Supporting Information

Two porous luminescent metal-organic frameworks: quantifiable evaluation of dynamic and static luminescent sensing mechanisms towards Fe^{3+}

Jun-Cheng Jin,[ab] Ling-Yan Pang,[a] Guo-Ping Yang,[a] Lei Hou[a] and Yao-Yu Wang*[a]

[a]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, College of Chemistry & Materials Science, Northwest University. Xi'an 710069, China.*

[b]*Technology Promotion Center of Nano Composite Material Preparation and Application; Anhui Provincial Laboratory of Biomimetic Sensor and Detecting Technology, West Anhui University, Anhui 237012 , China.*

The corresponding author, E-mail: wyaoyu@nwu.edu.cn; Tel: +86 29 88308031

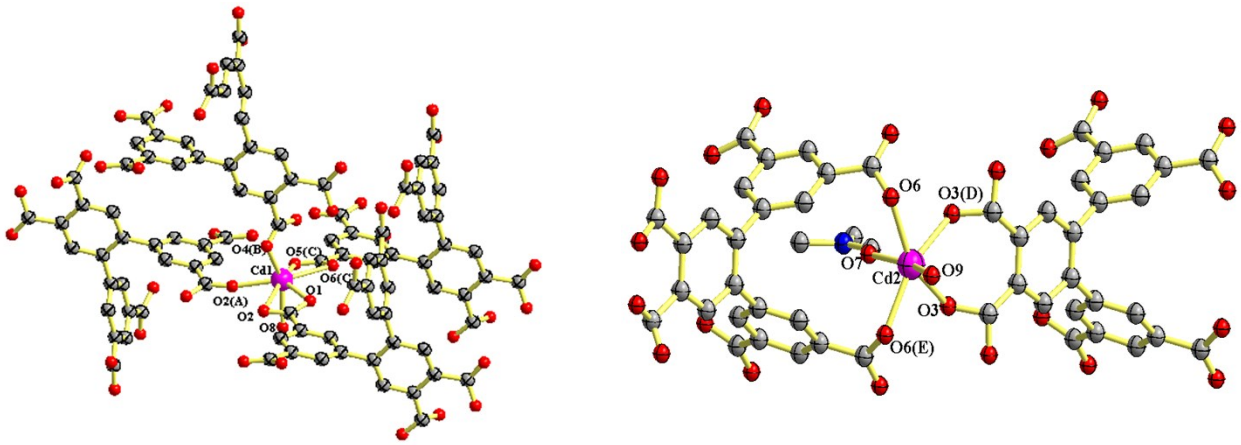


Fig. S1 Local coordination environments of the Cd(II) ions in **1**.

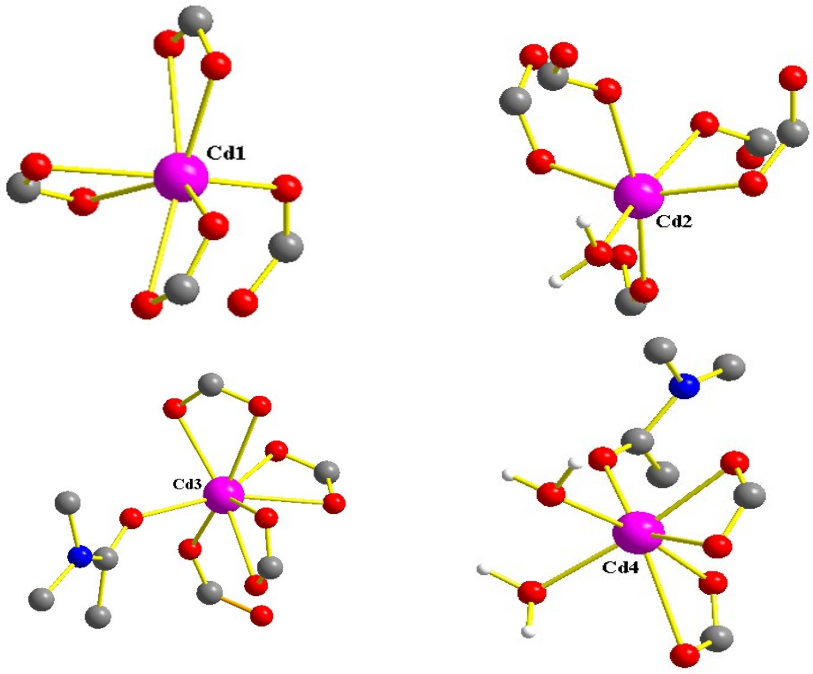


Fig. S2 The coordination modes of the Cd(II) ions in **2**.

a) b)

