Electronic Supplementary Material (ESI) for ChemComm.

Porous functionalized MOF self-evolution promoting molecule encapsulation and Hg^{2+} removal

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Supporting Information

1. Synthesis procedure of 1 and 2.

Synthesis of {[Zn(L)$_2$](H$_2$O)}$_n$ (1) Zn(CH$_3$COO)$_2$·4H$_2$O (0.021g, 0.1 mmol) and 3-aminoisonicotinic acid (L 0.014g, 0.1 mmol) were added in the mixture of DMF, acetonitrile and H$_2$O (2:2:1) at 100 °C. The colorless crystals of **1** were observed after 10 h. The yield was calculated to 84% based on HL. The chemical formula: $C_{12}H_{12}N_4O_5Zn$. Element analysis: C, 40.6(Calcd:40.3) H, 3.2(Calcd: 3.3) N, 16.0(Calcd: 15.6). IR (KBr, cm^{-1}): 3438m, 3318s, 1654m, 1576m, 1364m, 1074s, 796w, 690w, 591w.

Synthesis of {[Zn(L)$_2$](DMF)}$_n$ (2) The crystals of as-synthesized **1** (20 mg) were immersed in mixture of DMF and H$_2$O (4:1) for 15 days. The block crystals were obtained. The chemical formula is $C_{15}H_{17}N_5O_4Zn$, and the values(%) of element analysis is C, 43.6(Calcd: 43.2), H, 4.1(Calcd: 3.8), N, 16.9(Calcd: 16.5). IR (KBr, cm^{-1}): 3444m, 3425s, 1636m, 1587m, 1379m, 1085s, 809w, 681w, 588w.

2. Materials and physical measurements

All the supplies involved in this work were purchased from commercial sources. Element analysis results (C, N, H) were obtained by FLASH EA 1112 element analyzer.Thermogravimetric analysis (TGA) data were collected on the Netzsch STA 449C thermal analyzer. JASCO-750 uv - visible spectrophotometer was used to determine the solid diffuse reflectance spectrum.Infrared spectroscopy was performed on Bruker Tensor 27 spectrophotometer. A PANalytical X'Pert PRO diffractometer is used for mobile phone PXRD spectral data. X-ray photoelectron spectroscopy (XPS) were obtained with a Thermo Escalab 250 spectrometer. The concentration of metal ion in aqueous solution was tested by inductively coupled plasma optical emission spectrometry (ICP-OES) on a PerkinElmer Optima 8000 instrument.

3. Single crystal X-ray crystallography

The crystallographic data were collected on a Bruker D8 VENTURE diffractometer with Mo Kα radiation (λ = 0.71073 Å). The integration of the diffraction data, as well as the intensity corrections for the Lorentz and polarization effects, were performed using the SAINT program.[1] Semiempirical absorption correction was performed using SADABS program.[2] The structures were solved by direct methods and refined with a full matrix least-squares technique based on F^2 with the SHELXL crystallographic software package.[3] The hydrogen atoms except for those of water molecules were generated geometrically and refined isotropically using the riding model. Crystallographic data and structure processing parameters are summarized in Table S1. Selected bond lengths and bond angles are listed in Table S2.

[1] SAINT, Program for Data Extraction and Reduction Bruker AXS, Inc: Madison, WI, 2001.

[2] G. M. Sheldrick, SADABS, Program for Empirical Adsorption Correction of Area Detector Data University of Göttingen: Germany, 2003.

[3] G. M. Sheldrick A short history of SHELX. *Acta Crystallogr.*, A64 (2008) 112-122.

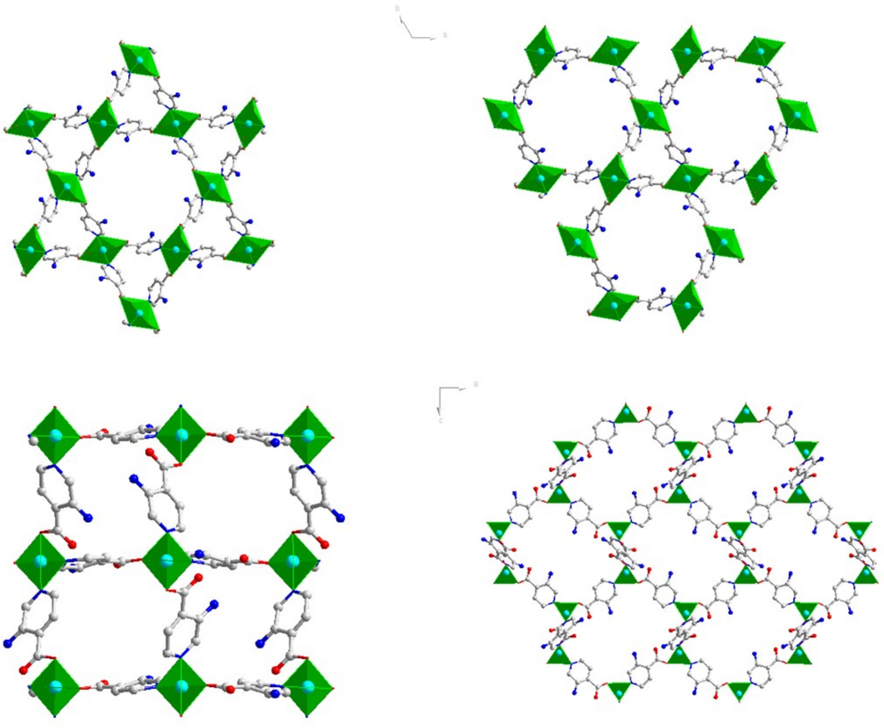


Fig. S1 (a) Supporting structure figure for **1**. (b) Supporting structure figure for **1**. (c) Square aperture of **2** in the direction of axis *c*. (d) View of **2** in the direction of axis *b*.

