

Electronic Supplementary Information (ESI)

Anionic Metal–Organic Framework for High-Efficiency Pollutant Removal and Selective Sensing of Fe(III) Ions†

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Materials and general methods

All solvents and starting materials for synthesis were purchased commercially and were used as received. Powder X-ray diffraction (PXRD) patterns were collected with a Bruker AXS D8 advanced automated diffractometer with Cu-K radiation. All UV/Vis spectra were measured on a SP-752(PC) UV-Vis spectrophotometer (Shanghai Spectrum Instrument Co., Ltd). Luminescence spectra for the solid samples and liquid samples were investigated with a Hitachi F-4500 fluorescence spectrophotometer and Varian Cary Eclipse Fluorescence spectrophotometer, respectively. Inductively coupled plasma-optical emission spectroscopy (ICP) was performed using a 700 Series ICPOES (Agilent Technologies).

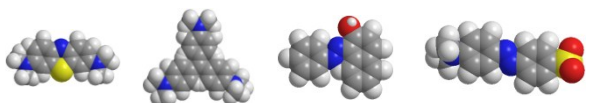
Synthesis of **gea-MOF-1**

The crystal of **gea-MOF-1** was synthesized according to references.¹ A solution of $Y(NO_3)_3 \cdot 6H_2O$ (8.6 mg, 0.0225 mmol), H_3BTB (6.6 mg, 0.015 mmol), 2-fluorobenzoic acid (95.2 mg, 0.675 mmol), DMF (2 ml) and H_2O (0.5 ml) was prepared in a 20 ml scintillation vial and subsequently heated to 378 K for 36 hours in a preheated oven.

Experimental details for Organic dye selective adsorption and separation

Freshly prepared **gea-MOF-1** (20 mg) was immersed in 5 mL DMF solutions of different organic dyes with the concentrations of 5×10^{-5} M. The release experiment was carried out after the completion of an ion-exchange process of Methylene blue (MB) on **gea-MOF-1**. Then, the as prepared $MB^+@gea-MOF-1$ was immersed in the saturated $NaNO_3$ DMF solution with the same volume.

Table S1 Molecular weight and dimensions of different dyes molecules.



Abbr	MB^+	MV^+	SD^0	MO^-
M_w	284.40	372.53	248.28	304.33
$x(\text{\AA})$	4.00	4.00	3.68	5.31
$y(\text{\AA})$	7.93	16.32	9.74	7.25
$z(\text{\AA})$	16.34	14.15	13.55	17.39

Table S2 The amounts of Y and Fe element in the sample of Fe³⁺@gea-MOF-1 after washing treatment.

