

A Stable 2D Luminescent Metal-Organic Framework as Highly Sensitive Sensor for Fe^{3+} and $\text{Cr}_2\text{O}_7^{2-}/\text{CrO}_4^{2-}$ in Water

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Supporting Information:

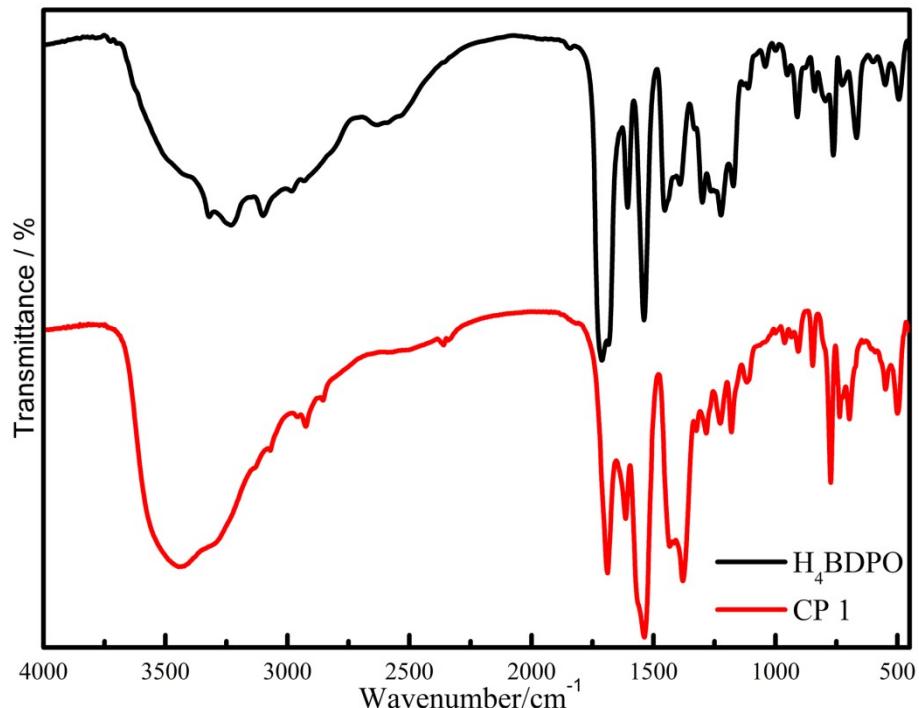


Fig. S1 The IR spectra of **1** and the H₄BDPO ligand at room temperature.

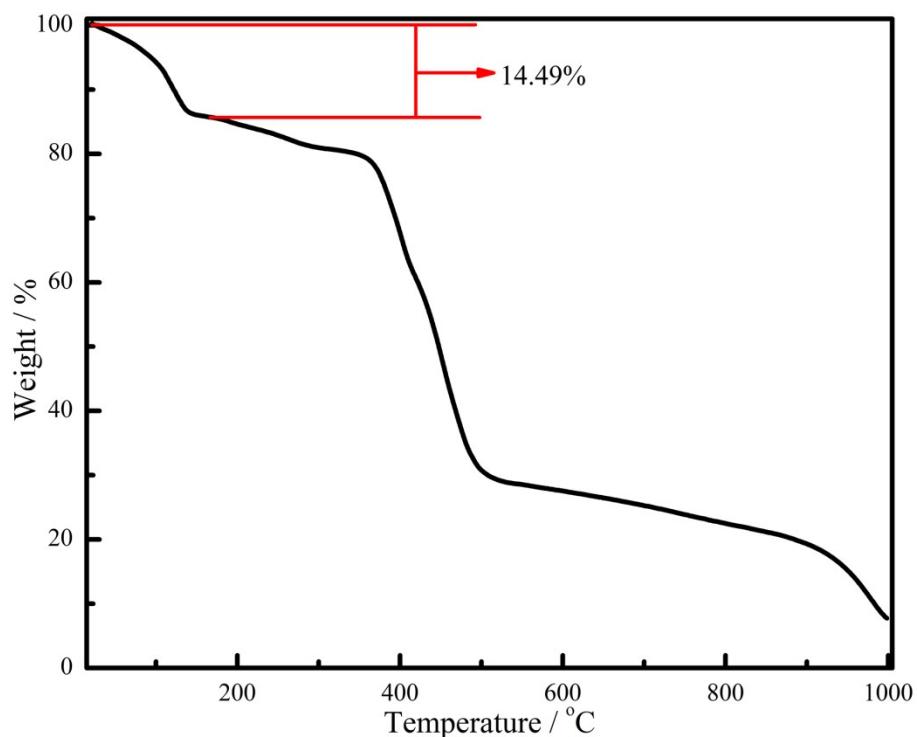


Fig. S2 The TG curve of **1** on crystalline samples under the N₂ atmosphere in the range of 25–1000 °C.

Table S1. *SHAPE* analysis of Cd1 ion in **1**.

Label	Shape	Symmetry	Distortion
HP-7	Heptagon	D_{7h}	33.055
HPY-7	Hexagonal pyramid	C_{6v}	23.061
PBPY-7	Pentagonal bipyramid	D_{5h}	1.717
COC-7	Capped octahedron	C_{3v}	7.041
CTPR-7	Capped trigonal prism	C_{2v}	5.191
JPBPY-7	Johnson pentagonal bipyramid	D_{5h}	4.962
JETPY-7	Johnson elongated triangular pyramid	C_{3v}	22.146

Table S2. *SHAPE* analysis of Cd2 ion in **1**.

