

Supporting Information

A New-AIE-ligand-based metal-organic framework “turn-on” sensor with extremely high sensitivity

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Table S1 Selected bond lengths(Å)and angles for **1**.

Bond	Lengths(Å)	Bond	Angles(°)
Cd(02)-O(1)	2.4531(19)	O(2)-Cd(02)-O(5)	152.65(8)
Cd(02)-O(2)	2.314(2)	O(2)-Cd(02)-N(00L)	103.06(9)
Cd(02)-O(3)	2.444(2)	O(5)-Cd(02)-N(00L)	81.16(7)
Cd(02)-O(4)	2.410(2)	O(2)-Cd(02)-N(1)	86.08(8)
Cd(02)-O(5)	2.3655(19)	O(5)-Cd(02)-N(1)	85.93(7)
Cd(02)-N(1)	2.395(2)	N(00L)-Cd(02)-N(1)	166.05(8)
Cd(02)-N(00L)	2.374(2)	O(2)-Cd(02)-O(4)	72.28(9)
		O(5)-Cd(02)-O(4)	81.24(8)
		N(00L)-Cd(02)-O(4)	85.64(8)

Symmetry transformations used to generate equivalent atoms: #1 $x-1/2, -y+1/2, z-1/2$;

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

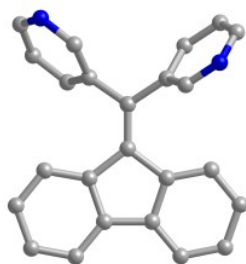


Figure S1. The crystal structure of 3-L (N: blue; C, gray; H atoms are omitted).

(a)

(b)

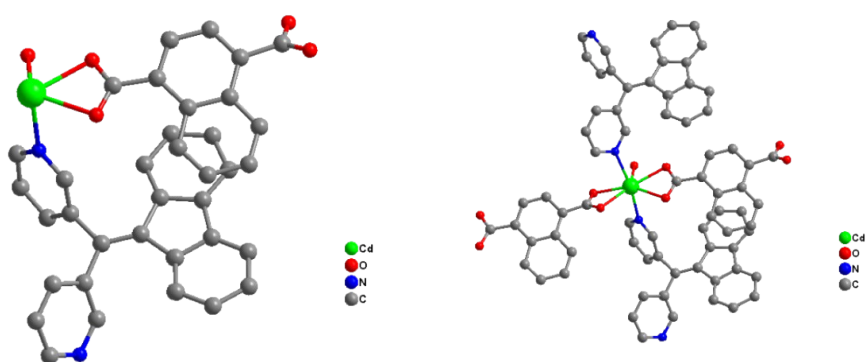


Figure S2. (a) the asymmetric unit of **1**; (b) the coordination environment of Cd.

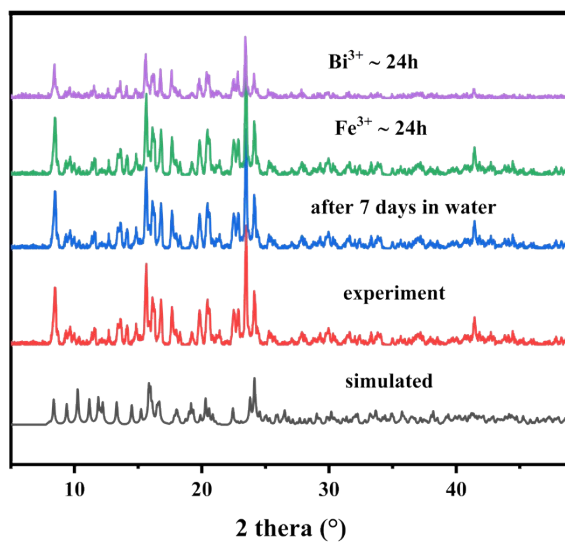


Figure S3. The PXRD analysis of **1**.

