pH-Regulated ratiometric luminescence Eu-MOF for rapid detection of toxic mycotoxin in moldy sugarcane

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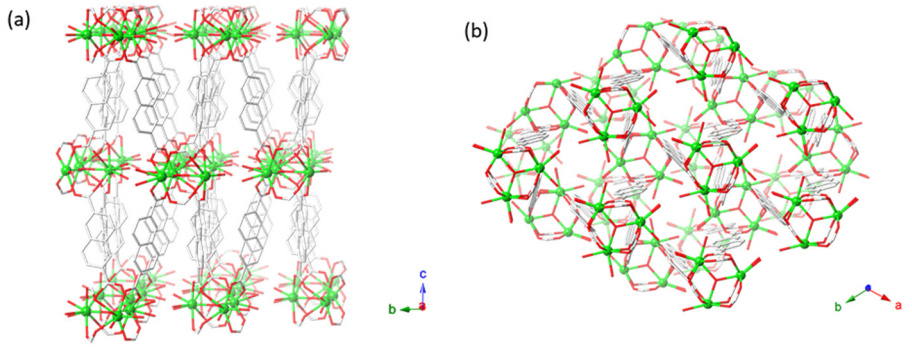

Fig. S1 Crystal structure of Eu-MOF (**2**) viewed along *a* axis and *c* axis.

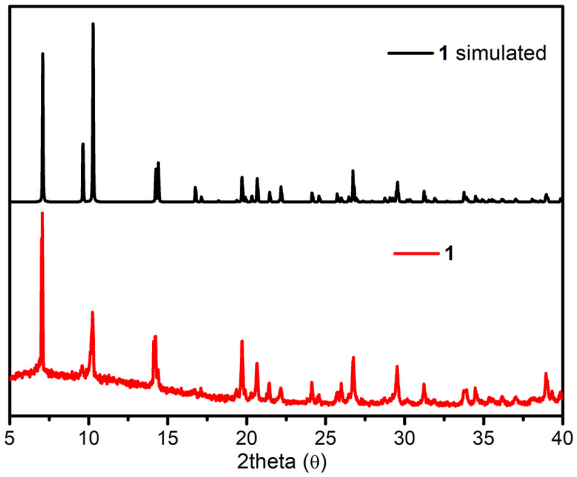

Fig. S2 Simulated and experimental powder X-ray diffraction patterns (PXRD) of the as-synthesized **1**.

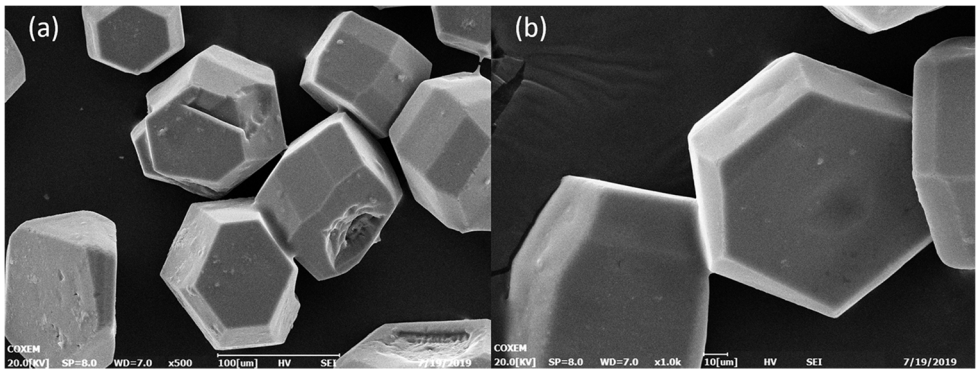

Fig. S3 SEM images of the as-synthesized **1**.