Label	Shape	Symmetry	Distortion
HP-6	Hexagon	D_{6h}	34.672
PPY-6	Pentagonal pyramid	C_{5v}	18.660
OC-6	Octahedron	O_h	6.946
TPR-6	Trigonal prism	D_{3h}	8.506
JPPY-6	Johnson pentagonal pyramid	C_{5v}	22.567

Table S3. Distance (Å) and angle (°) of hydrogen bonds for **1**.

D-H	d(D-H)	d(H···A)	∠DHA	d(D···A)	A
O8-H8	0.820	1.824	160.64	2.612	O2 [x, y+1, z]
O11-H11A	0.894	2.349	149.05	3.149	O5 [x+1/2, y-1/2, z]
O11-H11B	0.892	1.913	153.86	2.742	O4 [-x+1/2, -y+1/2, -z+1]
O12-H12A	0.943	2.260	115.78	2.801	O7 [x, y-1, z]
O13-H13B	0.875	1.862	151.65	2.664	O1 [-x+1/2, -y+3/2, -z+1]
O14-H14A	0.846	2.095	145.52	2.833	O9 [-x+1/2, y+1/2, -z+3/2]
O14-H14B	0.844	1.954	159.31	2.759	O15 [-x+1/2, y+1/2, -z+3/2]
N1-H1	0.860	2.178	112.92	2.635	O10
N1-H1	0.860	2.447	166.93	3.291	O16
N2-H2	0.860	2.325	159.06	3.143	O15
C6-H6	0.930	2.362	121.66	2.958	O9
C12-H12	0.930	2.203	123.21	2.821	O10
C16-H16	0.930	2.482	146.19	3.296	O15

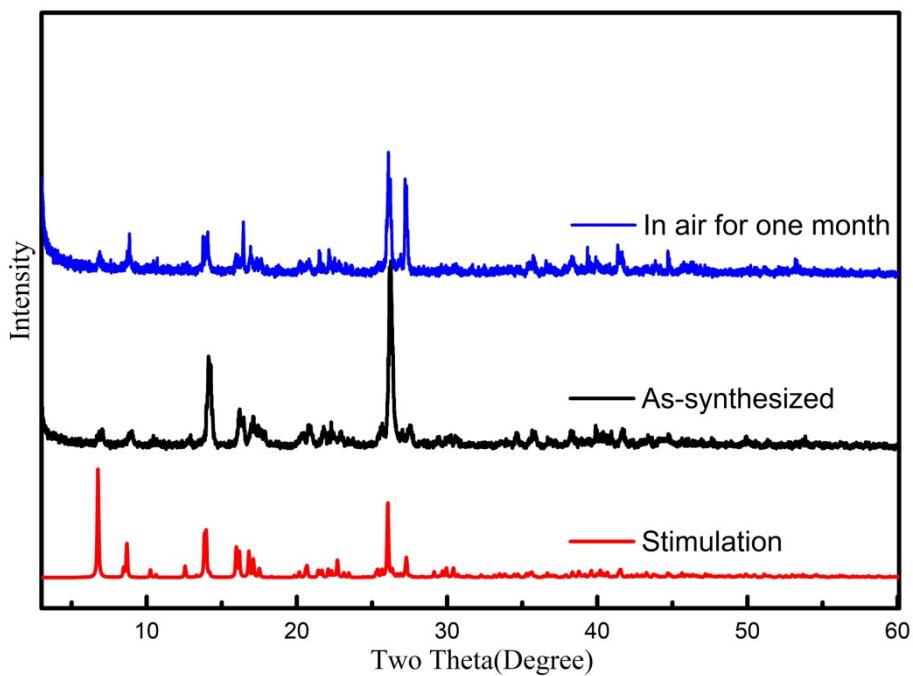


Fig. S3 PXRD patterns of simulated from the X-ray single structure of **1**, as-synthesized **1**, and **1** samples exposed in air for one month.

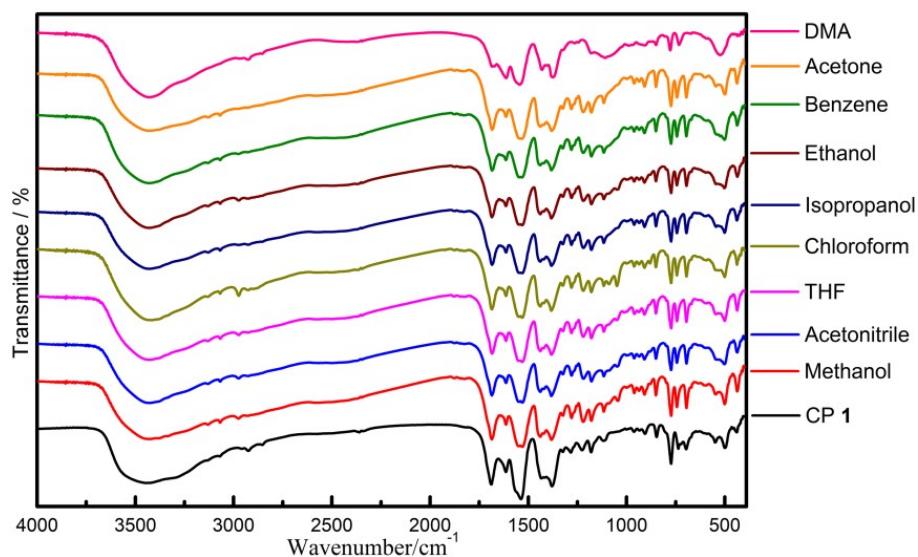


Fig. S4 IR spectra of **1** and **1** in the solutions of MeOH, CH₃CN, THF, CHCl₃, *i*-propanol, EtOH, benzene, acetone, and DMA for one week.

