excitation.

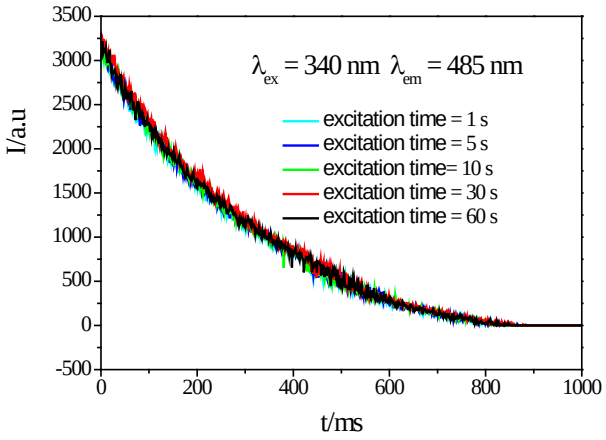

Figure S5. The afterglow intensity decay curve for the 485 nm emission after the excitation source is switched off at different times (*t*=1 s, 5s, 10 s, 30 s, 60 s)

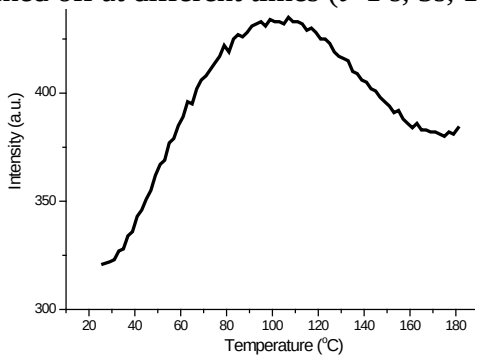

Figure S6. TL glow curves of **1** (the samples are excitated at 254 nm for 5 min).