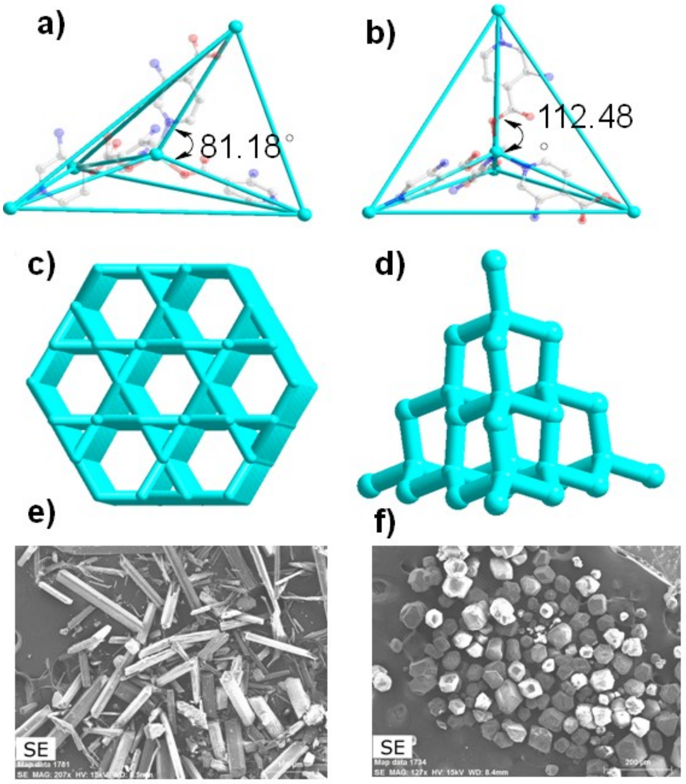


Fig. S2. The compare of **1** and **2**. (a) The spatial configuration of the structure of **1**. (b)The spatial configuration of the structure of **2**. (c) The model of hexagonal structure in **1**. (d) The model of diamond-like structure in **2**. (e) SEM image of **1**. (f) SEM image of **2**.

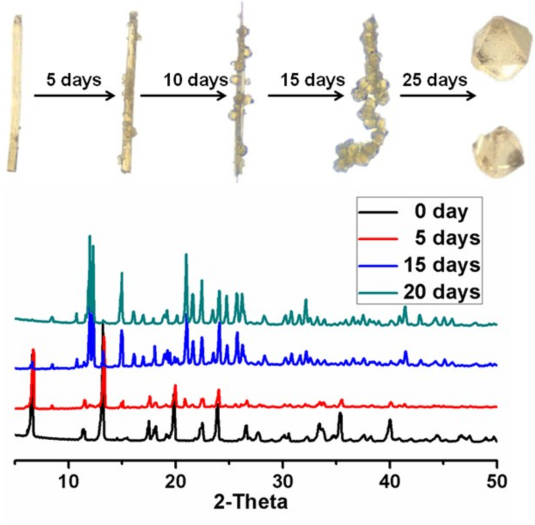


Fig. S3 The experimental PXRD patterns of **1**→**2** solvent-induced structure transformation.

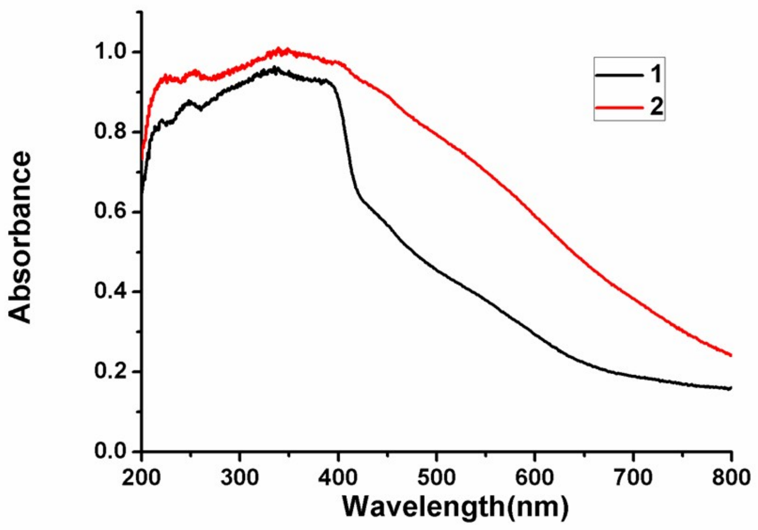


Fig. S4 The diffuse reflectance spectrum of **1** and **2**.