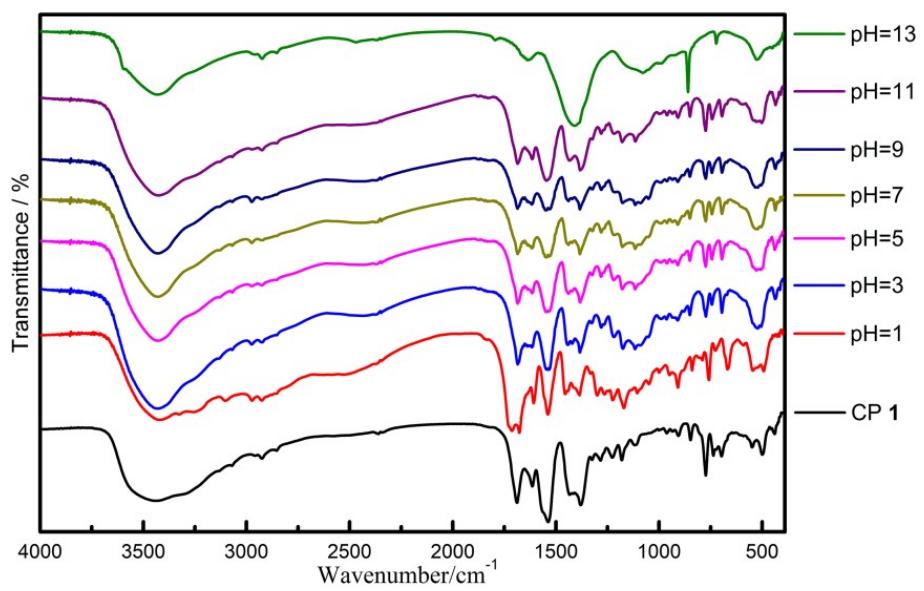


Fig. S5 IR spectra of **1** and **1** in the aqueous solutions ranging from pH = 1 to 13 for one week.

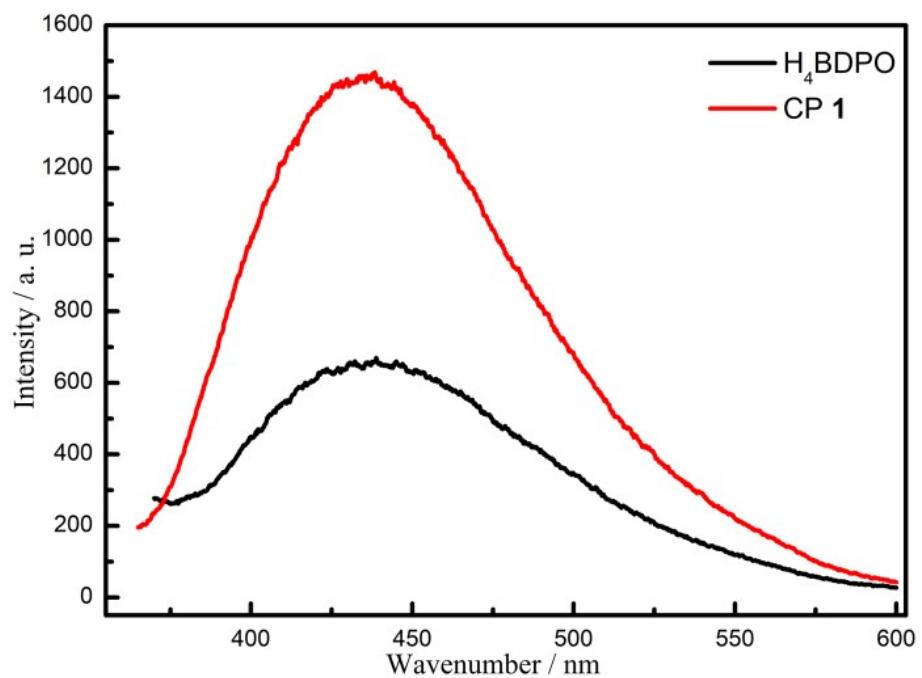


Fig. S6 The solid-state emission spectra of **1** and H₄BDPO ligand at room temperature ($\lambda_{\text{ex}} = 350$ nm).

Table S4. A comparison of selected MOFs-based luminescent sensors for the detection of Fe³⁺ ion.

