

***Electronic Supplementary Information (ESI)***

**Anionic lanthanide metal-organic frameworks with magnetic, fluorescence, and proton conductivity properties and selective adsorption of a cationic dye**

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**Table S1.** Selected bond lengths (Å) and angles (deg) for **1<sup>a</sup>**.

Gd1—O1	2.301(4)	Gd1—O5 <sup>iii</sup>	2.456(5)
Gd1—O2 <sup>i</sup>	2.434(5)	Gd1—O6 <sup>i</sup>	2.524(5)
Gd1—O3 <sup>ii</sup>	2.311(4)	Gd1—O7 <sup>iv</sup>	2.371(5)
Gd1—O4 <sup>iii</sup>	2.452(4)	Gd1—O11 <sup>v</sup>	2.374(5)
O1—Gd1—O2 <sup>i</sup>	76.9(2)	O2 <sup>i</sup> —Gd1—O4 <sup>iii</sup>	98.6(2)
O1—Gd1—O3 <sup>ii</sup>	78.6(2)	O2 <sup>i</sup> —Gd1—O5 <sup>iii</sup>	71.1(2)
O1—Gd1—O4 <sup>iii</sup>	132.43(19)	O2 <sup>i</sup> —Gd1—O6 <sup>i</sup>	52.2(2)
O1—Gd1—O5 <sup>iii</sup>	82.15(18)	O3 <sup>ii</sup> —Gd1—O2 <sup>i</sup>	84.8(2)
O1—Gd1—O6 <sup>i</sup>	126.10(18)	O3 <sup>ii</sup> —Gd1—O4 <sup>iii</sup>	148.9(2)
O1—Gd1—O7 <sup>iv</sup>	79.78(18)	O3 <sup>ii</sup> —Gd1—O5 <sup>iii</sup>	152.0(2)
O1—Gd1—O11 <sup>v</sup>	135.34(15)	O3 <sup>ii</sup> —Gd1—O6 <sup>i</sup>	80.21(17)
O4 <sup>iii</sup> —Gd1—O5 <sup>iii</sup>	52.7(2)	O3 <sup>ii</sup> —Gd1—O7 <sup>iv</sup>	117.21(16)
O4 <sup>iii</sup> —Gd1—O6 <sup>i</sup>	77.81(17)	O5 <sup>iii</sup> —Gd1—O6 <sup>i</sup>	95.3(2)
O7 <sup>iv</sup> —Gd1—O2 <sup>i</sup>	143.7(2)	O11 <sup>v</sup> —Gd1—O2 <sup>i</sup>	137.64(19)
O7 <sup>iv</sup> —Gd1—O4 <sup>iii</sup>	77.43(17)	O11 <sup>v</sup> —Gd1—O4 <sup>iii</sup>	78.52(17)
O7 <sup>iv</sup> —Gd1—O5 <sup>iii</sup>	78.6(2)	O11 <sup>v</sup> —Gd1—O5 <sup>iii</sup>	129.2(2)
O7 <sup>iv</sup> —Gd1—O6 <sup>i</sup>	152.73(19)	O11 <sup>v</sup> —Gd1—O6 <sup>i</sup>	86.46(17)

<sup>a</sup>Symmetry codes: (i)  $-x+y, -x+1, z-1/3$ ; (ii)  $-x+1, -x+y, -z+4/3$ ; (iii)  $y-1, x, -z+1$ ; (iv)  $-x, -x+y, -z+4/3$ ; (v)  $x-1, y-1, z$ .