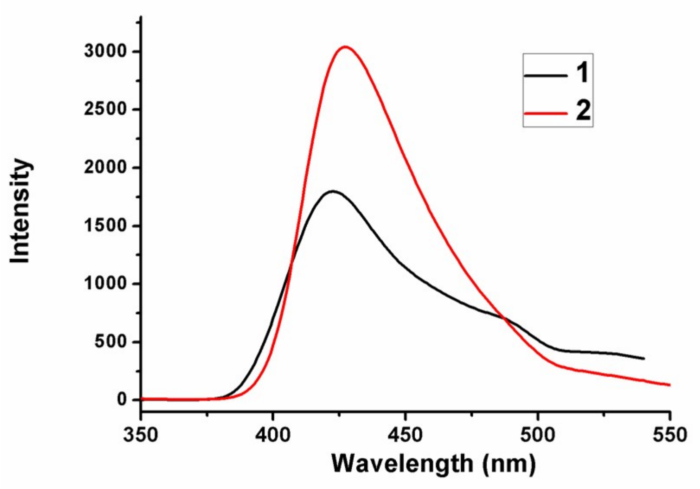


Fig. S5 The fluorescence spectrumof **1** and **2**.

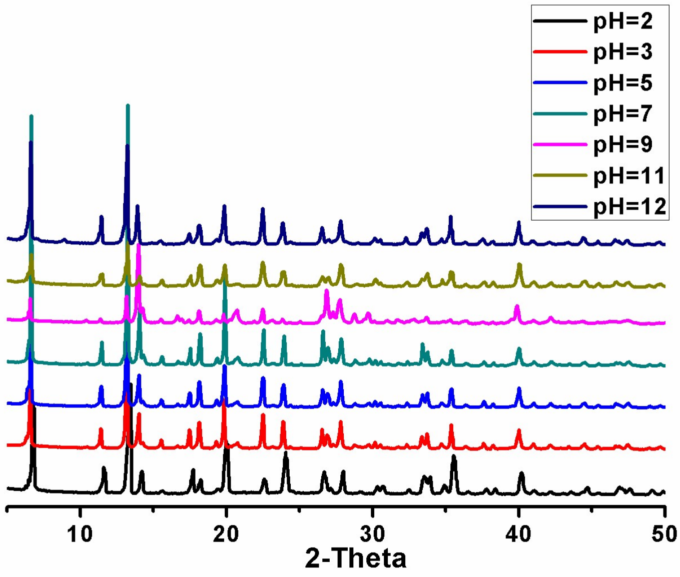


Fig. S6 The water stability for **1**.

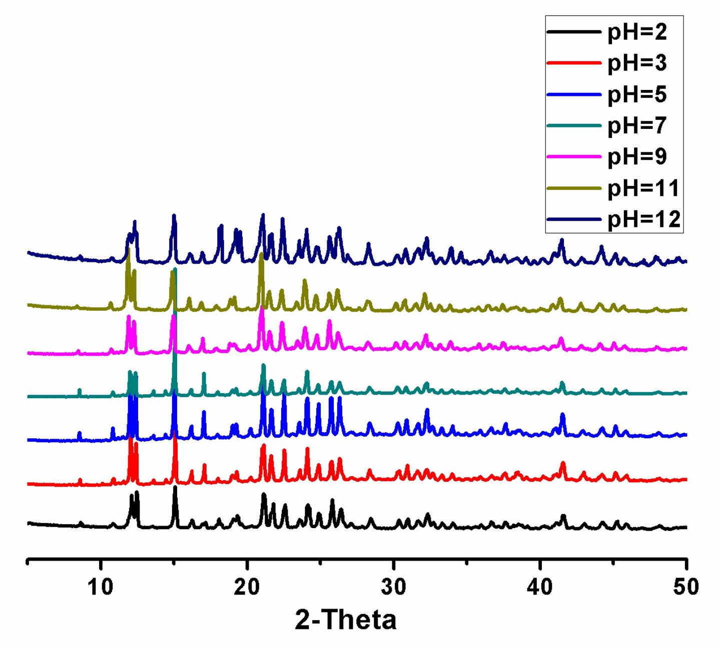


Fig. S7 The water stability for **2**.