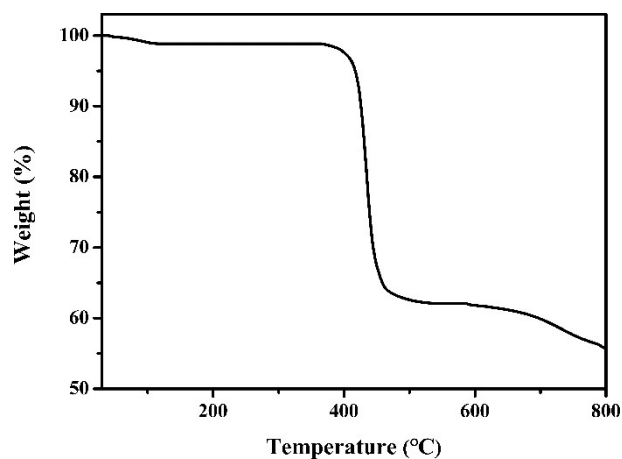


Figure S4. The thermogravimetric analyses (TGA) of **1**.

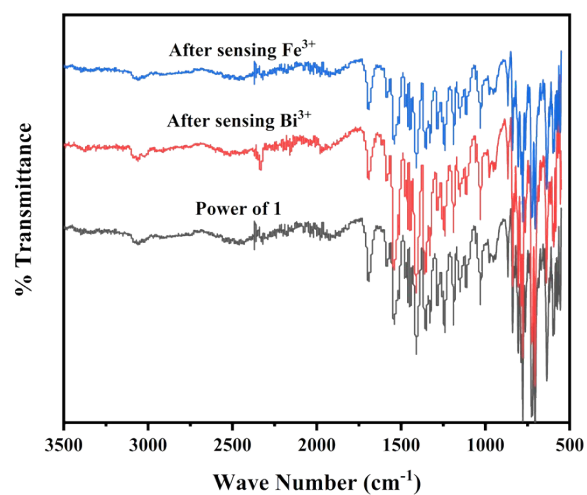


Figure S5. IR spectra of **1** before and after sensing Bi^{3+} and Fe^{3+} .

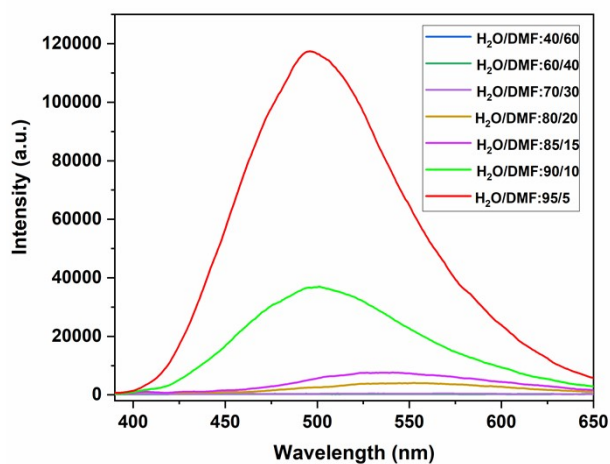


Figure S6. Luminescence spectra of **3-L** in DMF/water mixture with various water

fractions (f_w).

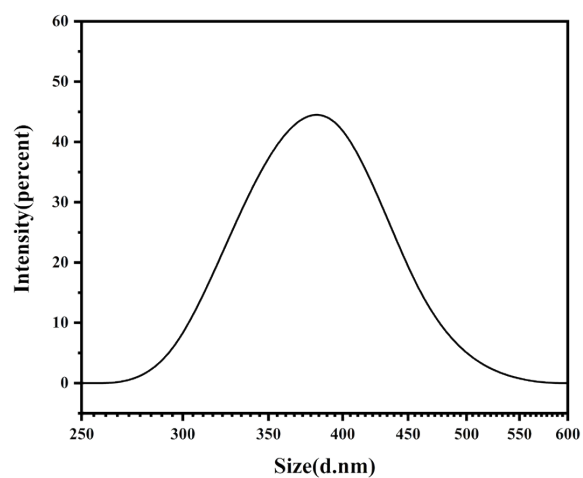


Figure S7. The particle size distribution of the suspension of **1** in H₂O.