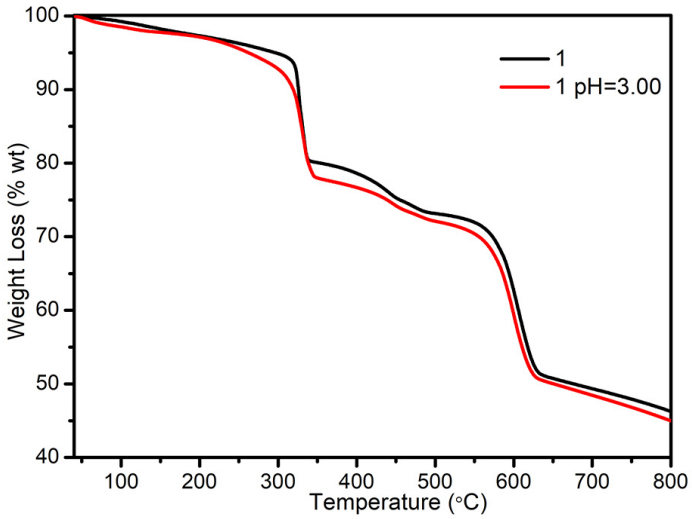

Fig. S4 TG curves of **1** and HCl-treated **1** (pH 3.00) in a N_2 flow from 40 °C to 800 °C.

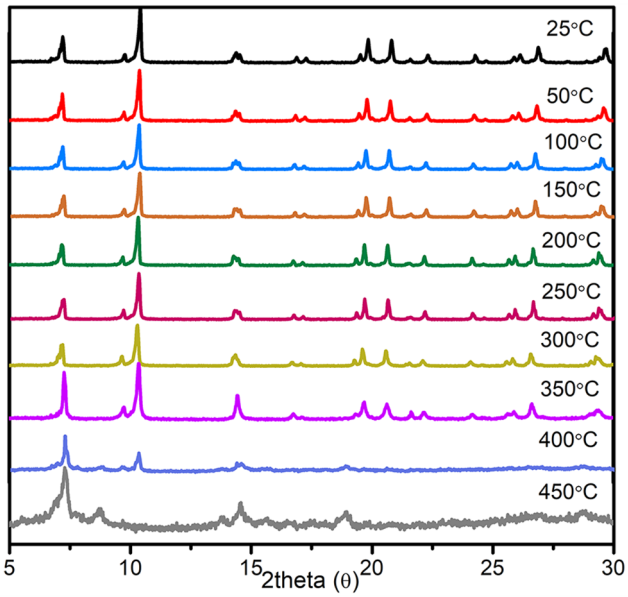

Fig. S5 In-situ PXRD patterns of **1** in a N_2 flow from 25 °C to 450 °C.

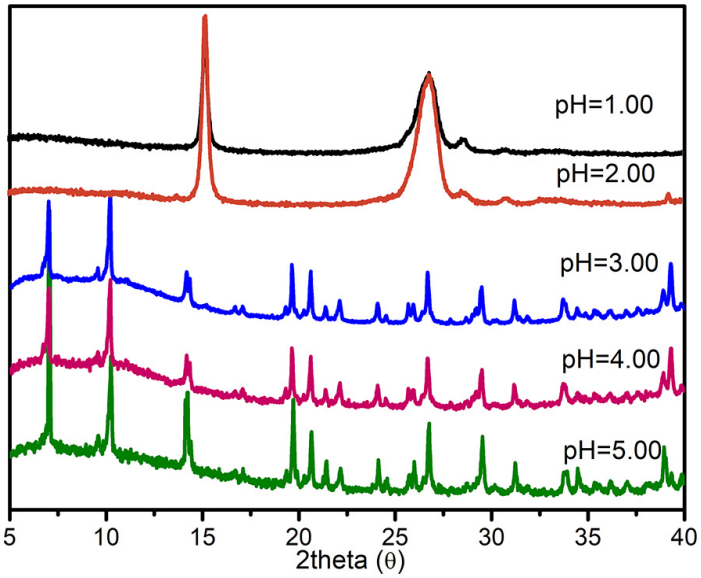

Fig. S6 PXRD patterns of **1** after immersed in HCl solutions at different pH (1.00 to 5.00) for 48 h.