**Table S2.** Selected bond lengths (Å) and angles (deg) for **2<sup>b</sup>**.

Dy01—O1 <sup>i</sup>	2.275(4)	Dy01—O4 <sup>iv</sup>	2.286(4)
Dy01—O8 <sup>ii</sup>	2.510(5)	Dy01—O5 <sup>v</sup>	2.443(5)
Dy01—O2 <sup>iii</sup>	2.350(5)	Dy01—O6 <sup>v</sup>	2.427(4)
Dy01—O3	2.349(4)	Dy01—O7 <sup>ii</sup>	2.400(5)
O1 <sup>i</sup> —Dy01—O2 <sup>iii</sup>	80.11(18)	O3—Dy01—O2 <sup>iii</sup>	77.14(19)
O1 <sup>i</sup> —Dy01—O3	135.12(15)	O3—Dy01—O5 <sup>v</sup>	128.93(19)
O1 <sup>i</sup> —Dy01—O4 <sup>iv</sup>	79.07(19)	O3—Dy01—O6 <sup>v</sup>	78.44(17)
O1 <sup>i</sup> —Dy01—O5 <sup>v</sup>	81.85(18)	O3—Dy01—O7 <sup>ii</sup>	138.05(18)
O1 <sup>i</sup> —Dy01—O6 <sup>v</sup>	132.92(19)	O3—Dy01—O8 <sup>ii</sup>	86.65(17)
O1 <sup>i</sup> —Dy01—O7 <sup>ii</sup>	76.88(18)	O4 <sup>iv</sup> —Dy01—O2 <sup>iii</sup>	118.29(16)
O1 <sup>i</sup> —Dy01—O8 <sup>ii</sup>	126.28(17)	O4 <sup>iv</sup> —Dy01—O3	78.5(2)
O2 <sup>iii</sup> —Dy01—O5 <sup>v</sup>	77.6(2)	O4 <sup>iv</sup> —Dy01—O5 <sup>v</sup>	152.2(2)
O2 <sup>iii</sup> —Dy01—O6 <sup>v</sup>	77.68(17)	O4 <sup>iv</sup> —Dy01—O6 <sup>v</sup>	147.8(2)
O2 <sup>iii</sup> —Dy01—O7 <sup>ii</sup>	143.7(2)	O4 <sup>iv</sup> —Dy01—O7 <sup>ii</sup>	84.4(2)
O2 <sup>iii</sup> —Dy01—O8 <sup>ii</sup>	152.17(18)	O4 <sup>iv</sup> —Dy01—O8 <sup>ii</sup>	79.48(18)
O5 <sup>v</sup> —Dy01—O8 <sup>ii</sup>	96.0(2)	O7 <sup>ii</sup> —Dy01—O5 <sup>v</sup>	71.6(2)
O7 <sup>ii</sup> —Dy01—O8 <sup>ii</sup>	52.44(19)	O7 <sup>ii</sup> —Dy01—O6 <sup>v</sup>	98.1(2)

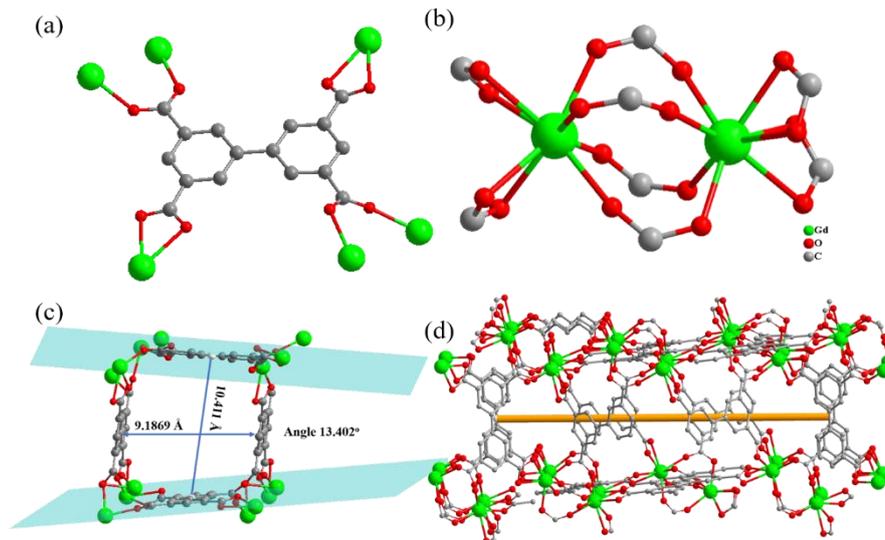
<sup>b</sup>Symmetry codes: (i)  $x, y+1, z$ ; (ii)  $-x+y+1, -x+2, z-1/3$ ; (iii)  $x-y, -y+1, -z+2/3$ ; (iv)  $x-y+1, -y+2, -z+2/3$ ; (v)  $-x+1, -x+y+1, -z+1/3$ .