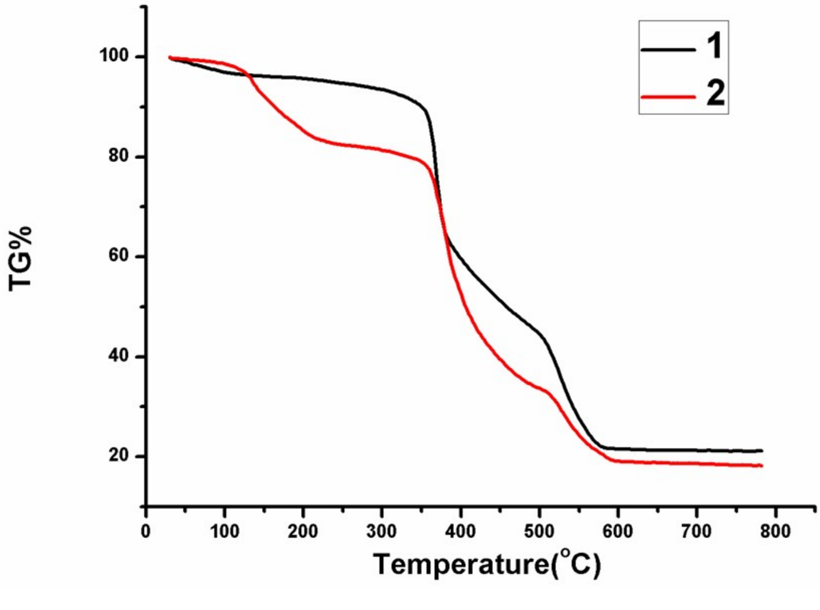


Fig. S8 Thermogravimetric analyses of **1** and **2**.

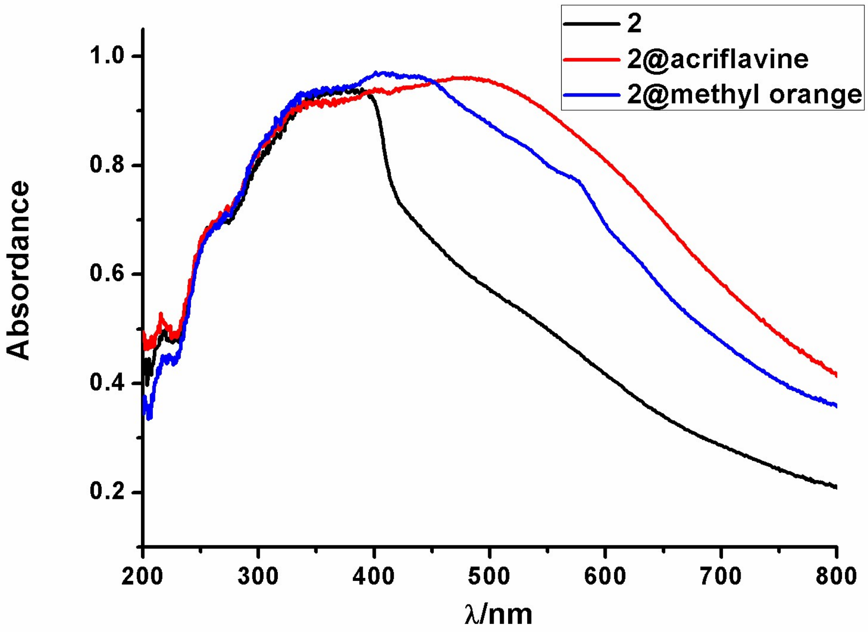


Fig. S9 The ultraviolet spectrum of **2**, **2@methyl orange** and **2@acriflavine**.

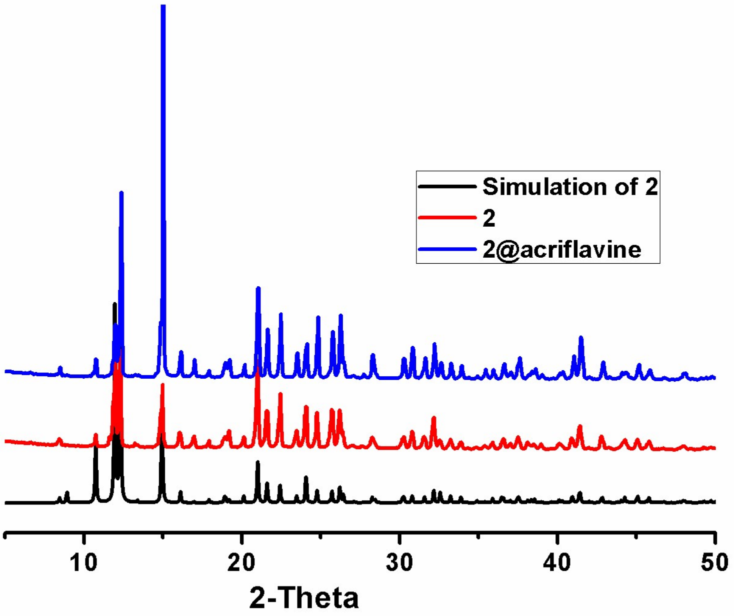


Fig. S10 The PXRD results of **2** and **2@acriflavine**.

