

Supporting information

A luminescent lanthanide MOF for selectively and ultra-high sensitively detecting Pb²⁺ ion in aqueous solution

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Fig. S1 The optical photograph of Tb-MOF.

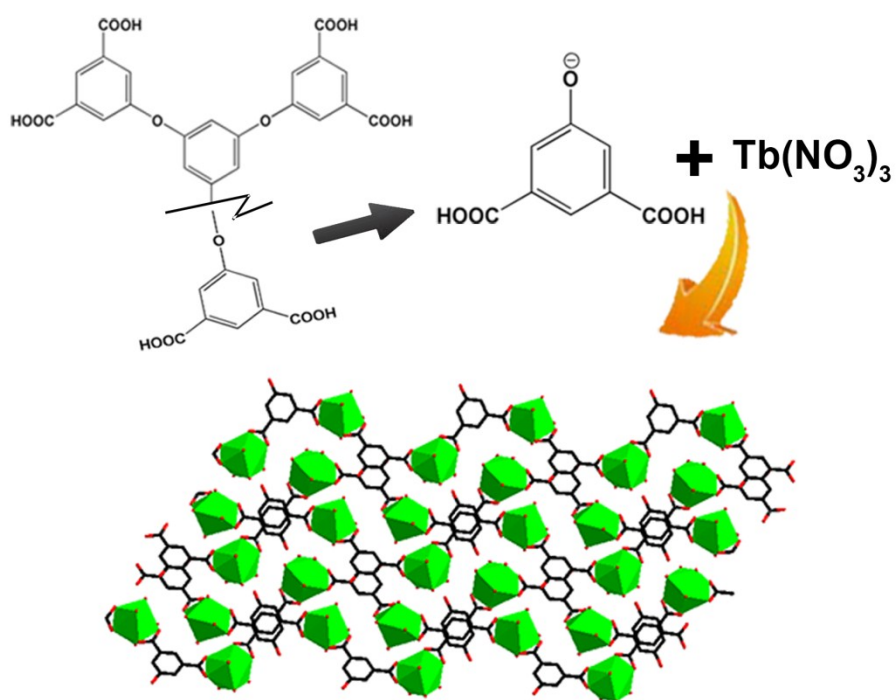


Fig. S2 The reaction process of hydrothermal synthesis Tb-MOF.

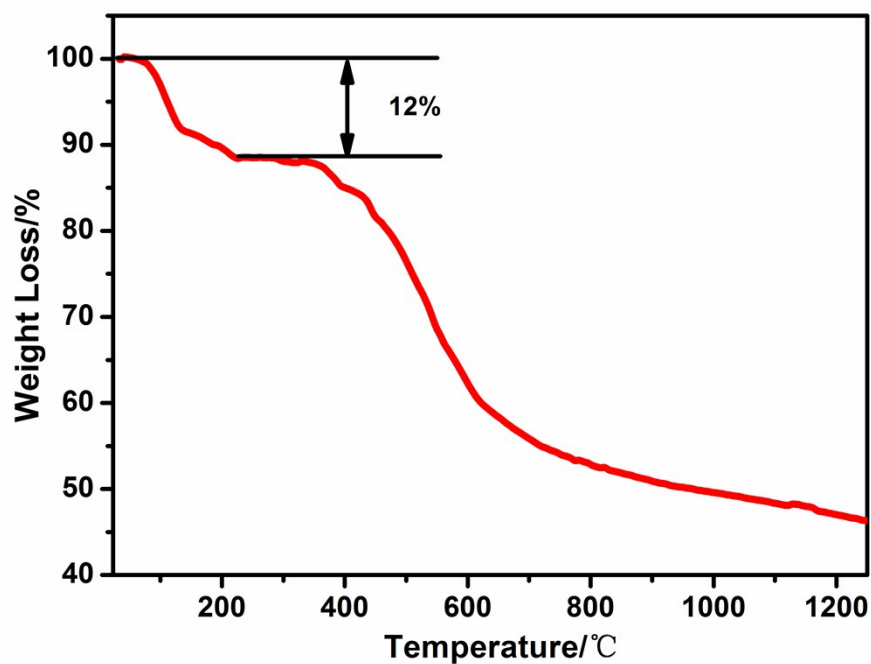


Fig. S3 The TGA plots of Tb-MOF under N₂ environment.