Sample	The mole ratio of Y: Fe
Fe ³⁺ @gea-MOF-1	127: 1

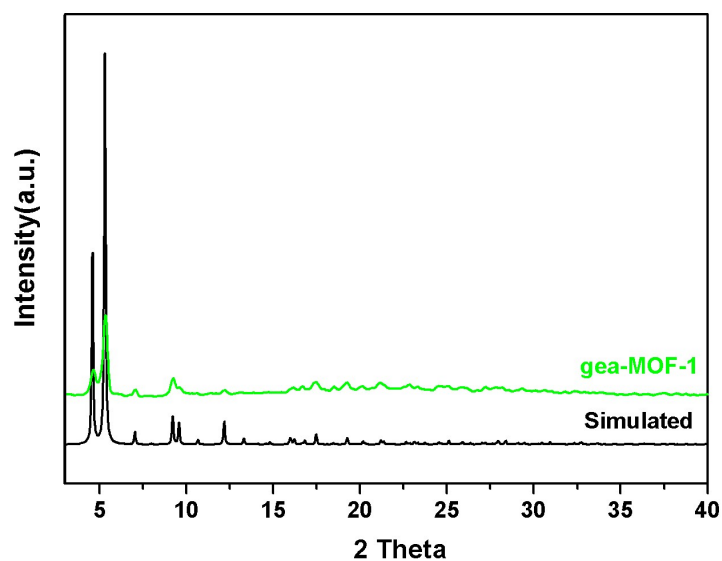


Fig. S1 Simulated and experimental PXRD patterns for gea-MOF-1

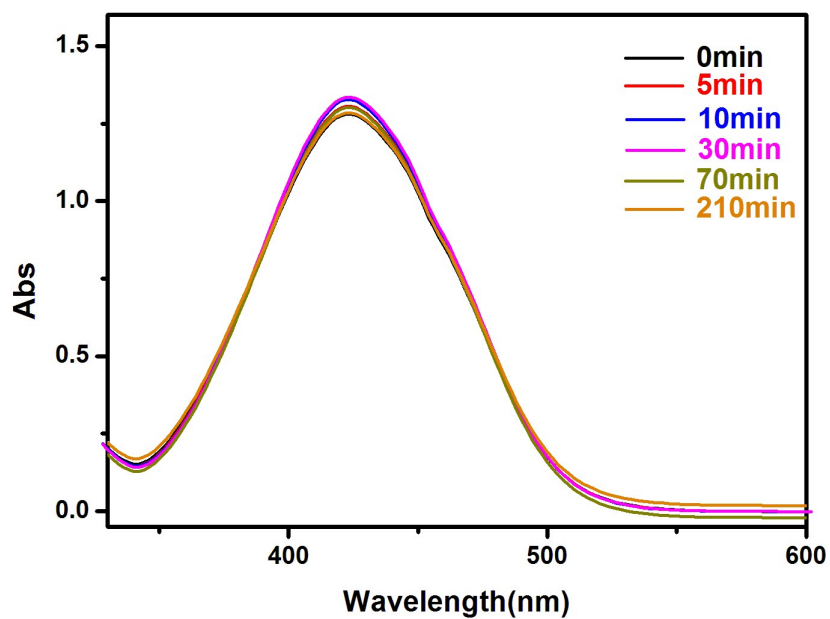


Fig. S2 UV-vis spectra of DMF solutions of MO⁻ in the presence of gea-MOF-1 monitored with time.

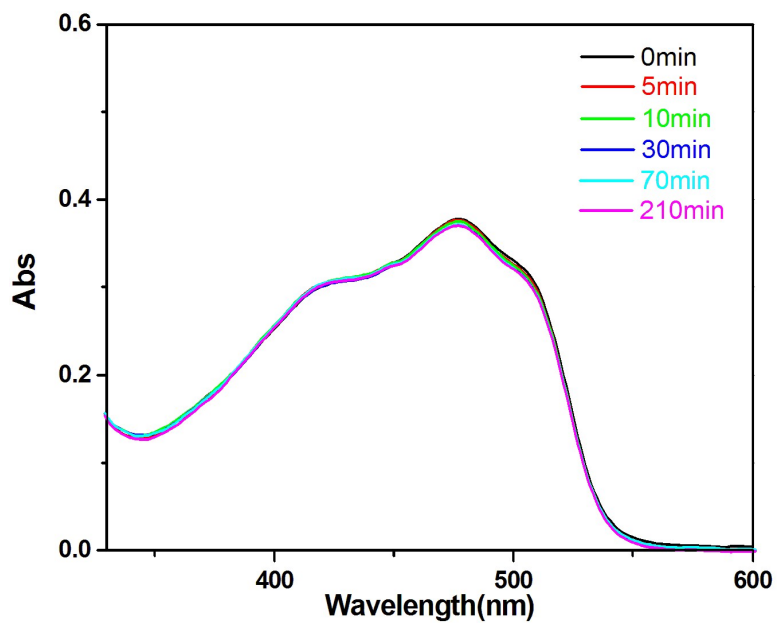


Fig. S3 UV-vis spectra of DMF solutions of SD⁰ in the presence of gea-MOF-1 monitored with time.