Coordination Polymers	Media	K _{sv} / (mol ⁻¹)	LOD / (mol·L ⁻¹)	Ref.
{[Cd ₃ (HBDPO) ₂ (H ₂ O) ₇]·4H ₂ O} _n (1)	H ₂ O	3.798 × 10 ⁴ 5.868 × 10 ³ (low concentration)	4.08 × 10 ⁻⁶	This work
{[Zn(L ¹)(dcdps)]} _n	H ₂ O	7.004 × 10 ³	6.21 × 10 ⁻⁵	S1
{Zn(L ¹)(bdc)} _n	H ₂ O	9.066 × 10 ³	4.45 × 10 ⁻⁵	S1
{[Cd(L ¹)(oba)]·0.5DMF} _n	H ₂ O	4.984 × 10 ³	1.152 × 10 ⁻⁴	S1
{[Cd(L ¹)(bdc)·2H ₂ O] 2DMF} _n	H ₂ O	6.387 × 10 ³	6.36 × 10 ⁻⁵	S1
{[Co ₃ (L ²) ₃ (phen) ₂]·4H ₂ O} _n	H ₂ O	8.10 × 10 ³	9.39 × 10 ⁻⁶	S2
{[Co ₃ (L ²) ₃ (2,2'-bipy) ₂]·8H ₂ O} _n	H ₂ O	6.27 × 10 ³	1.14 × 10 ⁻⁵	S2
{Cd ₂ (L ³)(2,2'-bipy)} _n	H ₂ O	2.99 × 10 ⁵	2.47 × 10 ⁻⁸	S3
{Cd ₂ (L ³)(H ₂ O) ₄ } _n	H ₂ O	1.23 × 10 ⁶	1.35 × 10 ⁻⁹	S3
[Zn ₃ (L ⁴) ₂ (2,2'-bipy)(μ ₃ -OH) ₂]·3H ₂ O	H ₂ O	2.3 × 10 ⁴	-	S4
{Cd(L ⁵)(bbibp)} _n	H ₂ O	6.83 × 10 ³	4.39 × 10 ⁻⁶	S5
{Cd ₃ ·L ⁶ ·(BTB) ₂ ·2DMF} _n	DMF	1.01 × 10 ⁴	1.12 × 10 ⁻⁶	S6

$\{(Cd_3O_2) \cdot L^6 \cdot btc\}_n$	DMF	1.31×10^4	2.29×10^{-6}	S6
$\{Cd_3(L^7)_2(Br-bdc)_6(DMF)_2\}_n$	DMF	5.25×10^4	1.37×10^{-9}	S7
$\{Cd_3(L^7)_2(NH_2-bdc)_6(DMF)_2\}_n$	DMF	3.23×10^4	2.23×10^{-9}	S7
$\{Cd_3(L^7)_2(bdc)_6(DMF)_2\}_n$	DMF	4.04×10^4	1.62×10^{-9}	S7
$\{[CoL^8_2Cl_2] \cdot 4CH_3OH\}_n$	EtOH	1.07×10^4	2.75×10^{-3}	S8
$\{[NiL^8_2Cl_2] \cdot 4CH_3OH\}_n$	EtOH	1.67×10^4	1.2×10^{-4}	S8
$\{[CoL^8_2Br_2] \cdot 4CH_3OH\}_n$	EtOH	3.33×10^4	8.7×10^{-4}	S8
$[Zr_6O_6(OH)_2(CF_3COO)_2(C_{11}H_5NO_4)_4(H_2O)_4]$	H ₂ O	2.25×10^7	1.7×10^{-9}	S9
$[Zn_2Na_2(TPHC)(4,4\text{-bipy})(DMF)] \cdot 8H_2O$	DMF	5.77×10^4	6.4×10^{-6}	S10
$[CH_3\text{-dpb}]_2[Mg_3(1,4\text{-ndc})_4(\mu\text{-H}_2O)_2(CH_3OH)(H_2O)] \cdot 1.5H_2O$	CH ₂ Cl ₂	1.6×10^4	4.70×10^{-4}	S11
FJI-C8·(Zn)	H ₂ O	8.245×10^3	2.33×10^{-5}	S12
$[Cd(5\text{-asba})(bimb)]_n$	H ₂ O	1.78×10^4	1.875×10^{-5}	S13
$[Zn_5(hfipbb)_4(trz)_2(H_2O)_2]$	H ₂ O	-	2.00×10^{-4}	S14
$\{[Cd(L^9)(HIP)] \cdot 2H_2O\}_n$	DMF	5.57×10^4	2.5×10^{-6}	S15

$\{(Me_2NH_2)[Zn_2(L^{10})(H_2O)] \cdot 0.5DMF\}_n$	DMF	7.83×10^3	1.45×10^{-8}	S16
$\{[Cd(L^{11})(BPDC)] \cdot 2H_2O\}_n$	H ₂ O	3.63×10^4	2.21×10^{-6}	S17
$\{[Cd(L^{11})(SDBA)(H_2O)] \cdot 0.5H_2O\}_n$	H ₂ O	3.59×10^4	7.14×10^{-6}	S17
$\{[Zn_3(mtrb)_3(btc)_2] \cdot 3H_2O\}$	H ₂ O	6.50×10^3	1.78×10^{-6}	S18
$\{[Zn(L^{12})(H_2O)_2] \cdot H_2O\}_n$	H ₂ O	1.09×10^5	5.6×10^{-7}	S19
$\{[Cd(L^{12})(H_2O)_2] \cdot 4H_2O\}_n$	H ₂ O	7.2×10^4	7.8×10^{-7}	S19
$\{[Zn_2(trz)_2(DBTDC-O_2)] \cdot DMAc\}_n$	H ₂ O	1.0×10^4	4.61×10^{-6}	S20
$[Zn(L^{13})_2] \cdot 2DMF$	H ₂ O	9.85×10^3	1.91×10^{-6}	S21
$[Zn_2(NO_3)_2(4,4'-bpy)_2(TBA)]_n$	H ₂ O	7.48×10^3	7.18×10^{-6}	S22
$[Zn_2(cptpy)(btc)(H_2O)]_n$	H ₂ O	5.46×10^3	4.33×10^{-6}	S23
$\{[Zn_3(HL^{14})2H_2O] \cdot 4H_2O\}_n$	H ₂ O	5.00×10^3	2.20×10^{-4}	S24
$\{[Me_2NH_2][Zn_2(HEDP)(BPDC)_{0.5}(H_2O)_2] \cdot H_2O\}_n$	H ₂ O	7.31×10^3	-	S25
$\{[Zn_3(L^{15})(OH)(H_2O)_5] \cdot NMP \cdot 2H_2O\}_n$	H ₂ O	4.7×10^4	7.7×10^{-5}	S26
$\{[Zn_2(L^{16})(5-AIP)_2] \cdot 3H_2O\}_n$	H ₂ O	4.475×10^3	1.29×10^{-6}	S27