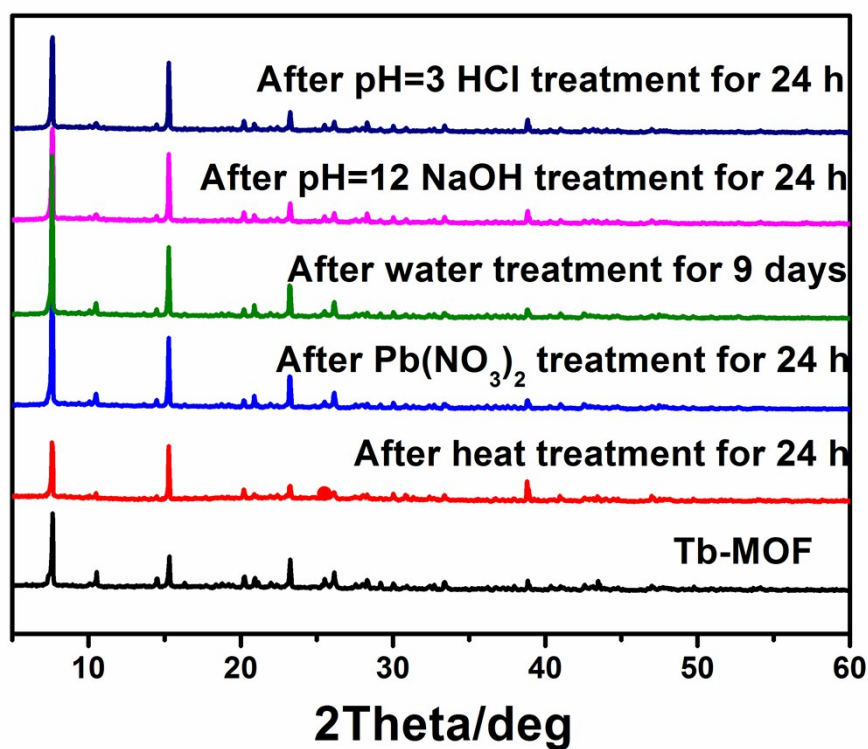


Fig. S4 PXRD patterns of Tb-MOF, upon the treatment with Pb (NO₃)₂ solution, water, pH = 12 NaOH solution, pH = 3 HCl, 6 solution.

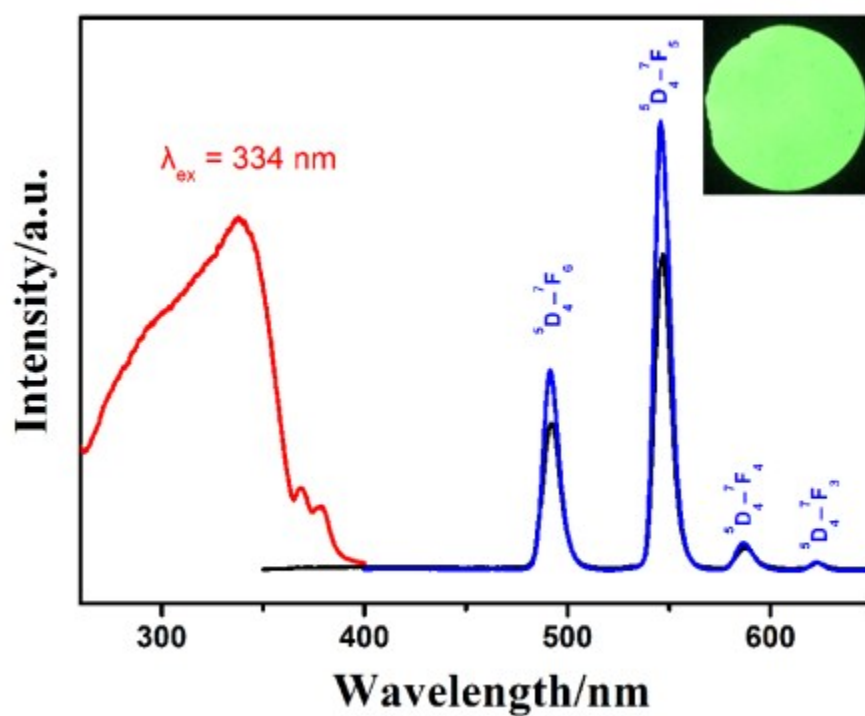


Fig. S5 The solid-state excitation (red) and emission (blue) spectra of Tb-MOF. Emission spectra of Tb-MOF in aqueous solution (black). The illustration is the corresponding fluorescence pictures under UV-light irradiation of 365 nm.