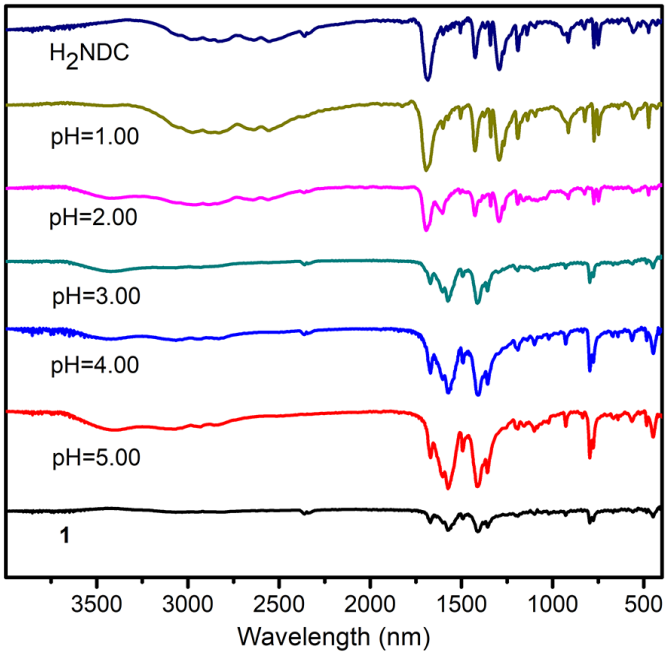

Fig. S7 IR spectra of **1**, the HCl-treated **1** (immersed in HCl solutions of pH from 1.00 to 5.00), and the ligand.

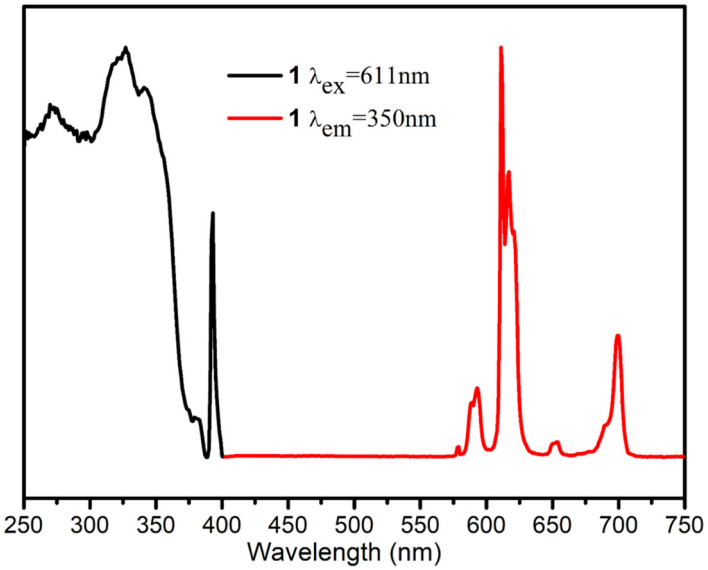

Fig. S8 The excitation (black line) and emission spectra (red line) of **1** in solid state.

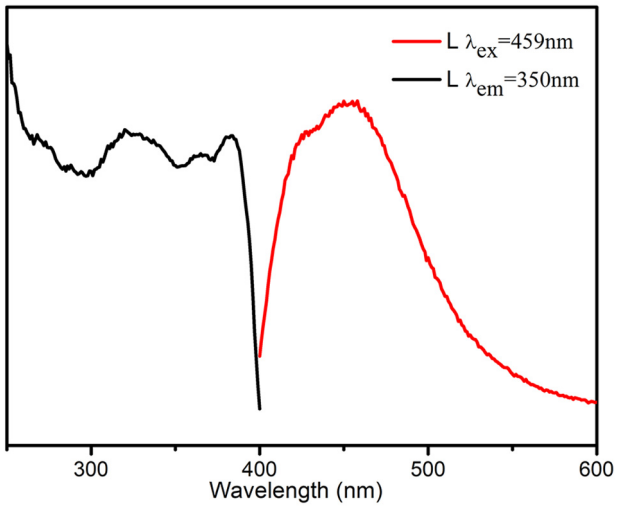

Fig. S9 The excitation (black line) and emission spectra (red line) of free ligand H_2NDC in solid state.

