

Electronic supplementary information (ESI)

Synthesis of a novel 2D zinc (II)-organic framework for photocatalytic degradation of organic dyes in water

Jian-Peng Dong, Zhen-Zhen Shi, Bo Li* and Li-Ya Wang*

Key Laboratory of Ecological Security for Water Source Region of Mid-line of South-to-North Water Diversion Project of Henan Province, Collaborative Innovation Center of Water Security for Water Source Region of Mid-line of South-to-North Diversion Project of Henan Province, College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, People's Republic of China.

Corresponding authors:

*(B. Li) E-mail: libony0107@nynu.edu.cn

*(L. Y. Wang) E-mail: wly@nynu.edu.cn

X-ray Crystallography

The single crystal X-ray diffraction data of **1** was collected using a Bruker SMART APEX II CCD diffractometer equipped with a graphite mono-chromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) at 293 (2) K. The SADABS program was used for absorption correction.¹ The structures were solved by direct methods and refined by the full-matrix least-squares method on F^2 .² The hydrogen atoms on ligands were placed in calculated positions and refined using the riding model. The hydrogens attached to water molecules were located from the difference Fourier maps and refined isotropically. Full crystallographic data for **1** have been deposited at the Cambridge Crystallographic Data Centre with the deposition number CCDC 1950609. Crystallographic data and structural refinement details of **1** are listed in Table S1. The selected bond lengths and angles are shown in Table S2.

Radical Trapping Experiments

The radical trapping experiments just have one more additional procedure than the Rh B photocatalytic process: the radical scavenger was added to the reaction system before the Xe lamp turned on. The specific dosage of *t*-BuOH, EDTA-2Na and BQ are 10mg, 10mg and 0.2 mL, respectively. The Rh B concentration changes were monitored by measuring the absorption intensity at its maximum absorbance wavelength of $\lambda = 554 \text{ nm}$ using a UV-visible spectrophotometer.

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

Formula	C ₁₃ H ₁₁ ZnNO ₆
Mr	342.6
Crystal system	monoclinic
space group	<i>P2₁/c</i>
<i>a</i> , Å	11.0839(6)
<i>b</i> , Å	16.4996(10)
<i>c</i> , Å	7.0477(4)
α , deg	90
β , deg	101.834(5)
γ , deg	90
<i>V</i> , Å ³	1261.49(13)
<i>Z</i>	4
D _c , g cm ⁻³	1.804
μ , mm ⁻¹	1.976
Unique. reflns/ <i>R_{int}</i>	2224/0.047
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.2446
w <i>R</i> ₂ (All data)	0.2511
GOF	1.089

Table S2. The selected bond lengths (Å) and angles (°) for **1**.

Zn1-O2B	1.973(4)	Zn1-O4	1.967(4)
Zn1-N1A	2.036(5)	Zn1-O1W	2.065(5)
Zn1-O3B	2.340(5)	O3B-Zn1-O2B	81.12(19)
O4-Zn1-N1A	131.2(2)	O2B-Zn1-N1A	119.6(2)
O4-Zn1-O1W	95.04(19)	O2B-Zn1-O1W	96.2(2)
O2B-Zn1-O3B	81.12(19)	N1A-Zn1-O1W	96.4(2)
N1A-Zn1-O3B	82.79(17)	O4-Zn1-O2B	105.95(18)
O3B-Zn1-O1W	176.29(19)	O1W-Zn1-O3B	176.29(19)

Symmetry transformations used to generate equivalent atoms: A: 1+x, y, z; B: x, 1.5-y, -0.5+z.

Table S3. Hydrogen bond lengths (Å) and angles (°) for **1**

D-H	A	d(D-H)	d(H...A)	<DHA	d(D...A)
O1W	O1D	0.85(2)	2.135(5)	135.84(2)	2.808(3)
O1W	O2C	0.82(3)	1.906(4)	164.65(3)	2.705(3)
O2WD	O1D	0.82(3)	2.207(5)	157.33(3)	2.980(2)
O2WD	O4	0.85(5)	2.276(5)	145.20(2)	3.021(2)
D: Donor; A: Acceptor					
Symmetry transformations used to generate equivalent atoms: C: 2-x, 0.5+y, 1.5-z; D: x, 1.5-y, 0.5+z.					

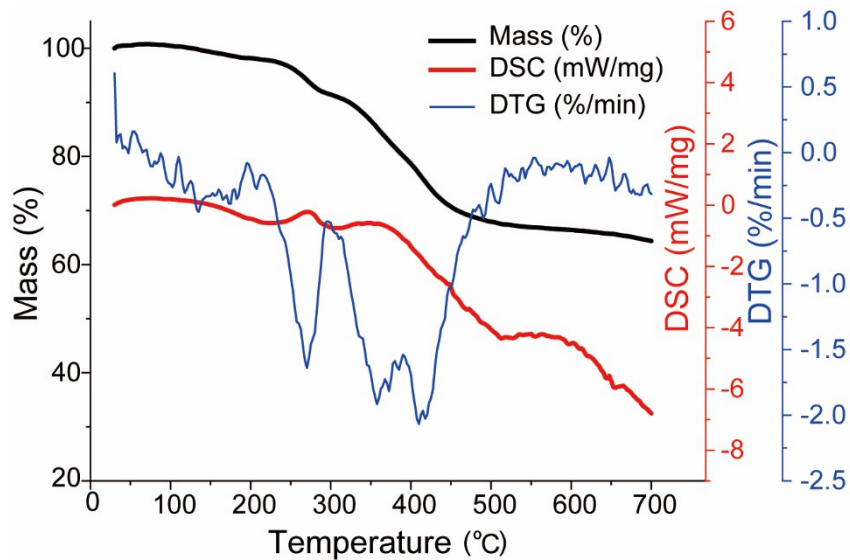


Fig. S1 TG, DTG and DSC curves for **1**.