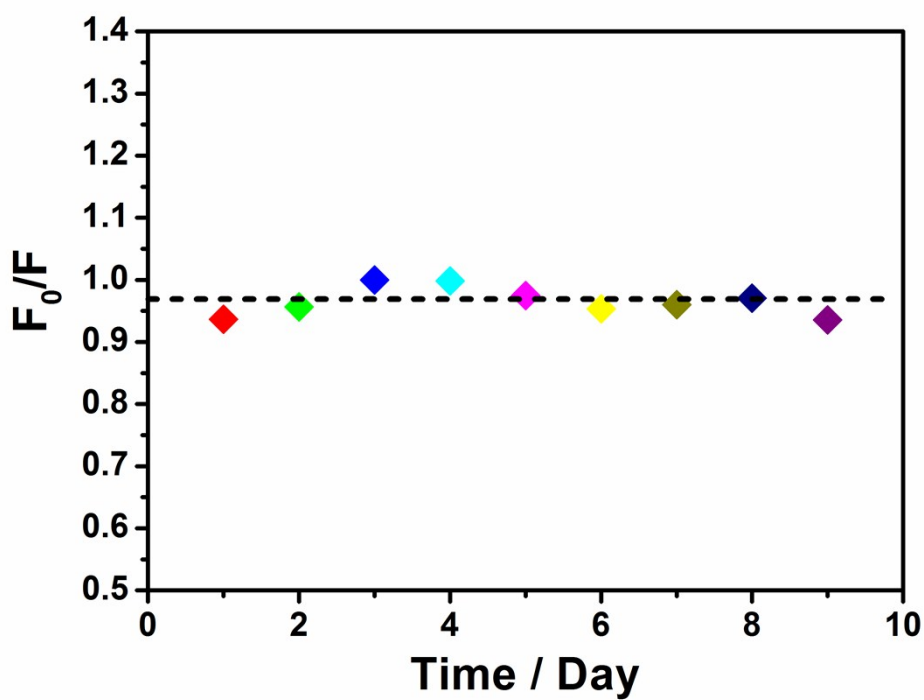


Fig. S6 Comparison of the dominated emission peaks (545 nm) of 1 after immersed in aqueous solution for 9 days.

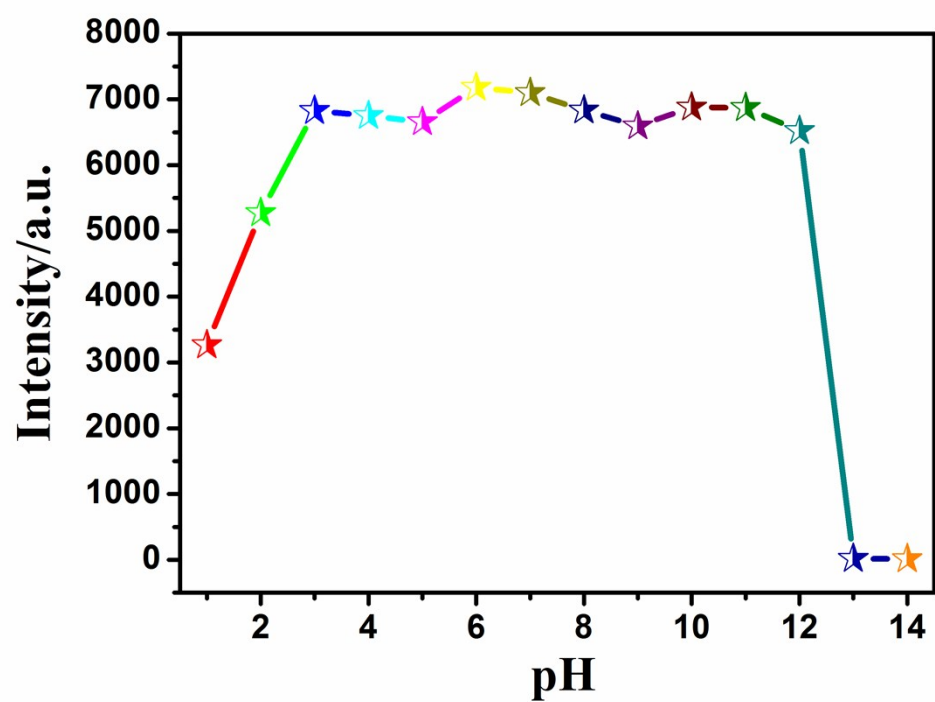


Fig. S7 Exposure various aqueous solutions with pH values from 1.0 to 14.0.