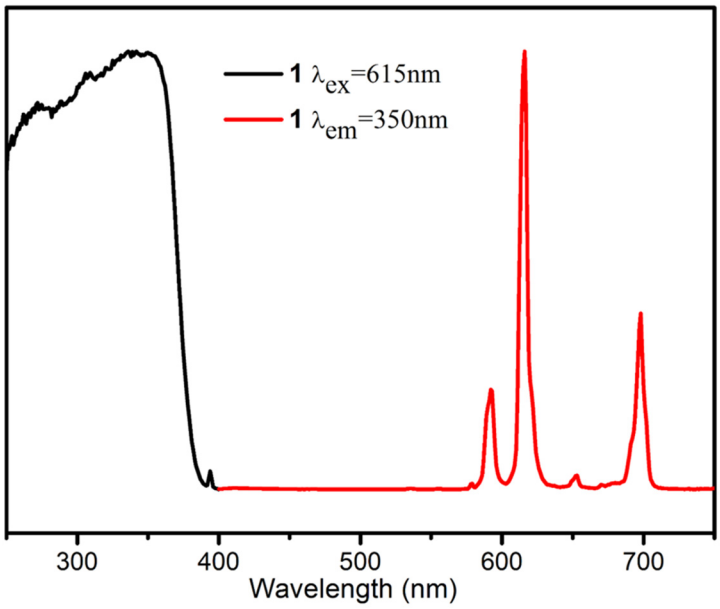

Fig. S10 The excitation (black line) and emission spectra (red line) of **1** dispersed in water.

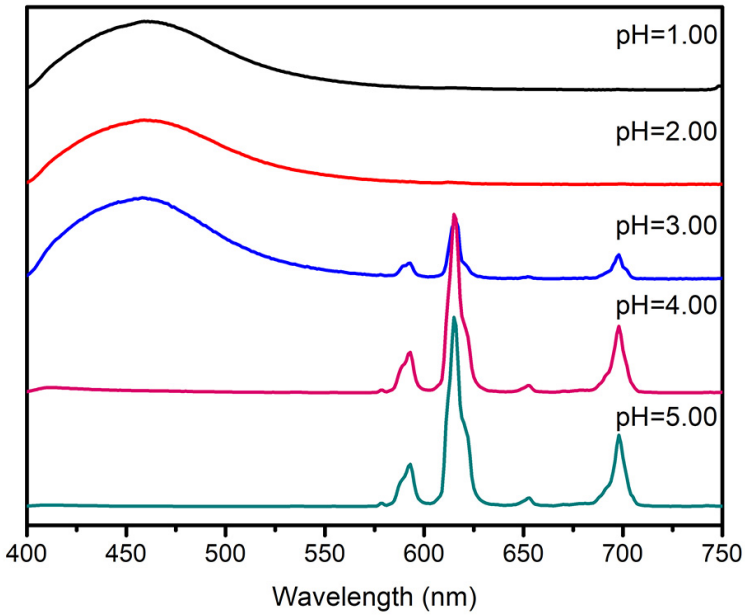

Fig. S11 Emission spectra (λ_{ex}=350 nm) of **1** after immersed in HCl solutions at different pH (1.00 to 5.00) for 48 h.

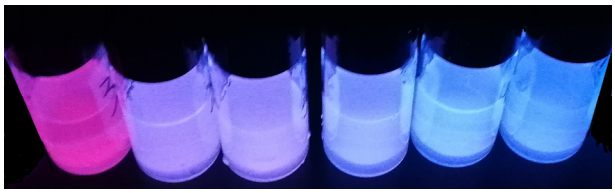

Fig. S12 Photographs of **1** in acidic aqueous solutions at different pH values (pH= 4.00 to 3.00) under the irradiation of 365 nm UV light.