**Table S3.** RhB adsorption capacity and adsorption time of MOFs.

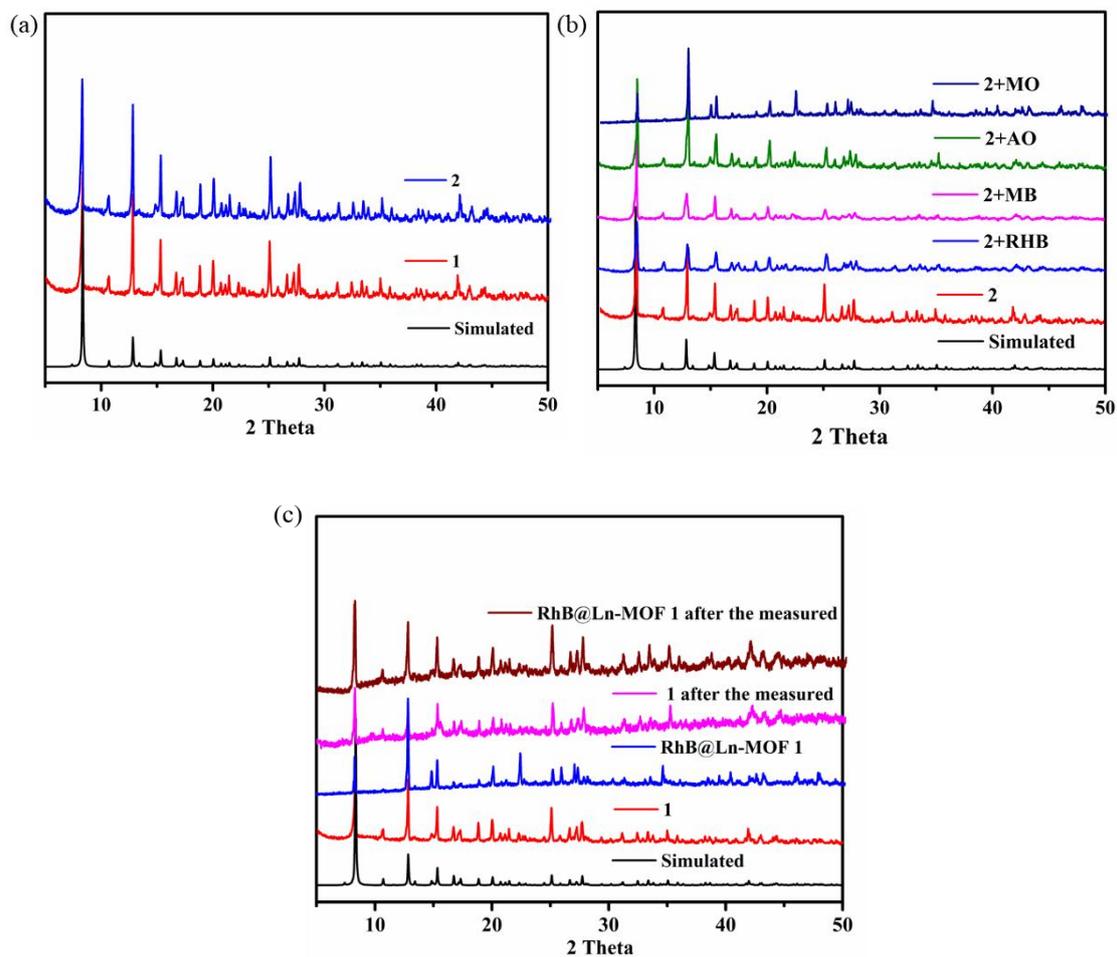
Dye	MOFs	Removalrate (mg/g)	Time (min)	Ref.
RhB	Ln-MOF 2	79.42	40	this work
	MIL-125(Ti)	59.92	180	S1
	Zn-MOF	3.75	60	S2
	POM@UiO-66	222.6	120	S3
	USTC-1	13.4	240	S4
	MIL-68(Al)	1111.11	10	S5
	MgFe <sub>2</sub> O <sub>4</sub> @MOF	219.78	5	S6
	Fe <sub>3</sub> O <sub>4</sub> /MIL-100(Fe)	28.36	90	S7