$\{\text{Zn}(\text{ATA})(\text{L}^{17})\}\cdot 2\text{H}_2\text{O}$	H_2O	5.57×10^{-4}	3.76×10^{-6}	S28
$\{\text{Cd}(\text{ATA})(\text{L}^{17})\}\cdot 2\text{H}_2\text{O}$	H_2O	3.838×10^{-3}	1.77×10^{-6}	S28
$\{\text{Cd}_2(\text{bptc})(2,2'\text{-bipy})_2(\text{H}_2\text{O})_2\}$	H_2O	8.61×10^3	1.02×10^{-5}	S29
$\{\text{Cd}_2(\text{bptc})(\text{phen})_2\}\cdot 4\text{H}_2\text{O}$	H_2O	3.07×10^3	2.17×10^{-5}	S29
$\{\text{Cd}_2(\text{bptc})(4,4'\text{-bipy})(\text{H}_2\text{O})_2\}\cdot 4\text{H}_2\text{O}$	H_2O	6.21×10^3	2.03×10^{-5}	S29
$[\text{Zn}_2(\text{L}^{18})_2(\text{bpe})_2(\text{H}_2\text{O})_2]$	H_2O	2.395×10^3	2.50×10^{-5}	S30
$[\text{Zr}_6\text{O}_4(\text{OH})_8(\text{H}_2\text{O})_4(\text{L}^{19})_2]$	H_2O	2.17×10^3	3.79×10^{-9}	S31
$[\text{Zr}_6\text{O}_4(\text{OH})_8(\text{H}_2\text{O})_4(\text{L}^{20})_2]$	H_2O	1.66×10^4	2.86×10^{-10}	S31
$[\text{H}_2\text{N}(\text{CH}_3)_2]_2[\text{Zn}_2\text{L}^{21}(\text{HPO}_3)_2]$	H_2O	3.96×10^5	1.16×10^{-7}	S32
$\{\text{Cd}_3(\mu_6\text{-cptc})_2(\text{py})_2\}\cdot 5\text{H}_2\text{O}$	H_2O	3.096×10^3	2.1×10^{-7}	S33
$\{\text{Zn}(\text{BIMB})(\text{HL}^{22})\}\cdot \text{H}_2\text{O}$	H_2O	2.21×10^4	2.29×10^{-5}	S34
$\{\text{Zn}_2(\text{BIBP})_2(\text{HL}^{22})_2\}\cdot 2\text{H}_2\text{O}$	H_2O	1.47×10^4	3.32×10^{-5}	S34
$[\text{Zn}(\text{DHT})(\text{BPP})]$	H_2O	1.77×10^4	4.46×10^{-7}	S35
$[\text{Zn}_2(\text{OH})(1,4\text{-ndc})_{1.5}(\text{Cz-3,6-bpy})]\cdot 2\text{H}_2\text{O}$	H_2O	7.176×10^3	4.60×10^{-6}	S36

[Zn(4-tkpvb)(BB) ₂]	H ₂ O	705	7.66×10^{-9}	S37
[Zn(μ_3 -L ²³)(H ₂ O) ₂]	H ₂ O	8.88×10^3	1.311×10^{-6}	S38
{Ni(1,4-bib) _{1.5} (TPA-Cl ₂)·H ₂ O} _n	H ₂ O	70	1.0×10^{-7}	S39
{[Cd ₃ (HL ²⁴) ₂ (H ₂ O) ₃]·3H ₂ O·2CH ₃ CN} _n	H ₂ O	1.04×10^4	9.06×10^{-5}	S40
PCN-604(Al)	H ₂ O	8.53×10^3	6.2×10^{-6}	S41
[Zn ₂ (3-bpah)(bpta)(H ₂ O)]·3H ₂ O	H ₂ O	9.8×10^{11}	1.0×10^{-6}	S42
[Zn ₄ (bptc) ₂ (NMP) ₃ (DMF)(H ₂ O) ₂] _n	EtOH/H ₂ O	4.12×10^3	-	S43
[Cd ₄ (bptc) ₂ (NMP) ₃ (DMF) ₂ (H ₂ O)] _n	EtOH/H ₂ O	6.57×10^3	-	S43
{[Zn ₂ (bptc)(DMA)(H ₂ O) ₂]·(DMA) ₂ ·H ₂ O} _n	EtOH/H ₂ O	3.76×10^3	-	S43
[Cd(Hcip)(bpea) _{0.5} (H ₂ O)] _n	DMF	4.10×10^4	3.24×10^{-6}	S44
[Zn _{1.5} (dttz)(Hdpa)] _n	DMF	1.79×10^4	1.45×10^{-6}	S45
[Ag(μ -aca)(μ_4 -bztpy) _{1/2}]	H ₂ O	1.25×10^4	6.85×10^{-6}	S46
[Ag(μ -bza)(μ -bpa)]	H ₂ O	3.93×10^3	5.17×10^{-5}	S46

Table S5. A comparison of selected MOFs-based luminescent sensors for the detection of $\text{Cr}_2\text{O}_7^{2-}$ ion.