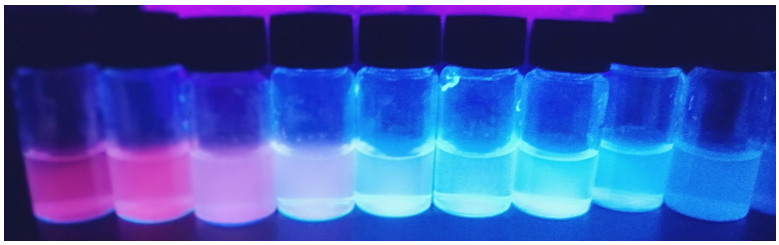

Fig. S13 Photographs of **1** in aqueous 3-NPA solutions at different concentrations (0.1 mM to 1.0 mM) under the irradiation of 365 nm UV light.

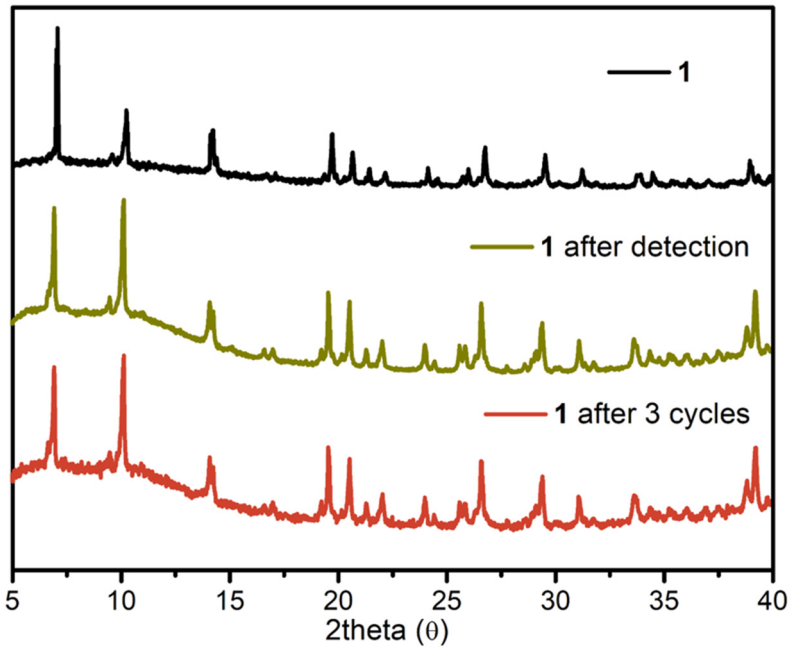

Fig. S14 PXRD patterns of **1**, **1** after sensing experiment, and **1** after three cycles of sensing experiments.

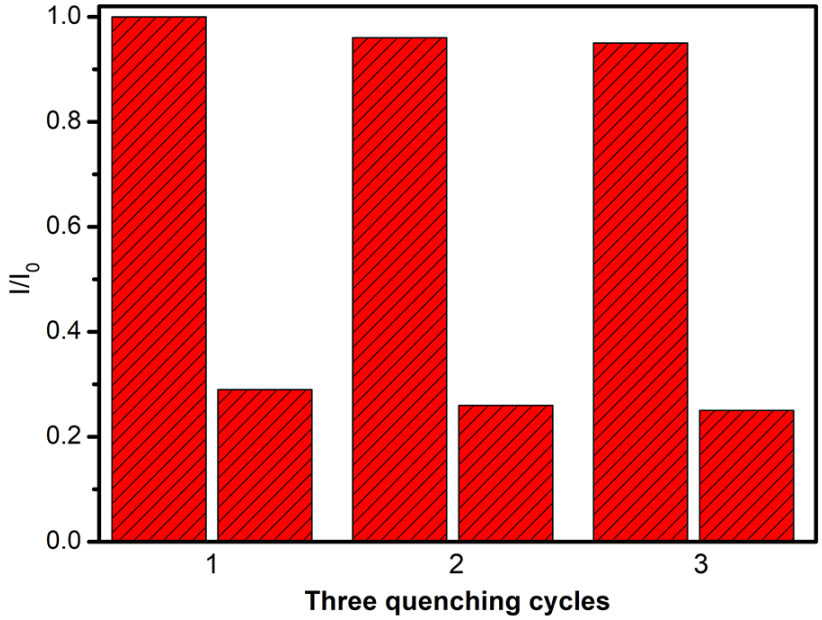

Fig. S15 Luminescence intensity ratio (I/I_0) at 615nm of three cycles of 3-NPA sensing experiments.