**Table S4.** Maximum  $\sigma$  values of Ln-MOF 1 and RhB@Ln-MOF 1 compared with the selected Ln-MOFs.

MOFs	$\sigma$ [S·cm <sup>-1</sup> ]	conditions	$E_a$ (eV)	Ref.
H[(N(Me) <sub>4</sub> ) <sub>2</sub> ][Gd <sub>3</sub> (NIPA) <sub>6</sub> ]·3H <sub>2</sub> O	$7.17 \times 10^{-2}$	75 °C-98% RH	0.13	S8
{[Er <sub>4</sub> (OH) <sub>4</sub> (L) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub> ]·4.6H <sub>2</sub> O·1.4CH <sub>3</sub> CN} <sub>n</sub>	$6.59 \times 10^{-3}$	80 °C-95% RH	0.32	S9
{[Ho <sub>4</sub> (OH) <sub>4</sub> (L) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub> ]·4.6H <sub>2</sub> O·1.4CH <sub>3</sub> CN} <sub>n</sub>	$4.56 \times 10^{-3}$	80 °C-95% RH	0.38	S9
{[Dy(DMTP-DC) <sub>1.5</sub> (H <sub>2</sub> O) <sub>3</sub> ]·H <sub>2</sub> O} <sub>n</sub>	$2.67 \times 10^{-4}$	55 °C-100% RH	0.20	S10
{[Nd <sub>2</sub> (HMIDC) <sub>2</sub> ( $\mu$ -C <sub>2</sub> O <sub>4</sub> )(H <sub>2</sub> O) <sub>3</sub> ]·4H <sub>2</sub> O} <sub>n</sub>	$2.25 \times 10^{-4}$	100°C-98% RH	0.71	S11
{[Gd(DMTP-DC) <sub>1.5</sub> (H <sub>2</sub> O) <sub>3</sub> ]·H <sub>2</sub> O} <sub>n</sub>	$1.62 \times 10^{-4}$	55°C-100% RH	0.27	S10
Ln-MOF 1	$1.02 \times 10^{-4}$	50 °C -90% RH	0.34	this work
JXNU-8(Eu)	$2.28 \times 10^{-5}$	80 °C-98% RH	0.18	S12
{[Gd <sub>4</sub> (OH) <sub>4</sub> (L) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub> ]·4.6H <sub>2</sub> O·1.4CH <sub>3</sub> CN} <sub>n</sub>	$2.02 \times 10^{-6}$	80 °C-95% RH	0.27	S9
RhB@Ln-MOF 1	$7.40 \times 10^{-8}$	50 °C -90% RH	0.45	this work



**Fig. S1** (a) the way a metal is connected to a ligand; (b) Secondary building unit; (c) the dihedral angles and distances between ligands; (d) the 1D channel in Ln-MOF 1.



**Fig. S2** The PXRD patterns of 1 and 2 (a), 2 after the adsorption of dyes (b), and RhB@Ln-MOF 1 and the sample after the proton conduction (c).

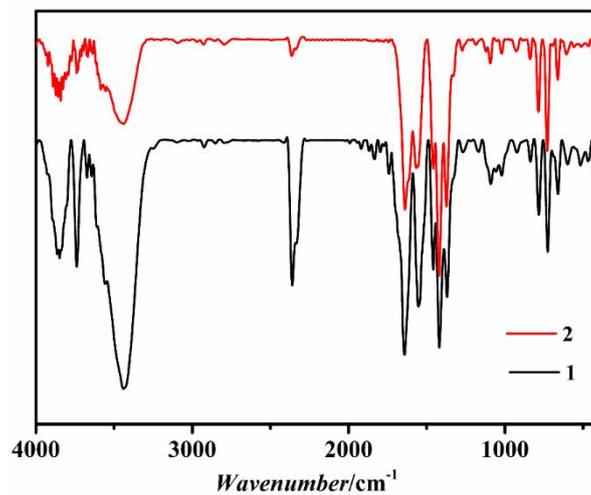


Fig. S3 The IR spectra of Ln-MOFs 1 and 2.