Coordination Polymers	Media	$K_{sv} / (\text{mol}^{-1})$	LOD / ($\text{mol}\cdot\text{L}^{-1}$)	Ref.
$\{\text{[Cd}_3(\text{HBDPO})_2(\text{H}_2\text{O})_7\}\cdot 4\text{H}_2\text{O}\}_n$ (1)	H_2O	2.691×10^4 5.635×10^3 (low concentration)	4.26×10^{-6}	This work
$\{\text{[Zn(L}^1\text{)}(\text{dcdps})]\}_n$	H_2O	4.456×10^4	1.03×10^{-5}	S1
$\{\text{[Zn(L}^1\text{)}(\text{bdc})\}_n$	H_2O	7.716×10^4	5.55×10^{-6}	S1
$\{\text{[Cd(L}^1\text{)}(\text{oba})]\cdot 0.5\text{DMF}\}_n$	H_2O	6.145×10^4	7.36×10^{-6}	S1
$\{\text{[Cd(L}^1\text{)}(\text{bdc})\cdot 2\text{H}_2\text{O]}\cdot 2\text{DMF}\}_n$	H_2O	4.248×10^4	1.05×10^{-5}	S1
$\{\text{[Co}_3(\text{L}^2)_3(\text{phen})_2\}\cdot 4\text{H}_2\text{O}\}_n$	H_2O	5.62×10^3	1.66×10^{-5}	S2
$\{\text{[Co}_3(\text{L}^2)_3(2,2'\text{-bipy})_2\}\cdot 8\text{H}_2\text{O}\}_n$	H_2O	4.13×10^3	2.12×10^{-5}	S2
$\{\text{Cd}_3\cdot \text{L}^6\cdot (\text{BTB})_2\cdot 2\text{DMF}\}_n$	DMF	2.06×10^4	1.4×10^{-6}	S6
$\{\text{(Cd}_3\text{O}_2\text{)}\cdot \text{L}^6\cdot \text{btc}\}_n$	DMF	2.44×10^4	1.2×10^{-6}	S6
$\{\text{[Cd(L}^{11}\text{)}(\text{BPDC})]\cdot 2\text{H}_2\text{O}\}_n$	H_2O	6.4×10^3	3.76×10^{-5}	S17
$\{\text{[Cd(L}^{11}\text{)}(\text{SDBA})(\text{H}_2\text{O})\}\cdot 0.5\text{H}_2\text{O}\}_n$	H_2O	4.97×10^3	4.86×10^{-5}	S17
$\{\text{[Zn}_3(\text{mtrb})_3(\text{btc})_2\}\cdot 3\text{H}_2\text{O}\}$	H_2O	4.62×10^3	2.83×10^{-6}	S18

$\{\text{Zn}(\text{L}^{12})(\text{H}_2\text{O})_2\} \cdot \text{H}_2\text{O}$	H_2O	9.1×10^4	7.3×10^{-6}	S19
$\{\text{Cd}(\text{L}^{12})(\text{H}_2\text{O})_2\} \cdot 4\text{H}_2\text{O}$	H_2O	3.58×10^4	8.2×10^{-6}	S19
$\{\text{Zn}_2(\text{trz})_2(\text{DBTDC-O}_2)\} \cdot \text{DMAc}$	H_2O	1.24×10^4	2.55×10^{-6}	S20
$[\text{Zn}(\text{L}^{13})_2] \cdot 2\text{DMF}$	H_2O	1.25×10^4	1.45×10^{-6}	S21
$\{\text{Me}_2\text{NH}_2\}[\text{Zn}_2(\text{HEDP})(\text{BPDC})_{0.5}(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$	H_2O	2.09×10^5	-	S25
$\{\text{Zn}_3(\text{L}^{15})(\text{OH})(\text{H}_2\text{O})_5\} \cdot \text{NMP} \cdot 2\text{H}_2\text{O}$	H_2O	6.6×10^4	6.05×10^{-5}	S26
$\{\text{Zn}(\text{ATA})(\text{L}^{17})\} \cdot 2\text{H}_2\text{O}$	H_2O	2.623×10^{-3}	4.3×10^{-7}	S28
$\{\text{Cd}(\text{ATA})(\text{L}^{17})\} \cdot 2\text{H}_2\text{O}$	H_2O	3.119×10^{-3}	1.9×10^{-7}	S28
$\{\text{Cd}_2(\text{bptc})(2,2'\text{-bipy})_2(\text{H}_2\text{O})_2\}$	H_2O	1.17×10^4	7.38×10^{-6}	S29
$\{\text{Cd}_2(\text{bptc})(\text{phen})_2\} \cdot 4\text{H}_2\text{O}$	H_2O	2.09×10^3	5.89×10^{-5}	S29
$\{\text{Cd}_2(\text{bptc})(4,4'\text{-bipy})(\text{H}_2\text{O})_2\} \cdot 4\text{H}_2\text{O}$	H_2O	9.34×10^3	1.36×10^{-5}	S29
$[\text{H}_2\text{N}(\text{CH}_3)_2]_2[\text{Zn}_2\text{L}^{21}(\text{HPO}_3)_2]$	H_2O	4.44×10^4	1.09×10^{-6}	S32
$\{\text{Zn}(\text{BIMB})(\text{HL}^{22})\} \cdot \text{H}_2\text{O}$	H_2O	2.08×10^4	2.51×10^{-5}	S34
$\{\text{Zn}_2(\text{BIBP})_2(\text{HL}^{22})_2\} \cdot 2\text{H}_2\text{O}$	H_2O	1.34×10^4	3.34×10^{-5}	S34