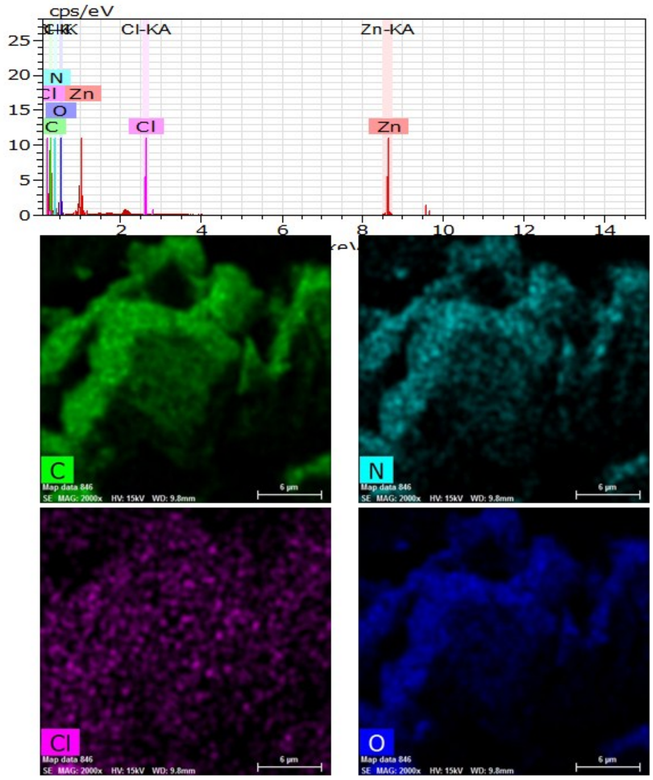


Fig. S11 The EDS spectra of **2@acriflavine**.

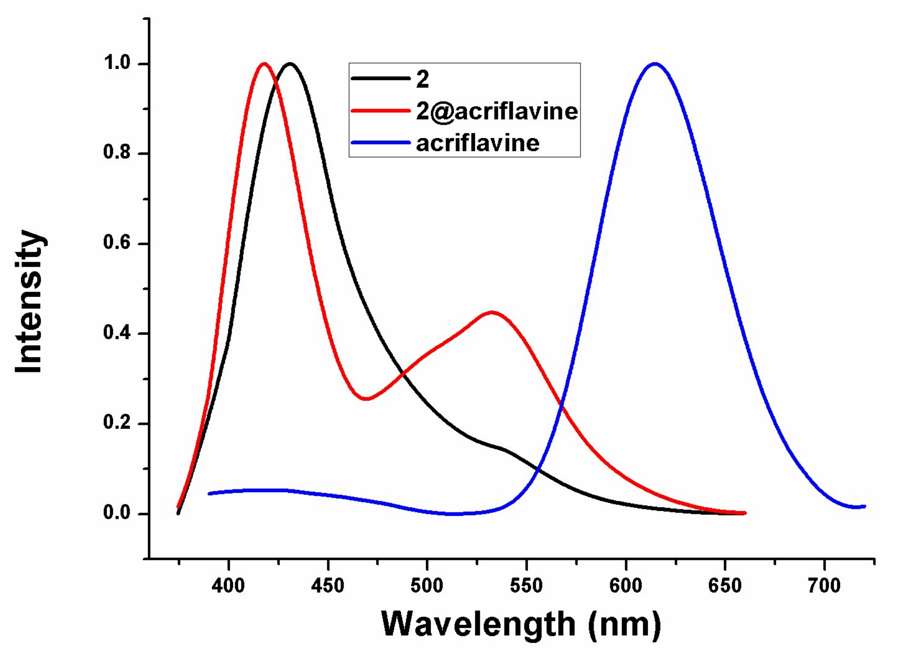


Fig. S12 The fluorescence spectra of **2@acriflavine**.

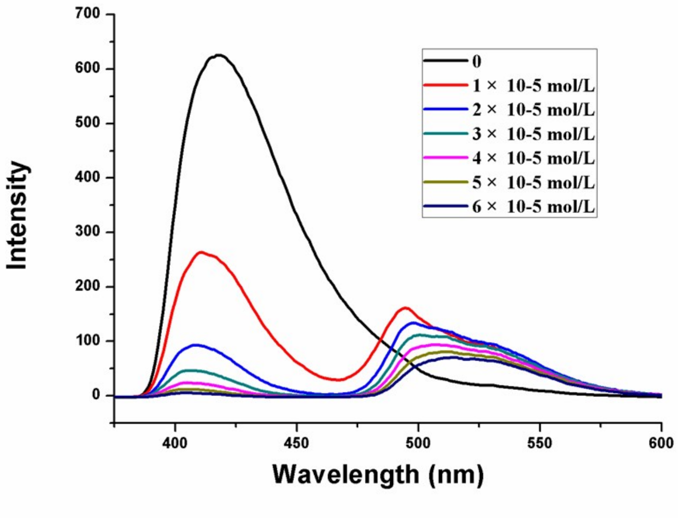


Fig. S13 The titration experiment of acriflavine into L.