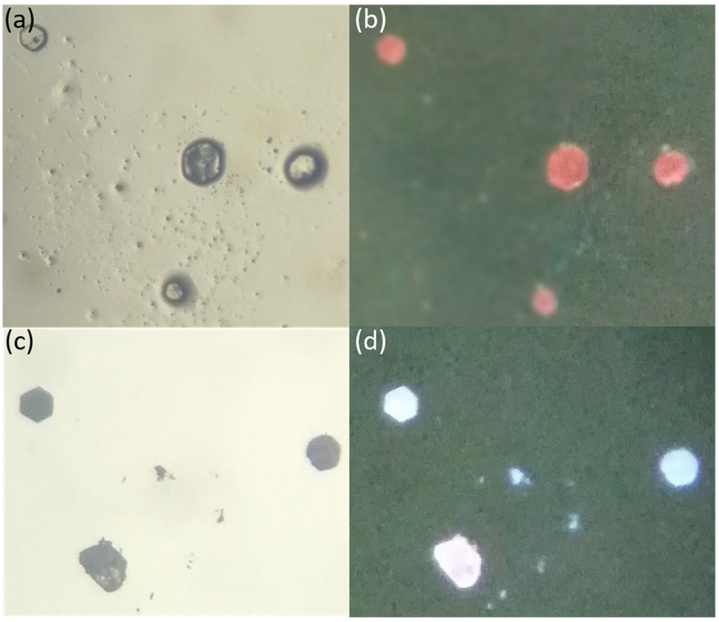

Fig. S16 Photo-micrographs of **1** before (a, b) and after (c, d) immersed in acidic aqueous solution (pH=3.00) under natural light (a, c) and UV light (b, d).

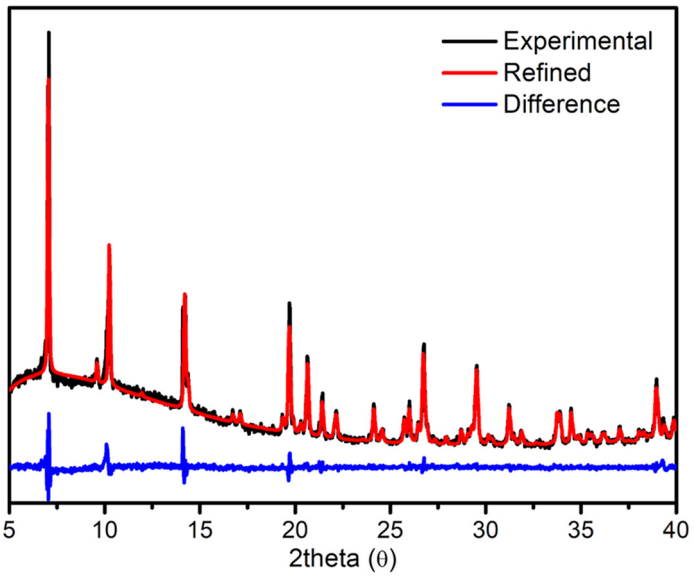

Fig. S17 Lebail fitting of PXRD patterns of **1**. Experimental (balck line), refined (red line) and the difference (below) patterns of **1**.