[Zn ₂ (OH)(1,4-ndc) _{1.5} (Cz-3,6-bpy)]·2H ₂ O	H ₂ O	1.17 × 10 ⁴	1.77 × 10 ⁻⁶	S36
{[Cd ₃ (HL ²⁴) ₂ (H ₂ O) ₃]·3H ₂ O·2CH ₃ CN} _n	H ₂ O	6.99 × 10 ³	1.17 × 10 ⁻⁴	S40
[Zn ₂ (3-bpah)(bpta)(H ₂ O)]·3H ₂ O	H ₂ O	9.3 × 10 ⁶	10 ⁻¹⁵	S42
[Ag(μ-aca)(μ ₄ -bztpy) _{1/2}]	H ₂ O	7.33 × 10 ³	3.68 × 10 ⁻⁵	S46
[Ag(μ-bza)(μ-bpa)]	H ₂ O	4.37 × 10 ⁴	1.03 × 10 ⁻⁵	S46
{Co(TBTA)(L ²⁵) ₂ } _n	H ₂ O	1.6286 × 10 ⁴	9.0 × 10 ⁻⁴	S47
{Co(TBTA)(L ²⁶) ₂ } _n	H ₂ O	1.2435 × 10 ⁴	1.51 × 10 ⁻³	S47
{Co(TBTA)(L ²⁷) _{1.5} } _n	H ₂ O	1.5997 × 10 ⁴	6.7 × 10 ⁻⁴	S47
USTS-7	H ₂ O	1.31 × 10 ⁴	2.2 × 10 ⁻⁶	S48
[Zn(tpbpc) ₂]·solvent	H ₂ O	1.13 × 10 ⁴	6.76 × 10 ⁻⁷	S49
{[Co _{1.5} (TBIP) _{1.5} (L ²⁸)]<·0.5H ₂ O} _n	H ₂ O	2.09 × 10 ⁴	9.9 × 10 ⁻⁵	S50
{[Cd ₁₀ (DDB) ₄ (bpz) ₈ (DMA)(H ₂ O) _{8.2}]<·2H ₂ O} _n	H ₂ O	2.27 × 10 ⁴	3.77 × 10 ⁻⁷	S51
[Zn(IPA)(L ²⁹)] _n	H ₂ O	1.37 × 10 ³	1.202 × 10 ⁻⁵	S52
[Cd(IPA)(L ²⁹)] _n	H ₂ O	2.91 × 10 ³	2.26 × 10 ⁻⁶	S52

$\{\text{Cd}_2\text{L}^{30}_2(\text{H}_2\text{O})_4\}\cdot\text{H}_2\text{O}$	H_2O	1.25×10^4	3.7×10^{-6}	S53
$\{\text{Zn}_2\text{L}^{30}_2(\text{H}_2\text{O})_4\}\cdot\text{H}_2\text{O}$	H_2O	1.77×10^4	2.6×10^{-6}	S53
$[\text{Cd}(4\text{-tkpvb})(5\text{-tert-BIPA})]$	H_2O	2.50×10^4	1.2×10^{-7}	S54
$[\text{Zn}(\text{L}^{31})(\text{BBI})\cdot(\text{H}_2\text{O})_2]$	H_2O	1.17×10^4	-	S55
$[\text{Cd}(\text{L}^{31})(\text{TPOM})_{0.75}]\cdot\text{xS}$	H_2O	1.345×10^4	-	S55
$\{\text{Zn}_2(\text{TPOM})(\text{NH}_2\text{-bdc})_2\}\cdot4\text{H}_2\text{O}$	DMF	7.59×10^3	3.9×10^{-6}	S56
$[\text{Zn(btz)}]$	H_2O	4.23×10^3	2.0×10^{-6}	S57
$\{\text{Zn}_2(\text{ttz})\text{H}_2\text{O}\}$	H_2O	2.19×10^3	1.00×10^{-5}	S57
$[\text{Cd}_3(\text{cpota})_2(\text{phen})_3]\cdot5\text{H}_2\text{O}$	H_2O	1.21×10^4	3.70×10^{-7}	S58
$[\text{Zn}(\text{NH}_2\text{-bdc})(4,4'\text{-bipy})]$	H_2O	7.62×10^3	1.30×10^{-6}	S59
$\{\text{Cd}_2(\text{HDDB})(\text{bib})_{1.5}(\text{H}_2\text{O})\}\cdot2.5\text{H}_2\text{O}$	H_2O	2.7×10^4	-	S60
$[\text{Cd}_2(\text{HDDB})(\text{m-bimb})]\cdot\text{H}_2\text{O}$	H_2O	1.8×10^4	-	S60
$\{\text{Cd}_2(\text{DDB})(\text{p-bimb})\}\cdot2.5\text{H}_2\text{O}\cdot0.5(\text{p-H}_2\text{bimb})$	H_2O	2.8×10^4	-	S60
$[\text{Cd}_2(\text{dpa})_2(\text{cda})\text{Cl}_2]$	H_2O	-	4.0×10^{-7}	S61

[Cd(dpa)₂(cda)]_n

H₂O

-

2.0×10^{-7}

S61

Table S6. A comparison of selected MOFs-based luminescent sensors for the detection of CrO_4^{2-} ion.