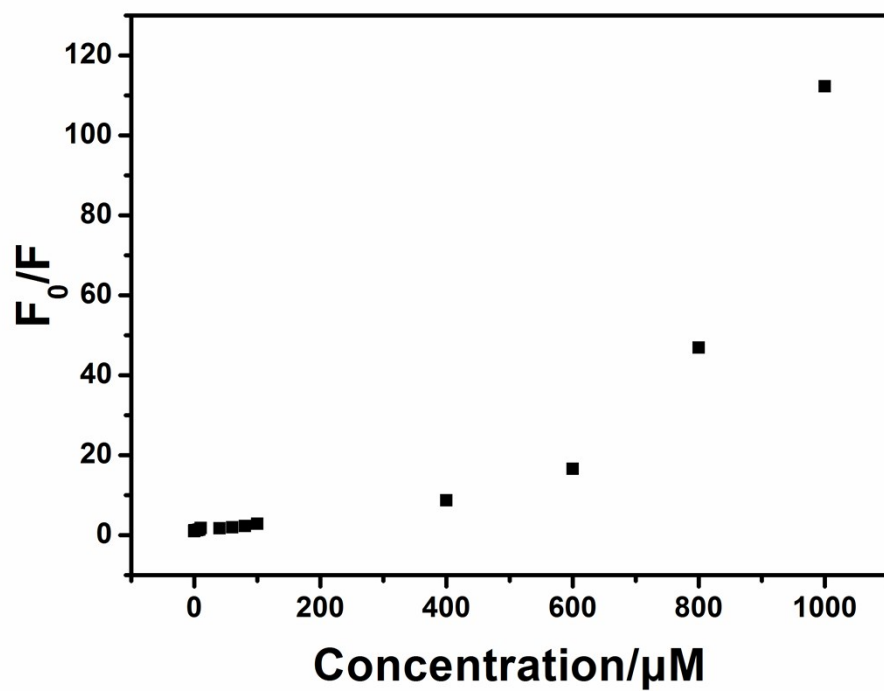


Fig. S8 Stern–Volmer plot for pb (II) in full concentration region

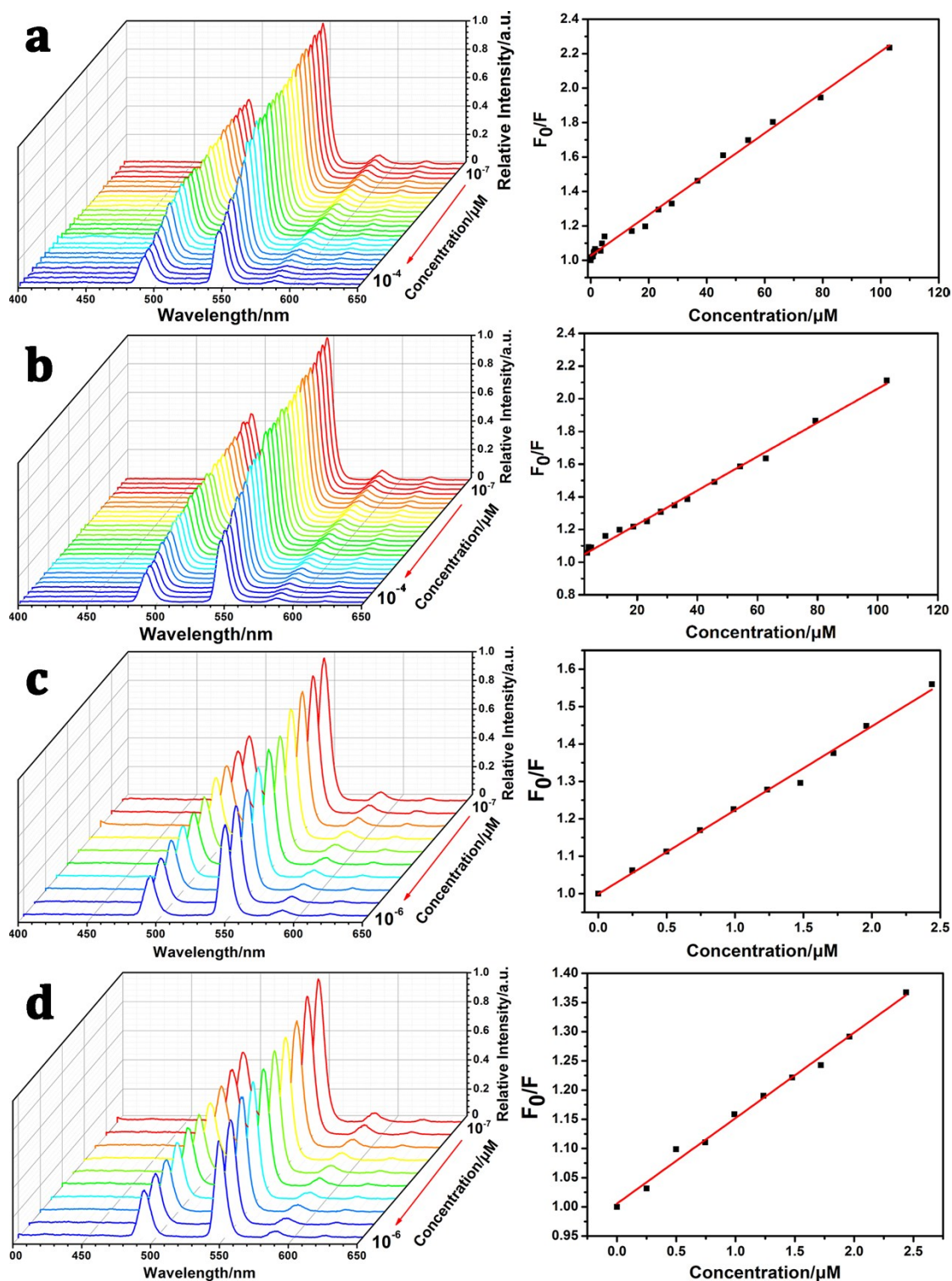


Fig S9 When the pH = 4(a), 5(b), 9(c), 11(d), the fluorescence spectra of Tb–MOF under different concentrations of