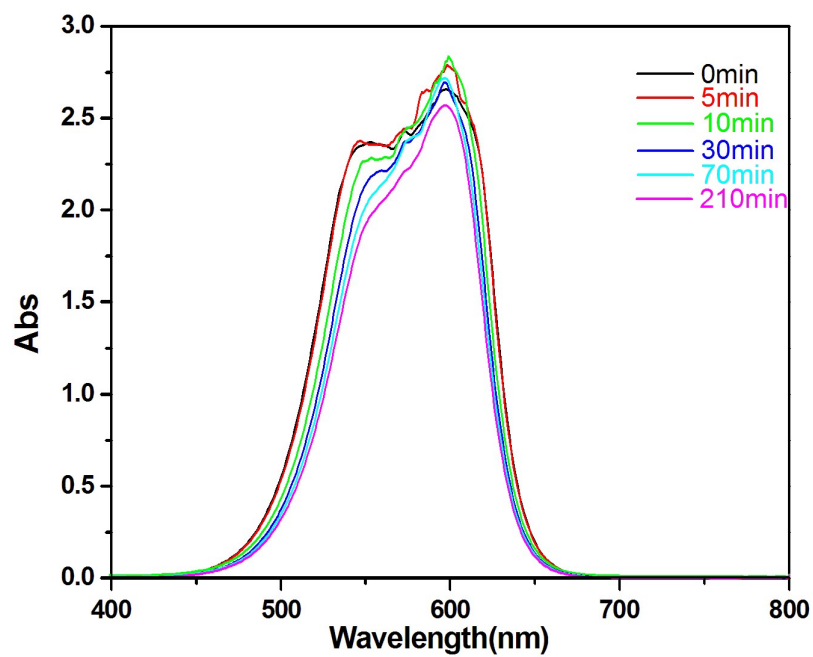


Fig. S4 UV-vis spectra of DMF solutions of SD⁰ in the presence of gea-MOF-1 monitored with time.

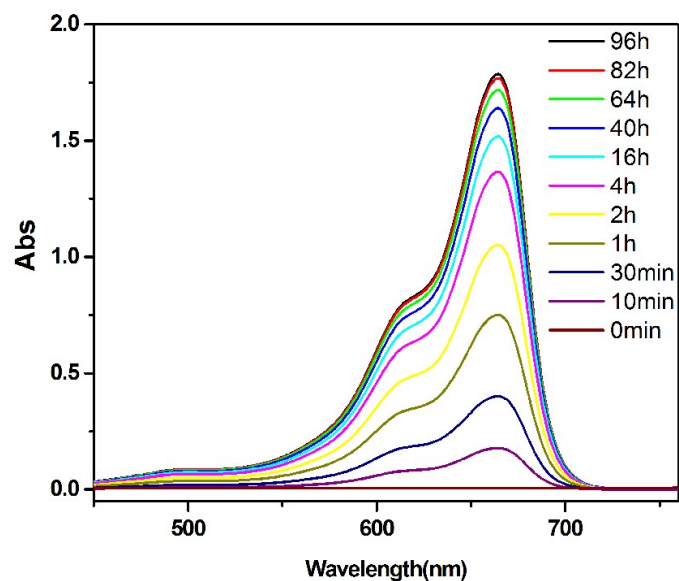


Fig. S5 Temporal evolution of UV-Vis absorption spectra of MB⁺ released from MB⁺@gea-MOF-1 in NaNO₃-containing DMF solution.

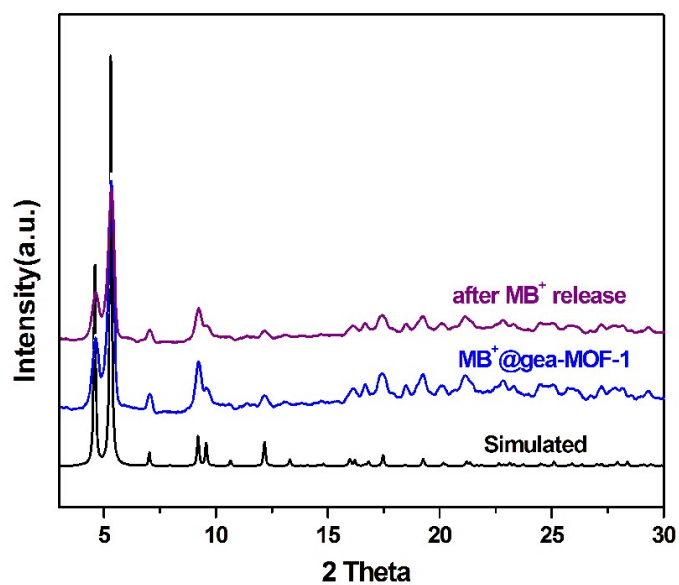


Fig. S6 PXRD patterns of gea-MOF-1 (black, simulated; blue, MB⁺@gea-MOF-1; violet, MB⁺@gea-MOF-1 after MB⁺ release).