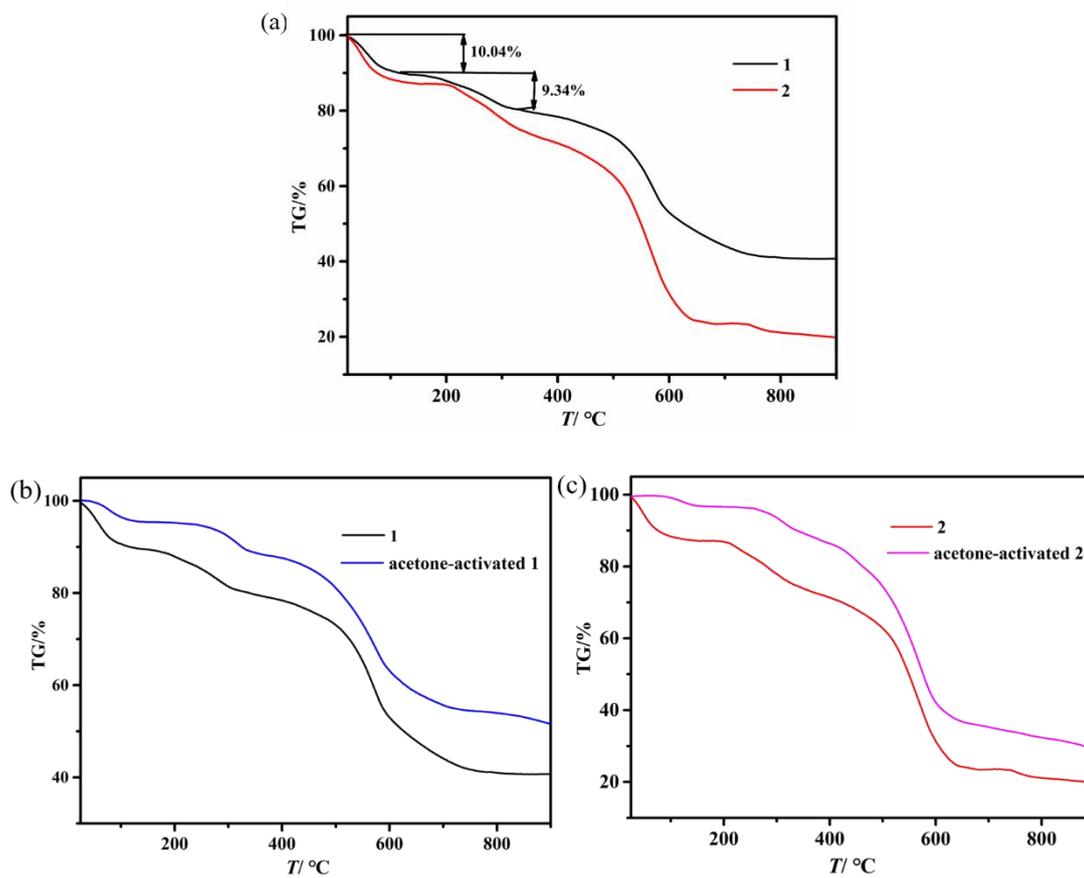


Fig. S4 The TG curves of Ln-MOFs 1 and 2 (a), and acetone-activated 1 (b) and 2 (c).

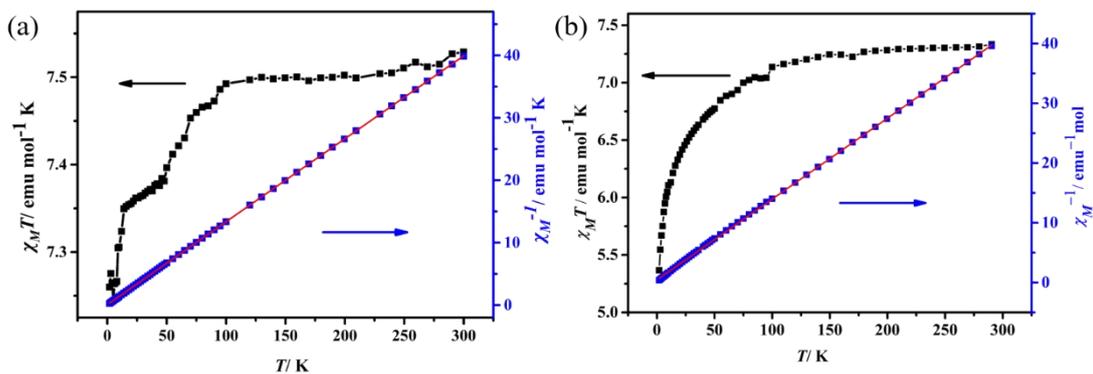


Fig. S5 Plots of  $\chi_M T$  vs  $T$  and  $\chi_M^{-1}$  vs  $T$  of Ln-MOFs **1** (a) and **2** (b). Red lines for the Curie-Weiss fitting.