Pb^{2+} aqueous solution (left), Linear relationship between the

fluorescence intensity and Pb^{2+} ion concentration at 545 nm (right)

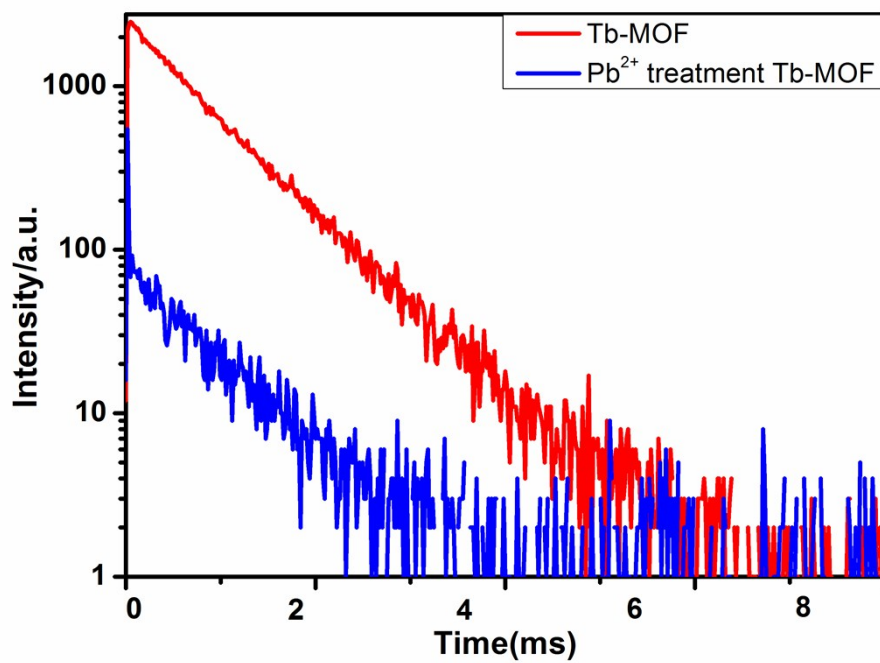


Fig S10 Fluorescence decay profile of Tb-MOF in the absence and presence of lead ions.