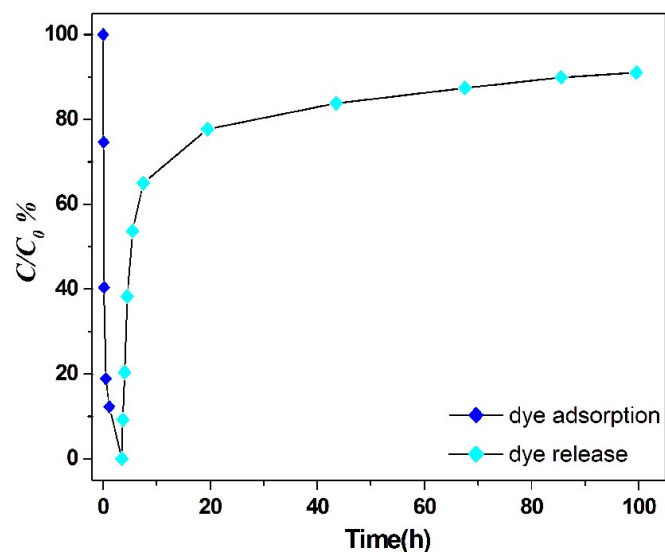


Fig. S7 The reversible adsorption and release of MB⁺ in a full ion-exchange and release cycle.

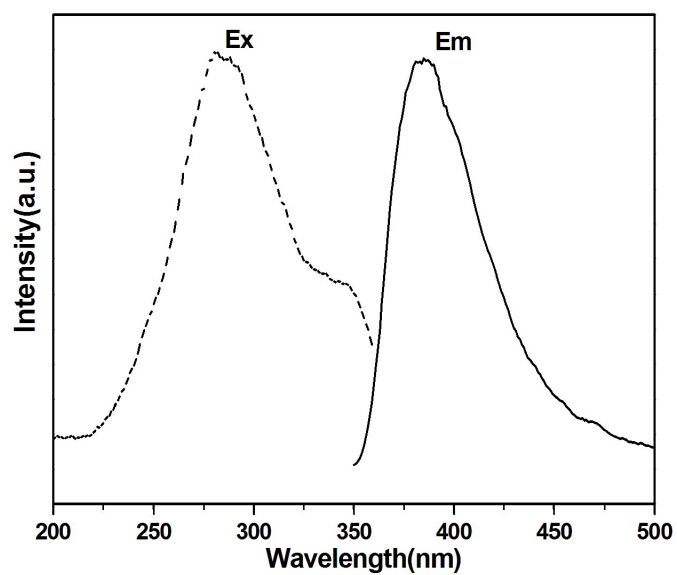


Fig. S8 Excitation (at 284 nm) and emission (at 385 nm) spectra of H₃BTB in the solid state at room temperature.

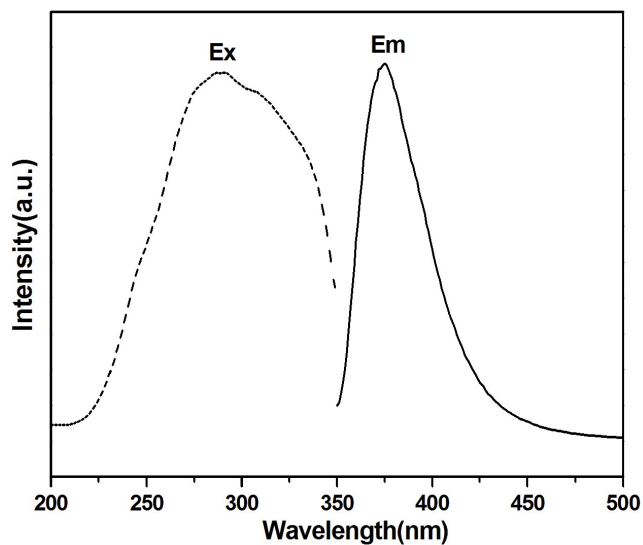


Fig. S9 Excitation (at 290 nm) and emission (at 375 nm) spectra of gea-MOF-1 in the solid state at room temperature.