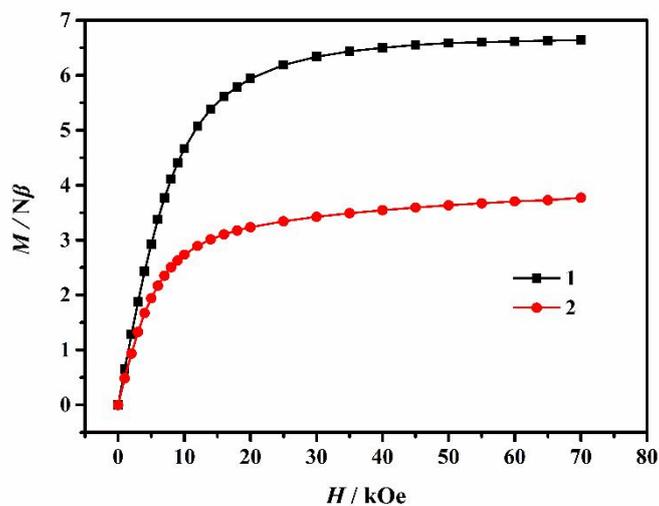


Fig. S6 Field dependence of the magnetizations of **1** and **2** at 2 K.

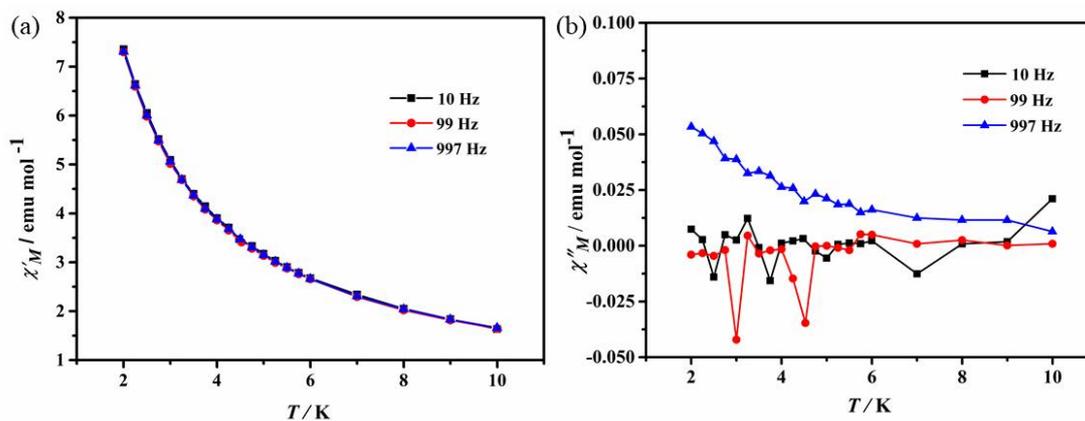


Fig. S7 Frequency dependence of the in-phase ( $\chi'$ ) and out-of-phase ( $\chi''$ ) ac susceptibility signals for **2** under zero-dc field.

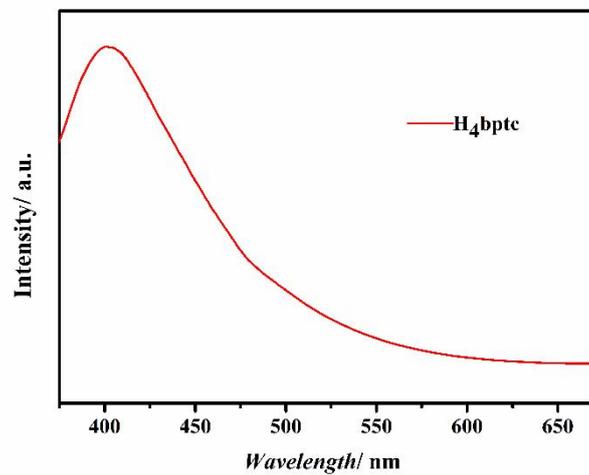


Fig. S8 The emission spectrum of H<sub>4</sub>bptc ( $\lambda_{\text{ex}} = 354$  nm).