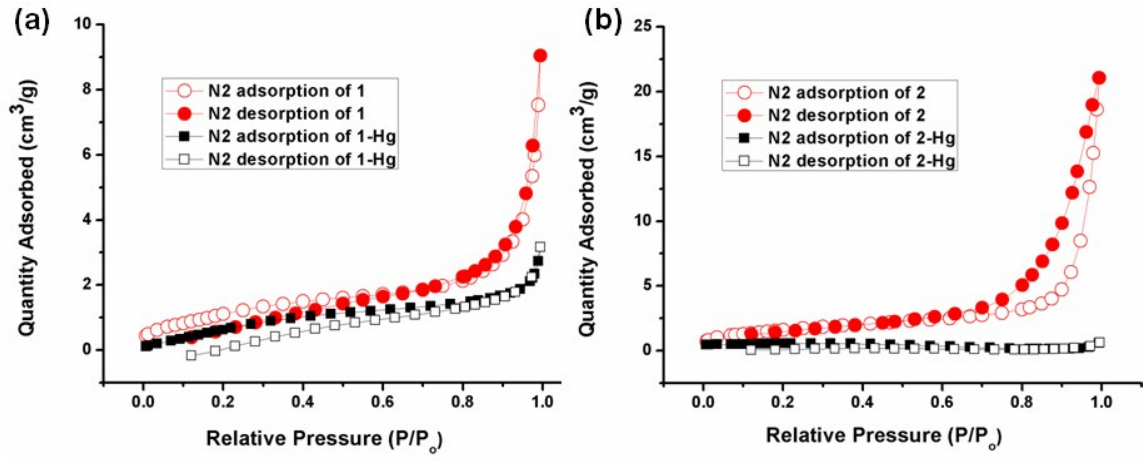
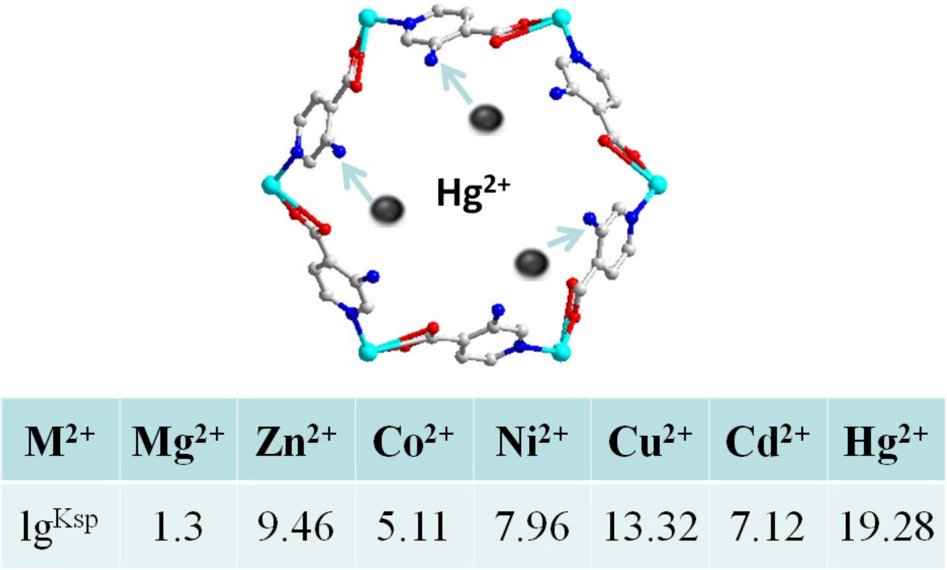


Fig. S14 N_2 adsorption and desorption isotherms (a): **1** and **1**-Hg; (b):**2** and **2**-Hg.



M^{2+}	Mg^{2+}	Zn^{2+}	Co^{2+}	Ni^{2+}	Cu^{2+}	Cd^{2+}	Hg^{2+}
lg^{Ksp}	1.3	9.46	5.11	7.96	13.32	7.12	19.28

Fig. S15 The stability coefficients lg^{Ksp} for $M(NH_2)_n$.

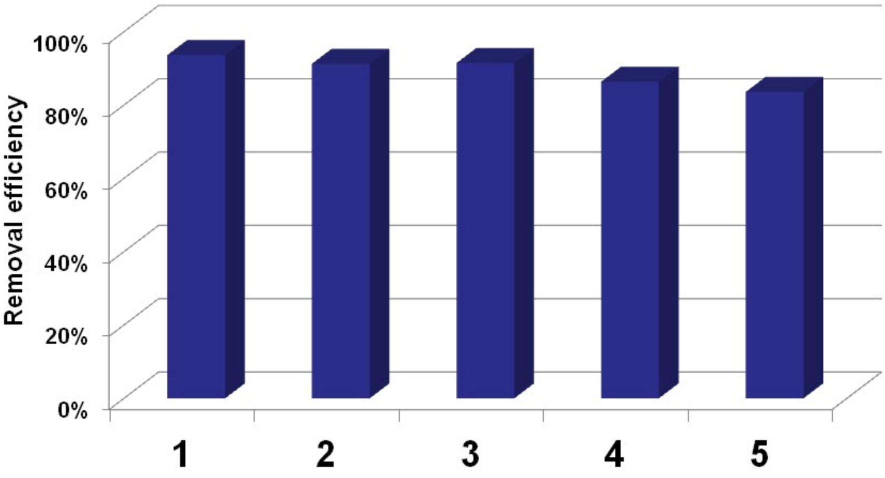
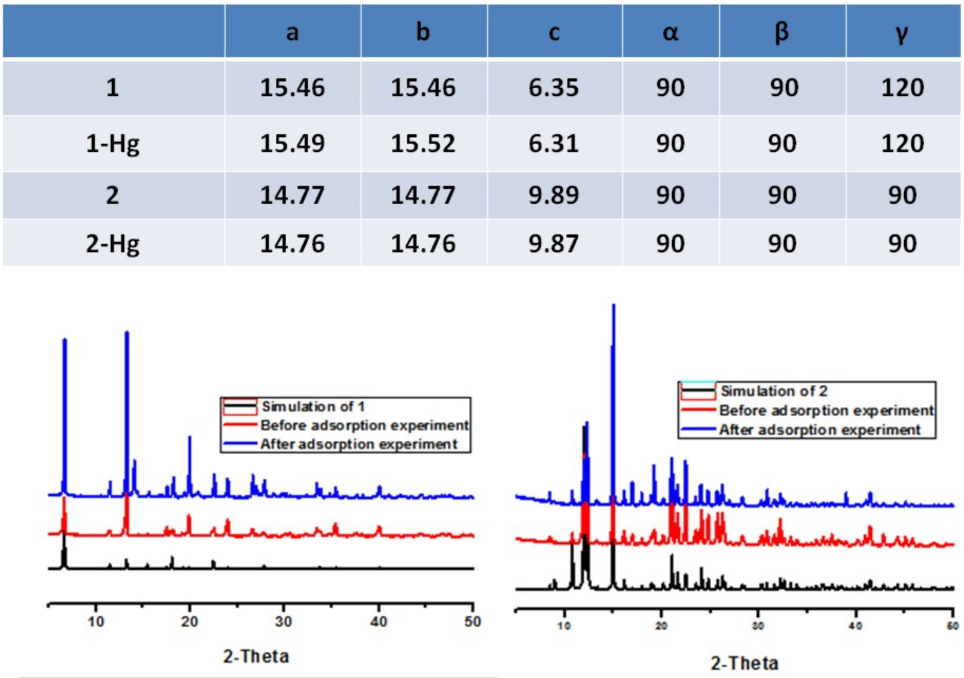