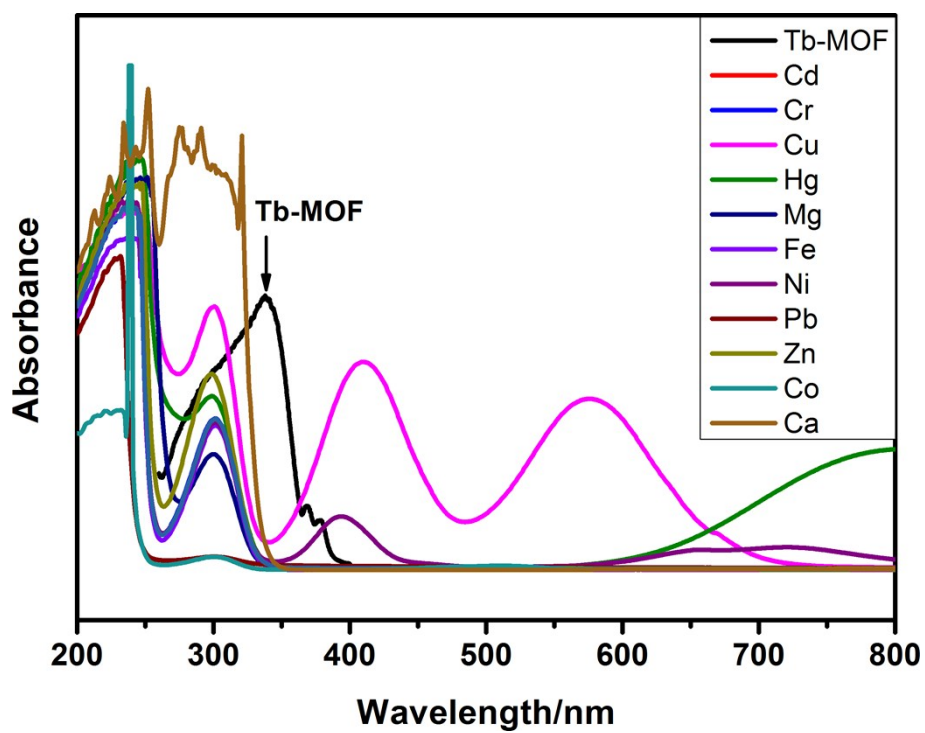


Fig S11 UV-vis absorption of aqueous solution containing different metal cations

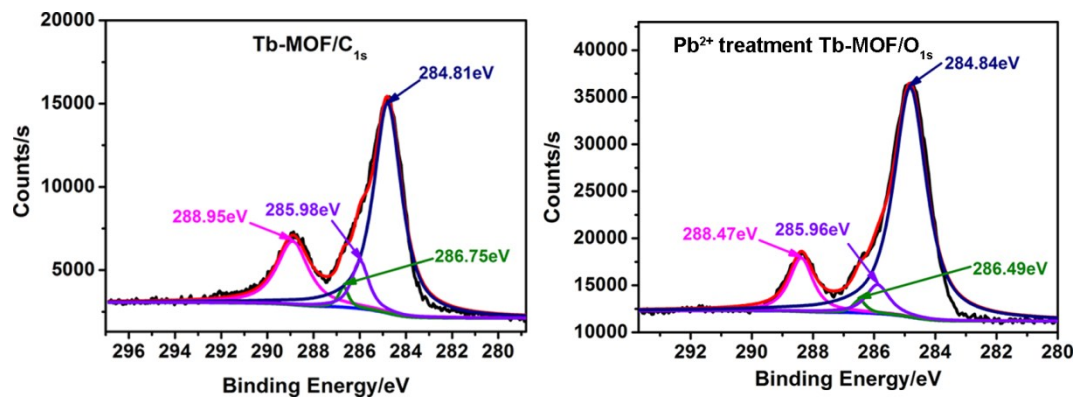


Fig. S12 C_{1s} XPS for Tb-MOF and Pb²⁺ treatment Tb-MOF

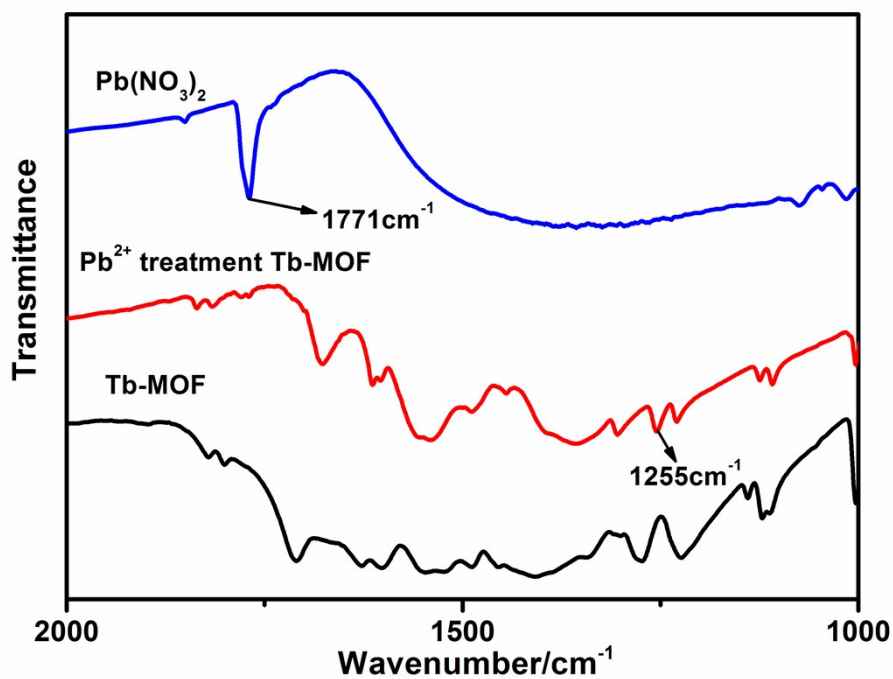