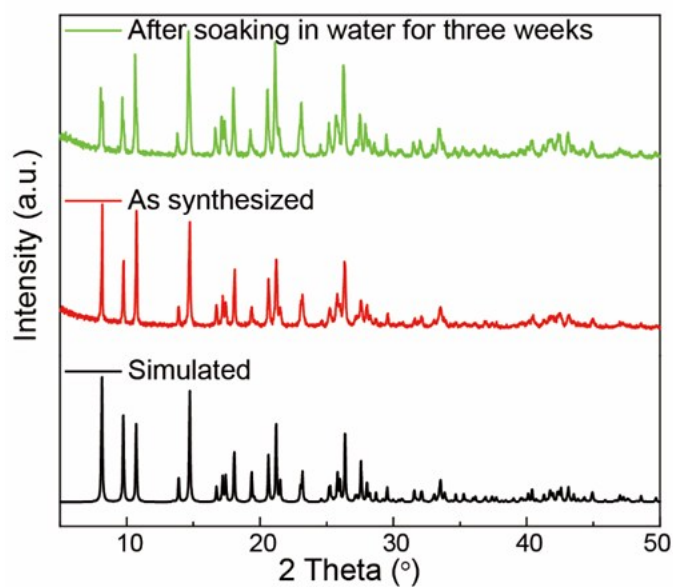


Fig. S2 PXRD patterns for **1**.

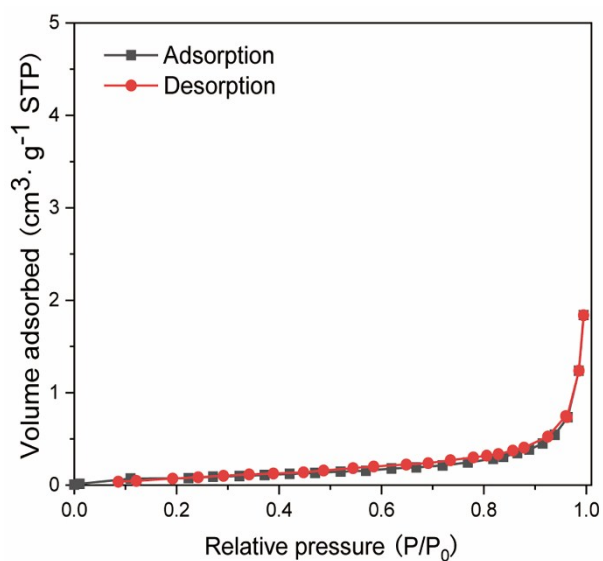


Fig. S3 N₂ sorption isotherm measured at 77 K.

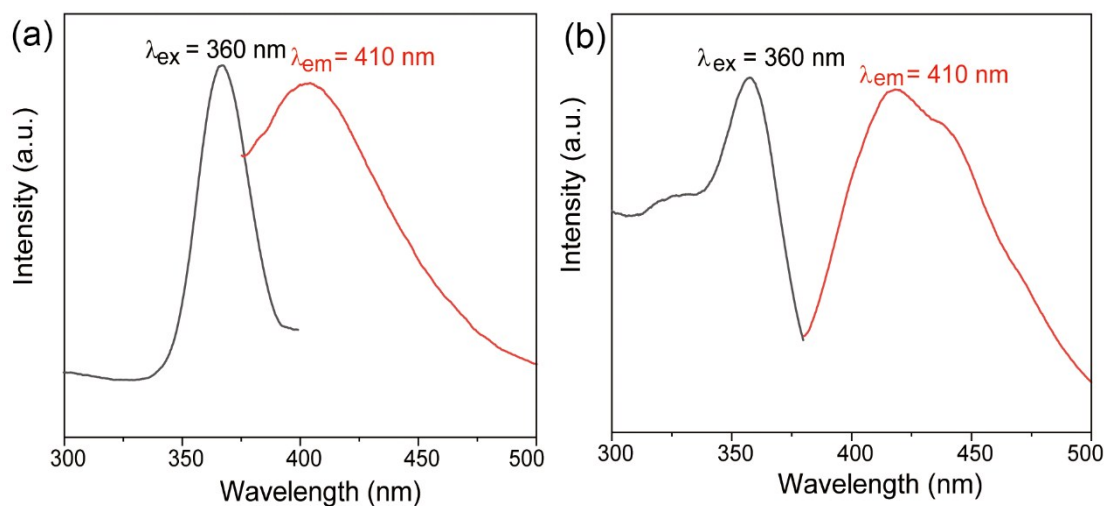


Fig. S4 The solid-state excitation and emission spectra of free H₂L ligands (a) and **1** (b) at room temperature.

References

- 1 G. M. Sheldrick, Program for Empirical Absorption Correction of Area Detector Data, University of Göttingen, Germany, 1996.
- 2 G. M. Sheldrick, SHELXS-97, Program for Crystal Structure Solution, Göttingen University, Göttingen, Germany, 1997.