Fig. S16 The reusability of **2** for Hg^{2+} adsorption.



	a	b	c	α	β	γ
1	**15.46**	**15.46**	**6.35**	**90**	**90**	**120**
1-Hg	**15.49**	**15.52**	**6.31**	**90**	**90**	**120**
2	**14.77**	**14.77**	**9.89**	**90**	**90**	**90**
2-Hg	**14.76**	**14.76**	**9.87**	**90**	**90**	**90**

Fig. S17 The reusability of **1** and **2** as adsorbent materials in the removal process.

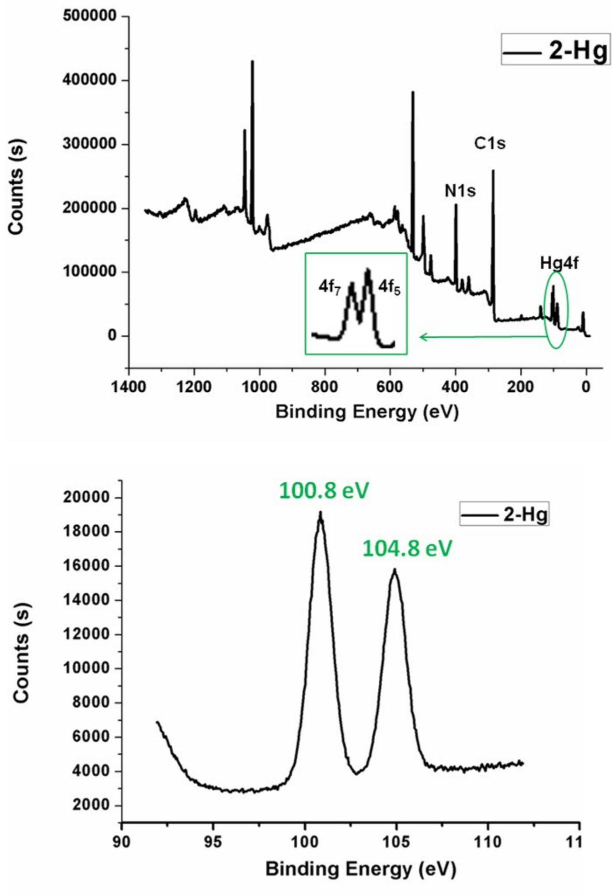


Fig. S18 The XPS spectrum of **2**-Hg.

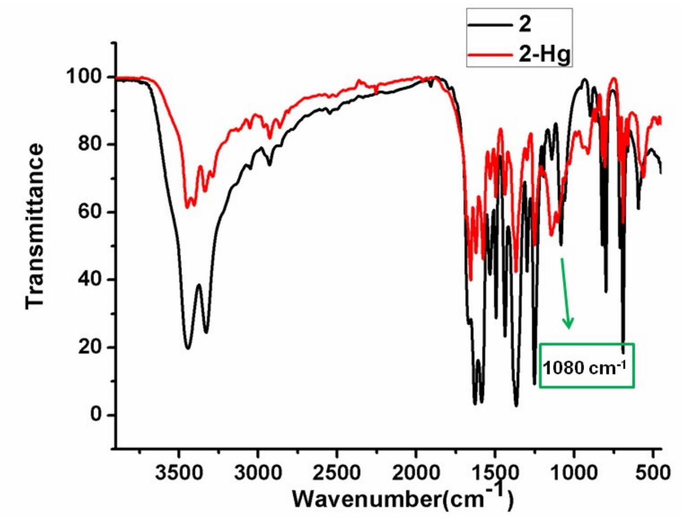


Fig. S19 The FT-IR spectra of **2** and **2**-Hg.