Fig. S13 FT-IR spectra of Pb(NO₃)₂, Tb-MOF and Pb²⁺ treatment Tb-MOF

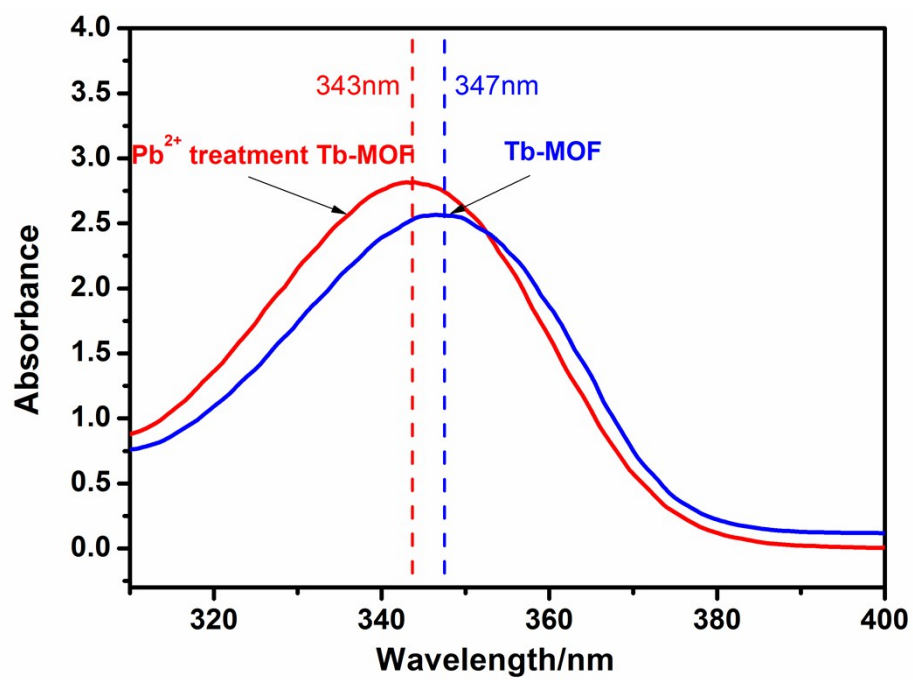


Fig. S14 Solid UV-vis spectra of Tb-MOF and Pb²⁺ treatment Tb-MOF

Table S1 Crystal data and structure refinement of compound Tb-MOF.