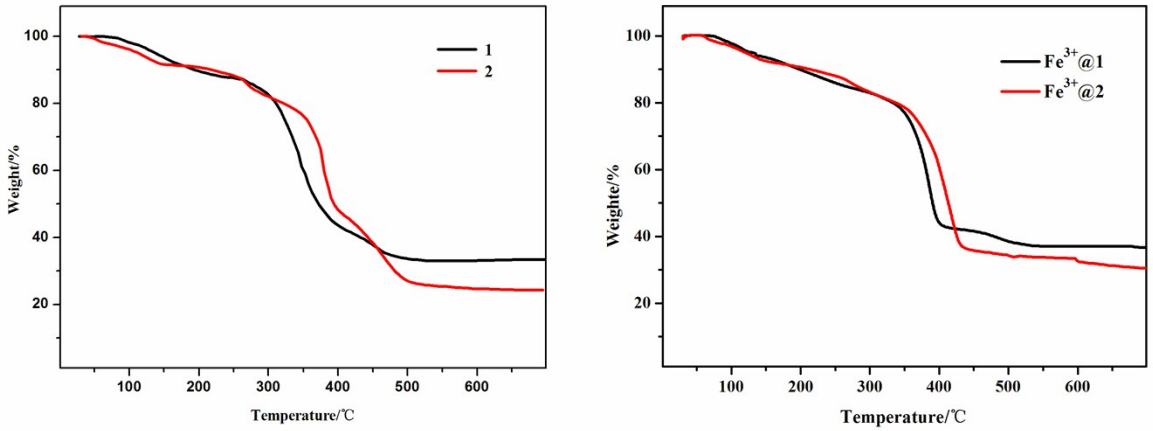


Fig. S3 (a) TGA plots of **1** and **2** under N_2 environment. Thermogravimetric analysis (TGA) reveals that **1** can be stable up to 245 ºC. The weight loss of 12.23 % corresponds to the loss of DMF and coordinated H_2O molecules (calc. 11.57%). For **2**, a total weight loss of 8.72% at 35−175 ºC, corresponding to the loss of 1.5DMA and $2H_2O$ guest molecules (calc. 8.69%). (b) The thermal stability of **Fe^{3+}@1** and **Fe^{3+}@2.**

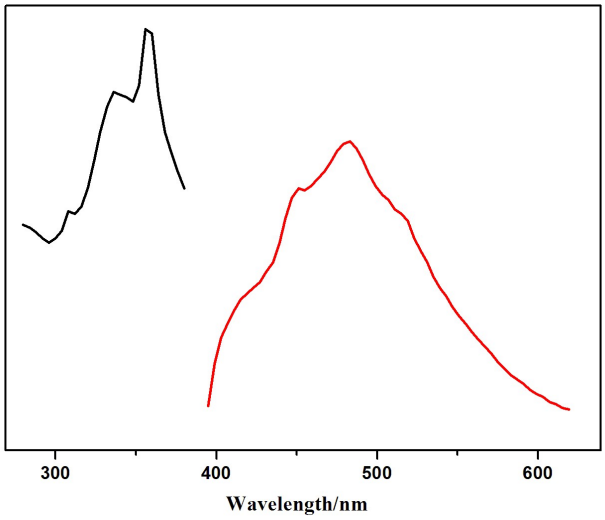
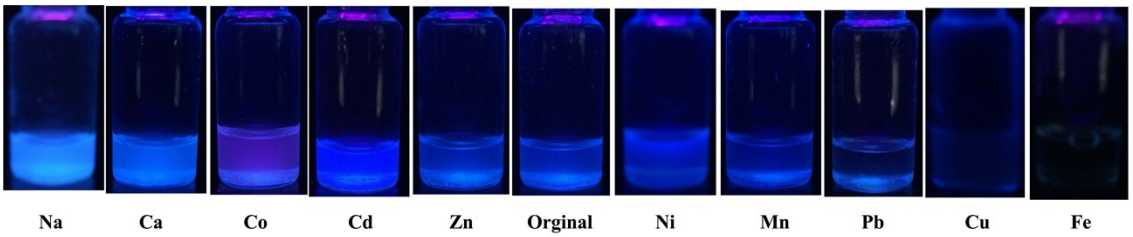


Fig. S4 Excitation and emission spectra of H_6dpa.

a)



b)

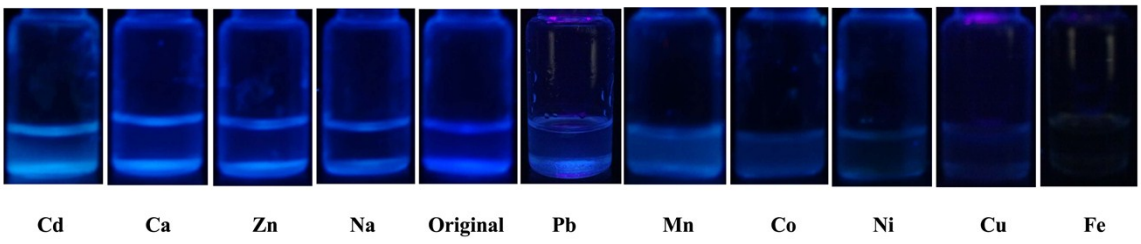


Fig. S5 The visual change on the addition of various $M(NO_3)_x$ with laboratory UV light (λ_{ex} = 254 nm; (a) for **1**; (b) for **2**].