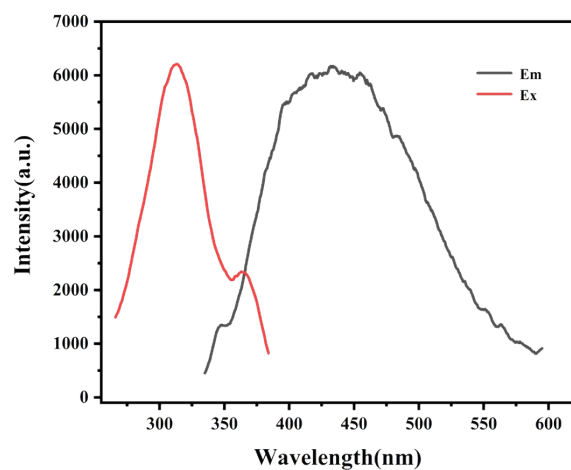


Figure S8. The excitation and emission spectra of the water suspensions of **1**.

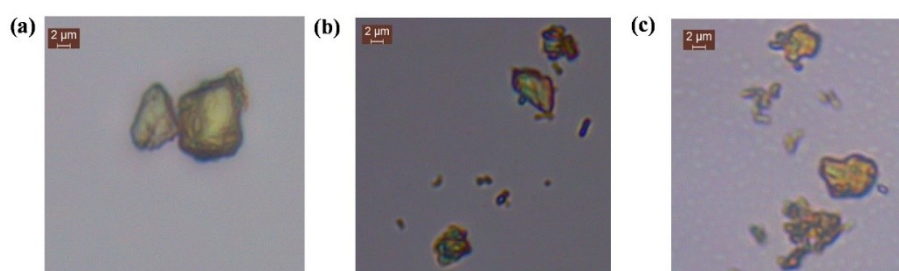


Figure S9. Optical images of **1** before and after sensing Bi³⁺ and Fe³⁺ achieved by Leica Microsystems.

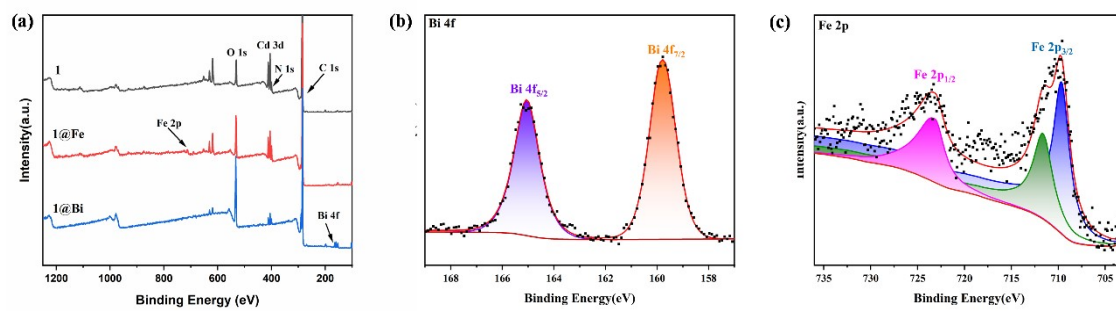


Figure S10. XPS spectra before and after sensing Bi^{3+} and Fe^{3+} : (a) total survey, (b) Bi 4f and (c) Fe 2p.

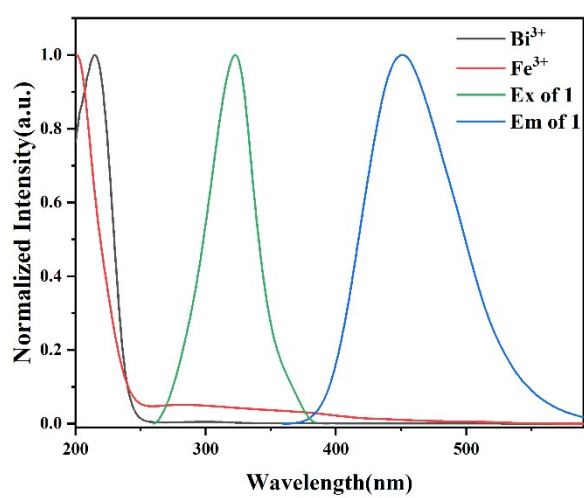


Figure S11. Absorption spectra of Bi^{3+} and Fe^{3+} and the excitation and emission of **1**.