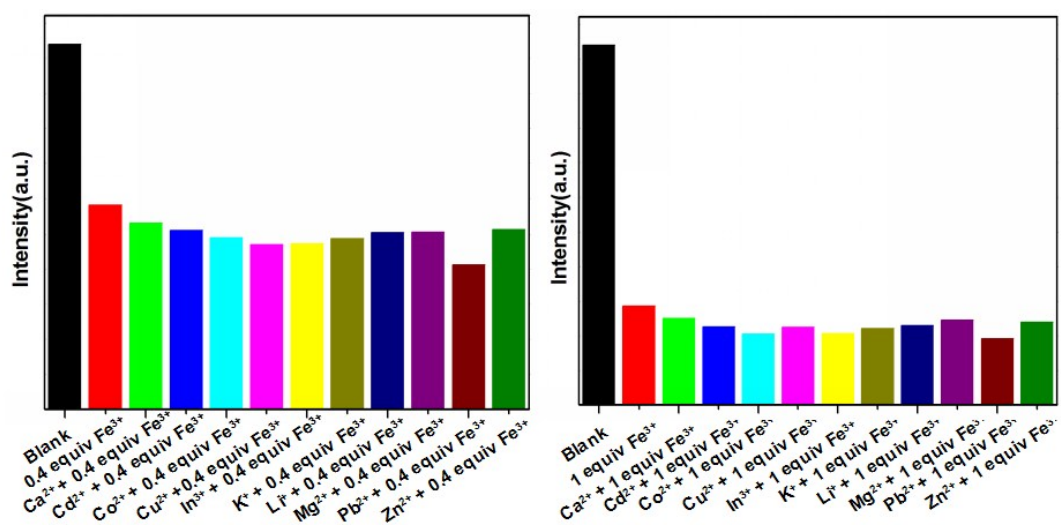


Fig. S10 Room-temperature luminescent intensity of gea-MOF-1 upon addition of 0.5 equiv of Fe^{3+} and 0.4 equiv of various metal ions (a) and with adding 1 equiv of Fe^{3+} and 1 equiv of other metal ions (b) in methanol ($\lambda_{\text{ex}} = 290 \text{ nm}$).

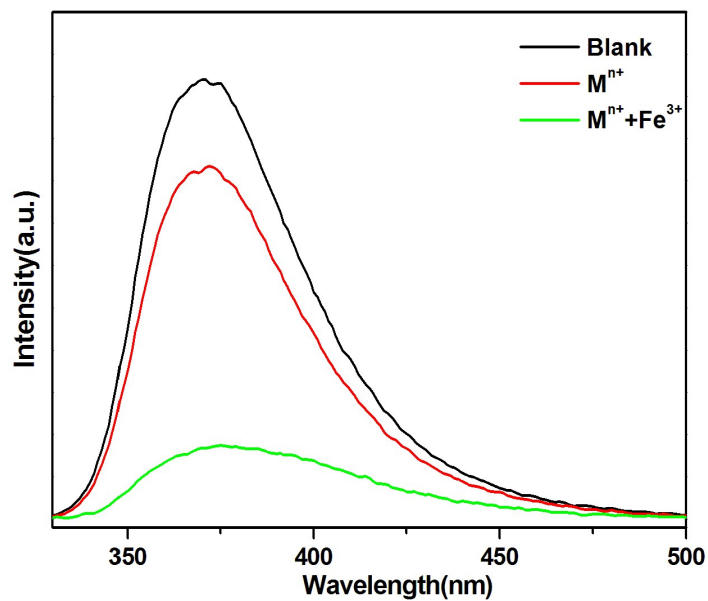


Fig. S11 Comparison of the photoluminescence intensity of gea-MOF-1 in methanol suspension with the introduction of other M^{n+} ions (Li^+ , Cd^{2+} , Pb^{2+} , Zn^{2+} , Mg^{2+} , Ca^{2+} , Co^{2+} , Cu^{2+} , In^{3+} , K^+) in the absence and presence of 1 equiv. Fe^{3+} ($\lambda_{ex}=290$ nm).