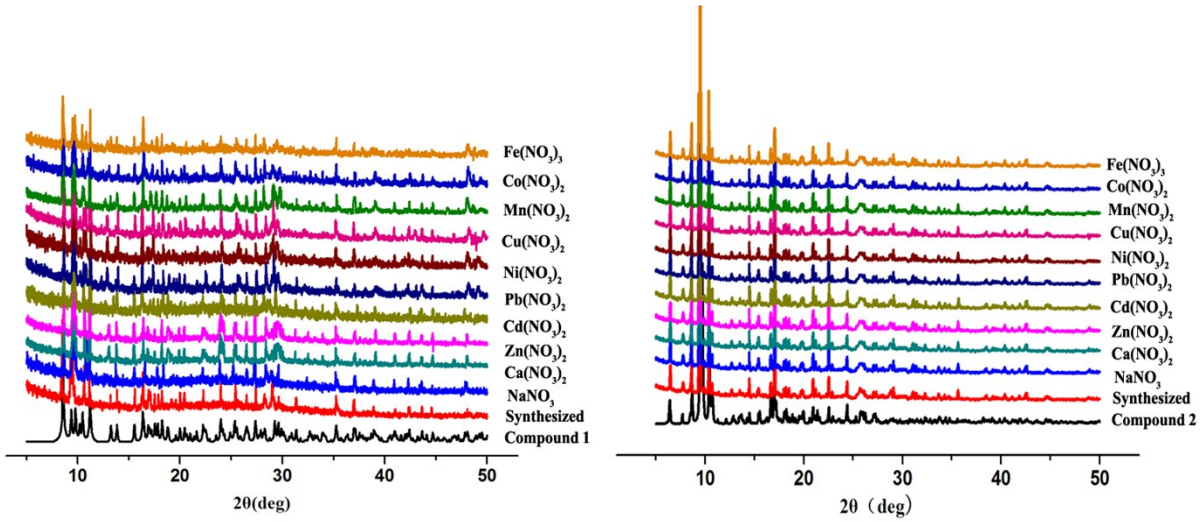


Fig. S6 PXRD patterns of $M(NO_3)_x$ immersion.