Table S1 Crystallographic data and structure refinement details for complexes **1** and **2.**

Compound	**1**	**2**
formula	$C_{12}H_{10}N_4O_4Zn$	$C_{12}H_{10}N_4O_4Zn$
Fw	339.61	339.61
T/K	293(2)	273.15
l (Mo–Ka)/Å	0.71073	0.71073
Crystsyst	hexagonal	orthorhombic
Space group	P62	P21212
a/Å	15.465(3)	14.7391(5)
b/Å	15.465(3)	14.7855(5)
c/Å	6.3597(13)	9.8812(4)
α (deg)	90	90
β (deg)	90	90
γ (deg)	120	90
V (Å3)	1317.2(6)	2153.36(14)
Z	4	4
Dcalcd(g cm-3)	1.284	1.048
F(000)	516.0	688.0
μ (mm^{-1})	1.415	1.154
GOF	0.777	1.085
R1 (I > 2σ(I))	0.0459	0.0288
wR2 (I > 2σ(I))	0.0192	0.0911

$R = [\sum||F_0| - |F_c|| / \sum|F_0|]$, $R_W = \sum_W [|F_0^2 - Fc^2|^2 / \sum_W (|F_w|^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and bond angles (deg) for **1** and **2** crystal structure description.

1			
Zn1-O21	1.9587(19)	C2-C3	1.401(3)
N1-C5	1.345(3)	O1-C6	1.220(3)
Zn1-O2	1.9587(19)	C3-C4	1.383(4)
N2-C2	1.357(4)	O2-C6	1.278(3)
Zn1-N12	2.032(2)	C3-C6	1.503(4)
C1-C2	1.394(4)	N1-C1	1.321(4)
Zn1-N13	2.032(2)	C4-C5	1.380(4)
O21-Zn1-O2	100.10(12)	C4-C3-C6	119.4(2)
N2-C2-C1	119.3(2)	C6-O2-Zn1	112.28(19)
O2-Zn1-N12	120.06(9)	C5-C4-C3	121.1(2)
N2-C2-C3	123.3(3)	C1-N1-Zn14	121.52(16)
O21-Zn1-N12	103.33(8)	N1-C5-C4	120.7(3)
C1-C2-C3	117.4(3)	C1-N1-C5	118.9(2)
O2-Zn1-N13	103.33(8)	O1-C6-O2	123.6(3)
C2-C3-C6	122.8(3)	C5-N1-Zn14	119.6(2)
O21-Zn1-N13	120.06(9)	O1-C6-C3	120.6(3)
C4-C3-C2	117.8(2)	N1-C1-C2	124.1(2)
N13-Zn1-N12	110.56(13)	O2-C6-C3	115.7(3)
Symmetry codes:	#1 1-X,1-Y,+Z; #2+Y,-X+Y,2/3+Z; #3 1-Y,1+X-Y,2/3+Z; #4 -Y+X,+X,-2/3+Z		

2			
Zn1-O2	1.959(2)	O3-C12	1.282(5)
N3-C11	1.325(5)	C4-C5	1.403(5)
Zn1-O31	1.948(3)	O4-C12	1.252(5)
N4-C8	1.313(5)	C7-C8	1.424(5)
Zn1-N12	2.063(3)	N1-C1	1.336(5)
C1-C2	1.366(5)	C8-C9	1.434(5)
Zn1-N3	2.034(3)	N1-C5	1.312(5)
C2-C3	1.363(5)	C9-C10	1.361(5)
O1-C6	1.231(4)	N2-C4	1.374(5)
C3-C4	1.421(5)	C9-C12	1.494(5)
O2-C6	1.285(4)	N3-C7	1.336(5)
C3-C6	1.507(4)	C10-C11	1.397(5)
O2-Zn1-N11	97.74(10)	O1-C6-C3	121.4(3)
N2-C4-C3	124.6(3)	C6-O2-Zn1	115.9(2)
O2-Zn1-N3	107.60(12)	O2-C6-C3	115.6(3)
N2-C4-C5	120.1(3)	C12-O3-Zn13	117.3(2)
O32-Zn1-O2	111.59(13)	N3-C7-C8	123.1(3)
C5-C4-C3	115.2(3)	C1-N1-Zn14	122.1(2)
O32-Zn1-N11	108.75(13)	N4-C8-C7	120.2(4)
N1-C5-C4	125.1(3)	C5-N1-Zn14	119.2(2)
O32-Zn1-N3	121.01(11)	N4-C8-C9	123.8(4)
O1-C6-O2	123.1(3)	C5-N1-C1	118.7(3)
N3-Zn1-N11	107.58(14)	C7-C8-C9	116.0(3)
O1-C6-C3	121.4(3)		
Symmetry codes:	11/2+X,3/2-Y,2-Z; 23/2-X,-1/2+Y,1-Z; 33/2-X,1/2+Y,1-Z; 4-1/2+X,3/2-Y,2-Z		