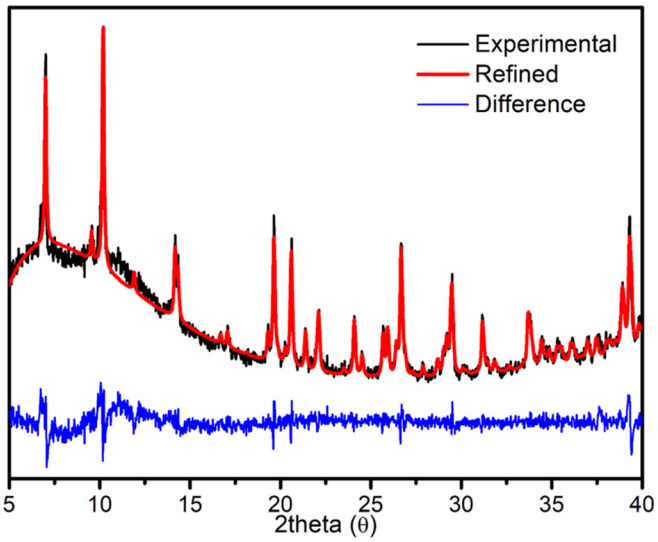

Fig. S18 Lebail fitting of PXRD patterns of **2**. Experimental (balck line), refined (red line) and the difference (below) patterns of **2**.

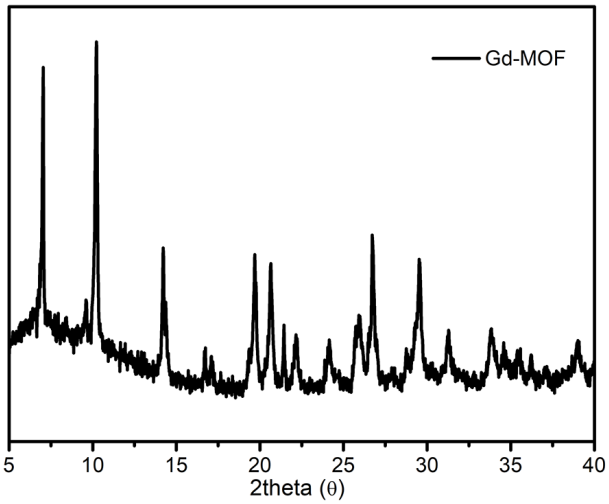

Fig. S19 PXRD pattern of Gd-MOF.

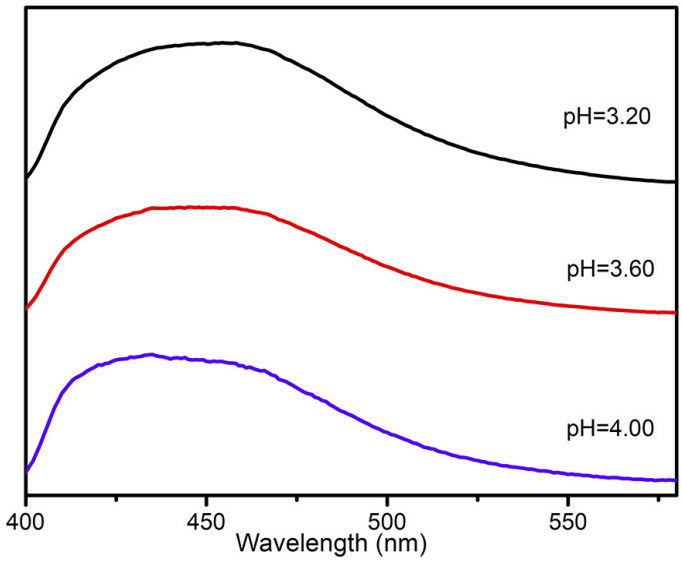

Fig. S20 Emission spectra (λ_{ex}=350 nm) of the aqueous solutions of Gd-MOF at different pH values.