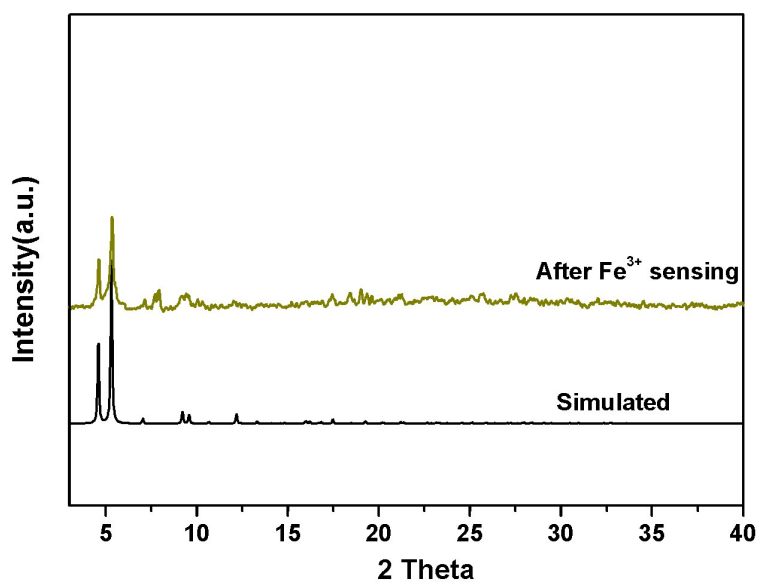


Fig. S12 The PXRD data of the simulated and 1 after Fe^{3+} sensing process.

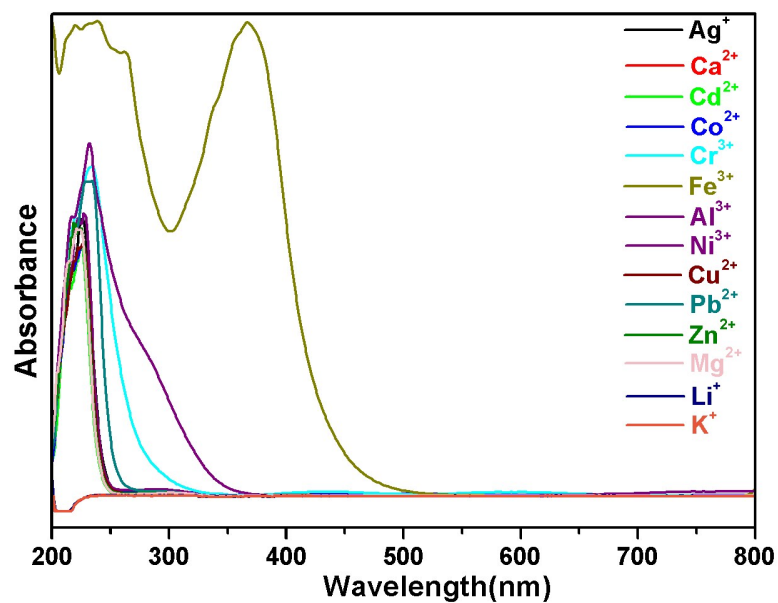


Fig. S13 UV-vis spectra of methanol solution containing different metal ions (10^{-3} M).

Reference:

[1] V. Guillerm, Ł. J. Weseliński, Y. Belmabkhout, A. J. Cairns, V. D'Elia, Ł. Wojtas, K. Adil and M. Eddaoudi, *Nat. chem.*, 2014, **6**, 673-680.