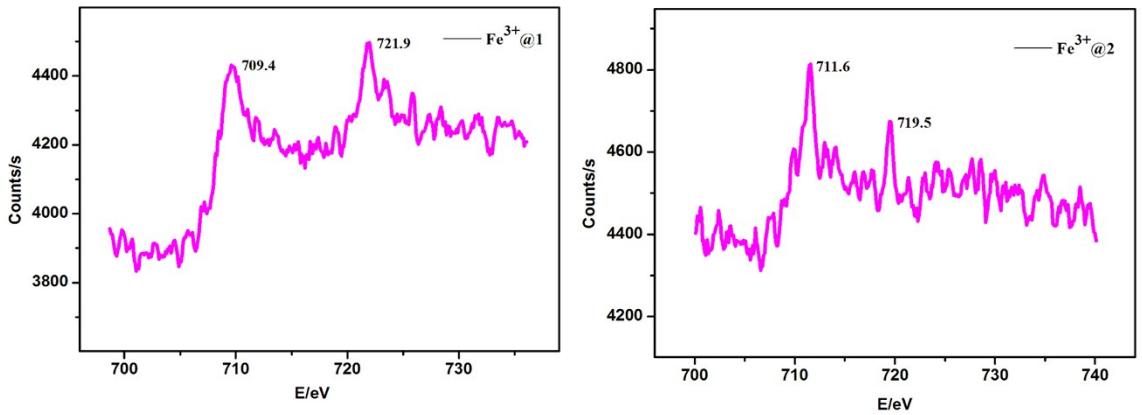


Fig. S7 The XPS of **Fe^{3+}@1** and **Fe^{3+}@2**

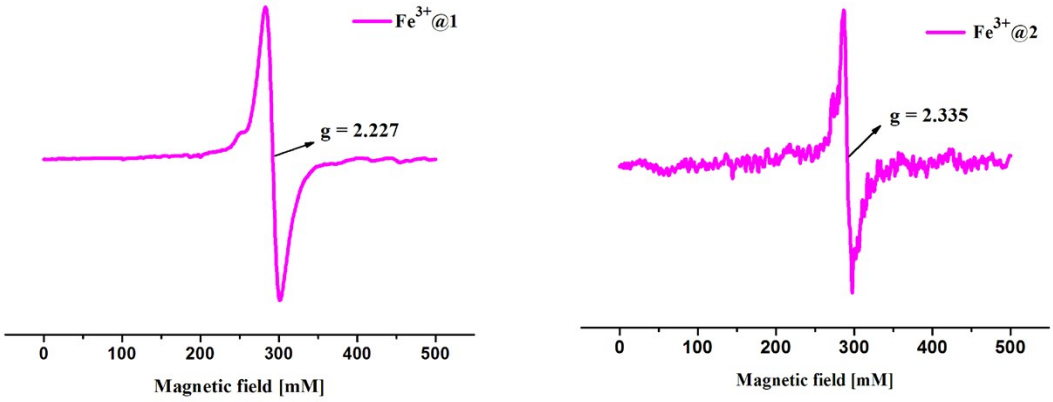


Fig. S8 Electron paramagnetic resonance (EPR) spectra of **Fe^{3+}@1** and **Fe^{3+}@2**

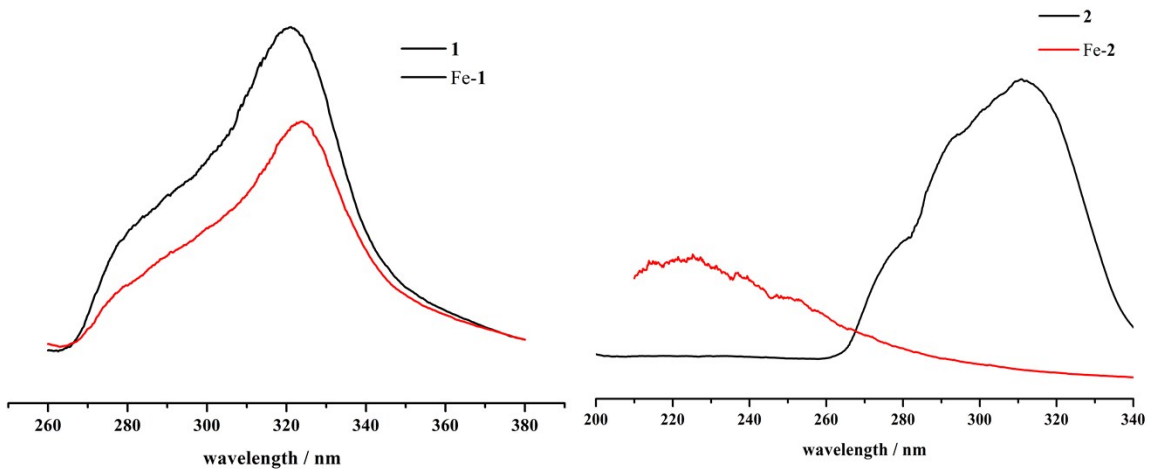


Fig. S9 The excitation peaks of **1** and **2** before and after the addition of $Fe(NO_3)_3$.

Table S1 The quantum yields of the compounds **1** and **2.**

Compounds	Excitation ranges/nm	Luminescence ranges/nm	η
1	310.00 - 327.00	351.00 - 455.00	0.15
2	300.00 - 322.00	354.00 - 387.00	0.19

Table S2 Selected crystallographic data for compounds **1** and **2.**

Compounds	1	2
Empirical formula	$C_{33}H_{35}Cd_3N_3O_{18}$	$C_{66}H_{75.5}Cd_4N_{5.5}O_{32.5}$
Formula mass	1098.87	1915.47
Crystal system	Monoclinic	Orthorhombic
Space group	*P21/m*	*P212121*
a [Å]	10.1085(13)	18.633(5)
b [Å]	18.918(2)	20.399(5)
c [Å]	11.0438(15)	20.852(5)
α/(°)	90	90
β/(°)	110.984(2)	90
γ/(°)	90	90
V [Å^3]	1971.9(4)	7926(3)
Z	2	4
μ [mm^{-1}]	1.682	1.134
F [000]	1080	3480
Reflections collected	3648	13861
Final R[a] indices	R_1 =0.0451	R_1 =0.0360
[I>2σ(I)]	wR_2 =0.1540	wR_2 =0.1043

[a] $R_1=\sum||F_o|-|F_c||/\sum|F_o|$, $wR_2=[\sum w(F_o^2- F_c^2)^2/ \sum w(F_o^2)^2]^{1/2}$