Compound	Tb-MOF
Formula	C ₈ H ₁₃ N ₀ O ₁₀ Tb
Formula weight	428.10
Crystal system	Monoclinic
Space group	C2/c
a (Å)	a = 19.7011(9)
b (Å)	b = 10.5118(5)
c (Å)	c = 17.6789(8)
V (Å ³)	3492.3(3)
Z	8
ρ_{calc} (mg·mm ⁻³)	1.628
F(000)	1648
μ (mm ⁻¹)	4.083
T(K)	296
Θ range	3.03-25.02
Reflections collected /unique	28194 / 3084 [R(int) = 0.0210]
Final R indices [I>2 σ]	0.0230
Final wR indices (F^2) [I>2 σ]	0.0783
Goodness of fit	1.118
Max/min $\Delta\rho$ (e Å ⁻³)	0.899 and -0.623

Table S2 Selected bond lengths [Å] and angles [°] for compound Tb-MOF.

O(7)-Tb(1)	2.443(3)	Tb(1)-O(2)	2.488(3)
O(1)-Tb(1)	2.383(3)	Tb(1)-O(3)	2.488(3)
Tb(1)-O(5)	2.385(3)	Tb(1)-O(6)#1	2.496(3)
Tb(1)-O(10)	2.391(3)	O(6)-Tb(1)#2	2.496(3)
Tb(1)-O(9)	2.402(4)	O(8)-Tb(1)#2	2.437(3)
Tb(1)-O(8)#1	2.437(3)		
O(1)-Tb(1)-O(5)	138.36(11)	O(7)-Tb(1)-O(2)	143.19(11)
O(1)-Tb(1)-O(10)	76.71(10)	O(5)-Tb(1)-O(2)	75.95(10)
O(5)-Tb(1)-O(10)	72.24(11)	O(10)-Tb(1)-O(2)	84.50(10)
O(1)-Tb(1)-O(9)	74.31(13)	O(9)-Tb(1)-O(2)	88.21(14)
O(5)-Tb(1)-O(9)	146.44(13)	O(8)#1-Tb(1)-O(2)	74.44(9)
O(10)-Tb(1)-O(9)	136.26(12)	O(7)-Tb(1)-O(2)	143.19(11)
O(1)-Tb(1)-O(8)#1	140.97(11)	O(1)-Tb(1)-O(3)	75.94(10)
O(5)-Tb(1)-O(8)#1	72.02(12)	O(5)-Tb(1)-O(3)	117.79(12)
O(10)-Tb(1)-O(8)#1	141.89(11)	O(10)-Tb(1)-O(3)	71.30(11)
O(9)-Tb(1)-O(8)#1	75.32(13)	O(9)-Tb(1)-O(3)	70.36(14)
O(1)-Tb(1)-O(7)	73.53(11)	O(8)#1-Tb(1)-O(3)	115.48(10)
O(5)-Tb(1)-O(7)	70.62(11)	O(7)-Tb(1)-O(3)	135.81(11)
O(10)-Tb(1)-O(7)	71.14(11)	O(2)-Tb(1)-O(3)	52.06(10)
O(9)-Tb(1)-O(7)	128.46(14)	O(1)-Tb(1)-O(6)#1	95.50(10)
O(8)#1-Tb(1)-O(7)	108.38(11)	O(5)-Tb(1)-O(6)#1	92.23(12)
O(1)-Tb(1)-O(2)	127.98(10)	O(10)-Tb(1)-O(6)#1	141.88(10)
O(5)-Tb(1)-O(2)	75.95(10)	O(9)-Tb(1)-O(6)#1	73.38(13)
O(10)-Tb(1)-O(2)	84.50(10)	O(8)#1-Tb(1)-O(6)#1	52.24(9)
O(9)-Tb(1)-O(2)	88.21(14)	O(7)-Tb(1)-O(6)#1	70.87(11)
O(8)#1-Tb(1)-O(2)	74.44(9)	O(2)-Tb(1)-O(6)#1	126.21(10)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+2,z-1/2 #2 x,-y+2,z+1/2

Table S3 Selected hydrogen bond lengths [Å] and angles [°] for compound Tb-MOF.

D-H...A	D-H	H...A	<DHA	D...A
O7-H7B...O6#1	0.850	1.984	152.73	2.767
O5-H5A...O3#2	0.850	2.089	126.85	2.687
O5-H5A...O1#2	0.850	2.652	154.22	3.438
O10-H10C... O8#3	0.960	1.841	139.82	2.648
O10-H10C... O2#4	0.960	2.535	125.65	3.191

Symmetry transformations used to generate equivalent atoms:

#1:-x+3/2, y-1/2, -z+3/2, #2:-x+3/2, y+1/2, -z+3/2, #3:-x+3/2, -y+3/2, -z+2, #4:-x+3/2, y-1/2, -z+3/2