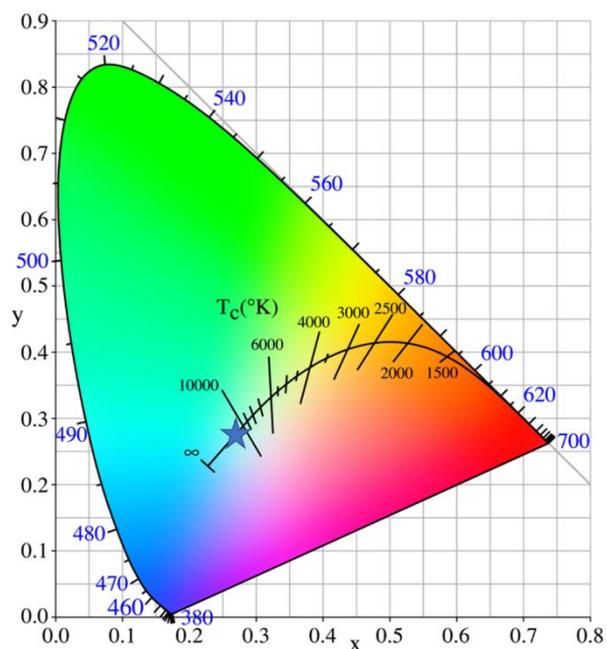
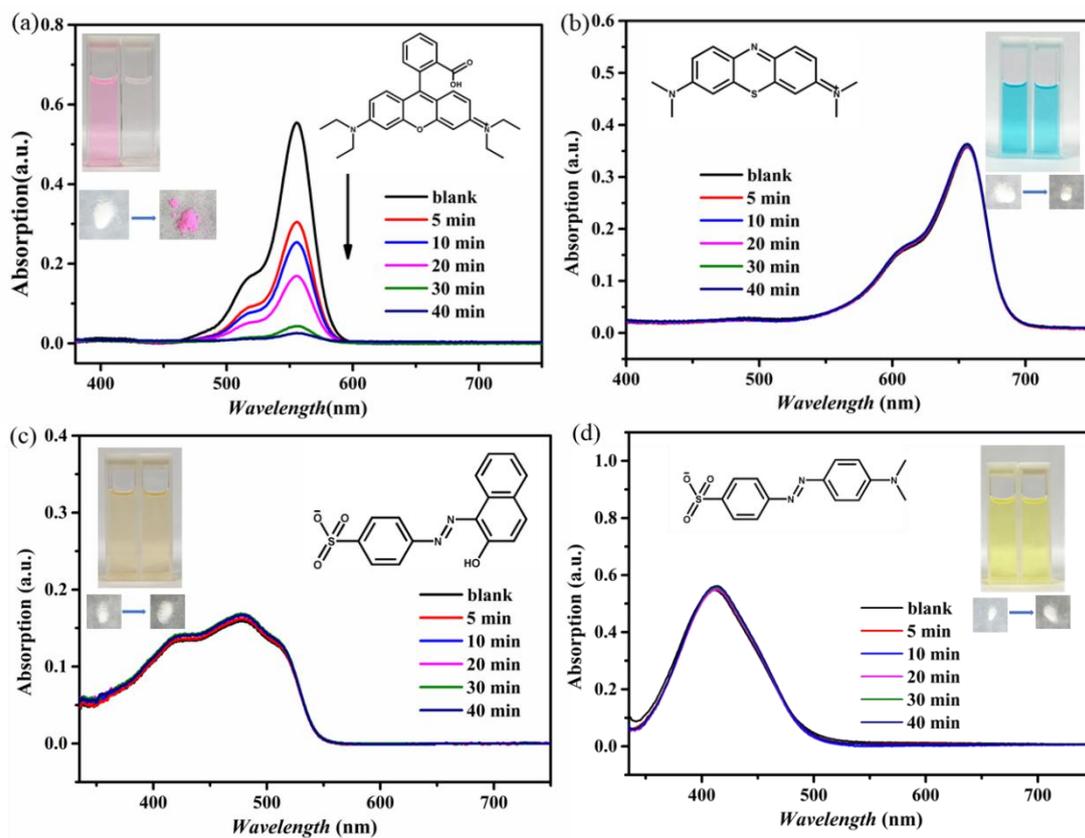
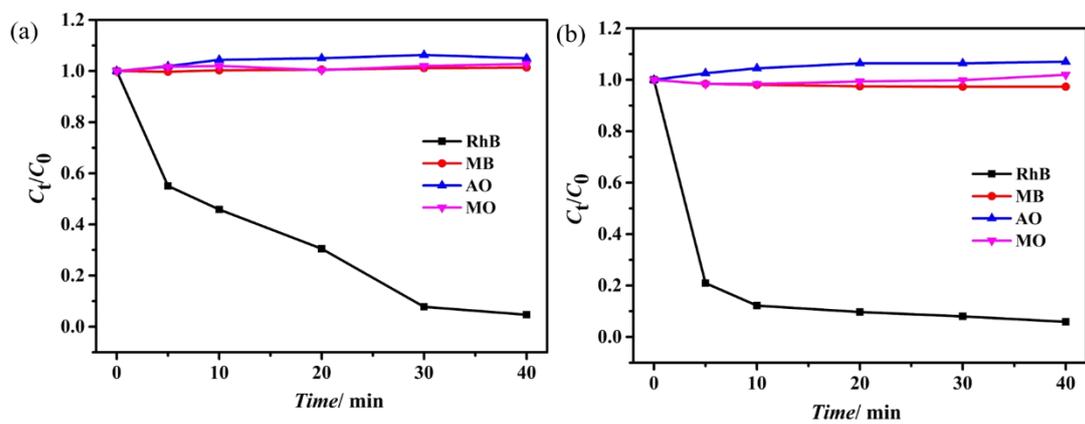