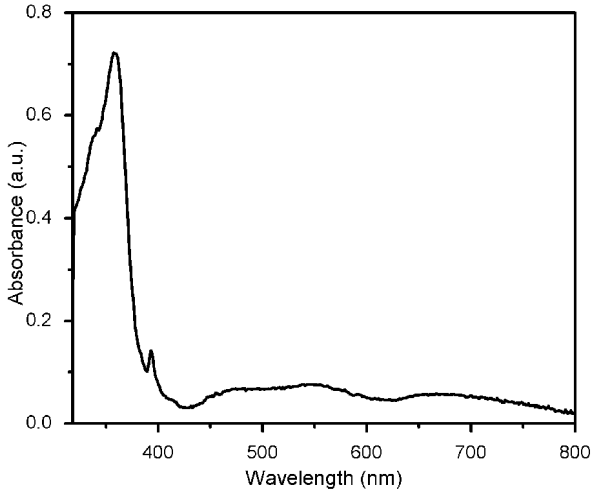

Fig. S21 UV-vis spectrum of **1**.

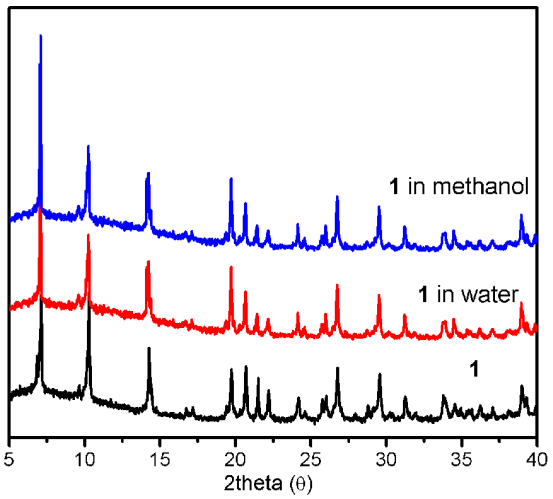

Fig. S22 PXRD patterns of **1**, soaked in water (pH = 5.00) for 48 hrs, and soaked in methanol for 48 hrs.

Tab. S1. Crystal data and structure refinement parameters for MOF 1 and 2.

Compound	Eu-MOF (1)	Eu-MOF (2)
Empirical fomula	$EuO_{0.33}(NDC)(H_2O)_{1.4}$	$EuO_{0.33}(NDC)(H_2O)_{1.4}$
M_r	393.81	393.81
Temperature(K)	299	299
Crystal size(mm)	0.08×0.06×0.03	0.08×0.06×0.03
Crystal system	Hexagonal	Hexagonal
Space group	$P6_3/m$	$P6_3/m$
a/Å	10.5515(5)	10.5589(1)
c/Å	24.7960(13)	24.8011(4)
α/°	90	90
β/°	90	90
γ/°	120	120
V/Å^3	2390.8(3)	2394.63(6)
Z	6	6
F(000)	1121	1121
Reflection collected	7139	11878
Independent reflections	1694	1736
GOF on F^2	1.131	1.104
Final R indexes [I>=4σ (I)]	0.0663	0.0689
Final R indexes [all data]	0.0739	0.0704
wR_2	0.2261	0.1958
Largest diff. peak and hole (e.Å^{-3})	-1.12/1.88	-1.17/1.55

Note: The occupancies of O4 and O5 are 0.35 and 0.7, respectively.

Tab. S2. Bond lengths of Eu ions in MOF 1 and 2.

Compound	Eu-MOF (1)	Eu-MOF (2)
Eu(1)-O(1)	2.337(7)	2.338(6)
Eu(1)-O(2)	2.343(9)	2.356(9)
Eu(1)-O(3)	2.389(9)	2.397(9)
Eu(1)-O(4)	2.38(3)	2.31(2)
Eu(1)-O(5)	2.41(2)	2.40(2)
Eu(1)-Eu(1)#1	4.048(11)	4.050(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y, -x, z

Tab. S3. Crystal data and Lebail fitting parameters for MOF 1 and 2.

Compound	Eu-MOF (1)	Eu-MOF (2)
Temperature(K)	293	293
Space group	$P6_3/m$	$P6_3/m$
a/Å	10.54305(0)	10.54765(0)
c/Å	24.79595(6)	24.77871(2)
R_p	0.0593	0.0559
R_{wp}	0.0844	0.0700
GOOF	1.89	1.58