Fig. S9 CIE chromaticity diagram showing the color coordinates of Ln-MOF 2 under the excitation of 328 nm.



**Fig. S10** UV-vis absorption spectra of **1** adsorbed RhB (a), MB (b), AO (c) and MO (d) in acetone solutions during the adsorption process.



**Fig. S11** Corresponding plots of  $C_t/C_0$  of dyes versus time during the adsorption of **1** (a) and **2** (b).

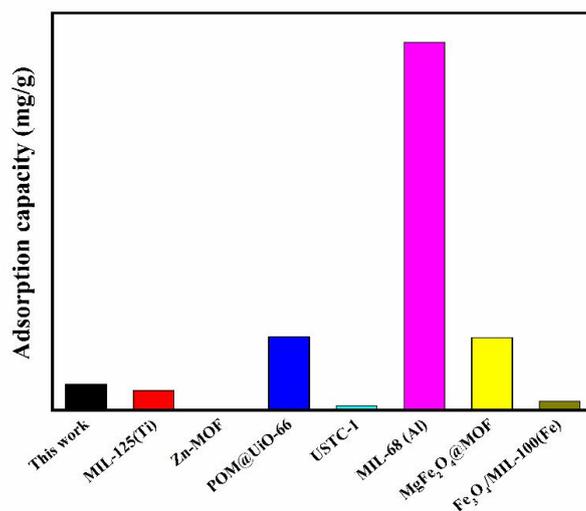


Fig. S12 The RhB adsorption capacity of different MOFs.

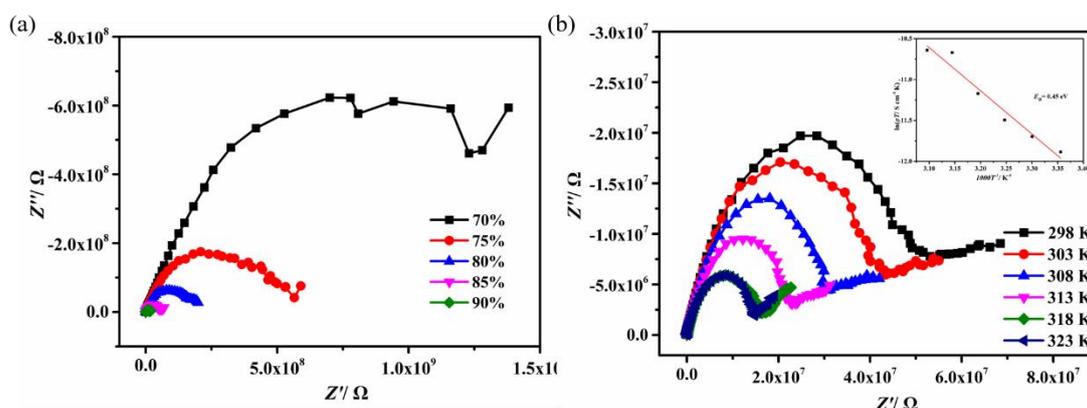


Fig. S13 (a) Nyquist plots for RhB@Ln-MOF **1** at different RHs and  $T = 323$  K. (b) Nyquist plots for RhB@Ln-MOF **1** at different temperatures and 90% RH; Arrhenius plots of the conductivity of RhB@Ln-MOF **1** (inset).

## References

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