Coordination Polymers	Media	$K_{sv} / (\text{mol}^{-1})$	LOD / ($\text{mol}\cdot\text{L}^{-1}$)	Ref.
{[Cd ₃ (HBDPO) ₂ (H ₂ O) ₇]·4H ₂ O} _n (1)	H ₂ O	1.614×10^3 1.400×10^3 (low concentration)	1.71×10^{-5}	This work
{Cd ₂ (L ³)(2,2'-bipy)} _n	H ₂ O	4.51×10^5	1.12×10^{-8}	S3
{Cd ₂ (L ³)(H ₂ O) ₄ } _n	H ₂ O	3.61×10^5	2.23×10^{-8}	S3
{[Zn ₃ (mtrb) ₃ (btc) ₂]·3H ₂ O}	H ₂ O	2.77×10^3	4.52×10^{-6}	S18
{[Zn(L ¹²)(H ₂ O) ₂]·H ₂ O} _n	H ₂ O	4.1×10^4	5.7×10^{-6}	S19
{[Cd(L ¹²)(H ₂ O) ₂]·4H ₂ O} _n	H ₂ O	3.03×10^4	6.8×10^{-6}	S19
[Zn(L ¹³) ₂]·2DMF	H ₂ O	1.34×10^4	1.14×10^{-6}	S21
{[Zn ₃ (L ¹⁵)(OH)(H ₂ O) ₅]·NMP·2H ₂ O} _n	H ₂ O	1.30×10^4	4.29×10^{-4}	S26
{[Zn(ATA)(L ¹⁷)]·2H ₂ O} _n	H ₂ O	1.485×10^{-3}	2.5×10^{-7}	S28
{[Cd(ATA)(L ¹⁷)]·2H ₂ O} _n	H ₂ O	9.7×10^{-4}	1.8×10^{-7}	S28
{[Cd ₂ (bptc)(2,2'-bipy) ₂ (H ₂ O) ₂]} _n	H ₂ O	7.95×10^3	7.79×10^{-6}	S29
{[Cd ₂ (bptc)(phen) ₂]·4H ₂ O} _n	H ₂ O	1.09×10^3	1.06×10^{-4}	S29

$\{\text{Cd}_2(\text{bptc})(4,4'\text{-bipy})(\text{H}_2\text{O})_2\} \cdot 4\text{H}_2\text{O}$	H_2O	5.38×10^3	1.60×10^{-5}	S29
$\{\text{Zn}(\text{BIMB})(\text{HL}^{22})\} \cdot \text{H}_2\text{O}$	H_2O	1.70×10^4	2.67×10^{-5}	S34
$\{\text{Zn}_2(\text{BIBP})_2(\text{HL}^{22})_2\} \cdot 2\text{H}_2\text{O}$	H_2O	1.20×10^4	4.16×10^{-5}	S34
$[\text{Zn}_2(\text{OH})(1,4\text{-ndc})_{1.5}(\text{Cz-3,6-bpy})] \cdot 2\text{H}_2\text{O}$	H_2O	9.08×10^3	1.10×10^{-6}	S36
$[\text{Zn}(4\text{-tkpvb})(\text{BB})_2]$	H_2O	923	1.21×10^{-8}	S37
$\{\text{Cd}_3(\text{HL}^{24})_2(\text{H}_2\text{O})_3\} \cdot 3\text{H}_2\text{O} \cdot 2\text{CH}_3\text{CN}$	H_2O	1.41×10^4	8.65×10^{-5}	S40
$[\text{Zn}(\text{tpbpc})_2] \cdot \text{solvent}$	H_2O	1.65×10^5	4.66×10^{-8}	S49
$\{\text{Cd}_{10}(\text{DDB})_4(\text{bpz})_8(\text{DMA})(\text{H}_2\text{O})_{8.2}\} \cdot 2\text{H}_2\text{O}$	H_2O	2.59×10^4	3.31×10^{-7}	S51
$[\text{Zn}(\text{IPA})(\text{L}^{29})]$	H_2O	1.00×10^3	1.833×10^{-5}	S52
$[\text{Cd}(\text{IPA})(\text{L}^{29})]$	H_2O	1.30×10^3	2.52×10^{-6}	S52
$\{\text{Cd}_2\text{L}^{30}(\text{H}_2\text{O})_4\} \cdot \text{H}_2\text{O}$	H_2O	1.21×10^4	3.8×10^{-6}	S53
$\{\text{Zn}_2\text{L}^{30}(\text{H}_2\text{O})_4\} \cdot \text{H}_2\text{O}$	H_2O	1.95×10^4	2.3×10^{-6}	S53
$[\text{Cd}(4\text{-tkpvb})(5\text{-tert-BIPA})]$	H_2O	4.68×10^4	8×10^{-8}	S54
$\{\text{Zn}_2(\text{TPOM})(\text{NH}_2\text{-bdc})_2\} \cdot 4\text{H}_2\text{O}$	DMF	4.45×10^3	4.8×10^{-6}	S56

[Zn(btz)] _n	H ₂ O	3.19×10^3	1.0×10^{-5}	S57
{[Zn ₂ (ttz)H ₂ O] _n }	H ₂ O	2.35×10^3	1.00×10^{-5}	S57
[Cd ₃ (cptota) ₂ (phen) ₃]·5H ₂ O	H ₂ O	6.9×10^3	4.18×10^{-7}	S58
[Zn(NH ₂ -bdc)(4,4'-bipy)] _n	H ₂ O	4.56×10^3	2.21×10^{-6}	S59
{[Cd ₂ (HDDB)(bib) _{1.5} (H ₂ O)]·2.5H ₂ O} _n	H ₂ O	4.7×10^3	-	S60
[Cd ₂ (HDDB)(m-bimb)]·H ₂ O _n	H ₂ O	2.5×10^3	-	S60
{[Cd ₂ (DDB)(p-bimb)]·2.5H ₂ O·0.5(p-H ₂ bimb)} _n	H ₂ O	6.0×10^3	-	S60

Abbreviations:

$L^1 = 4,4'$ -(2,5-Bis(methylthio)-1,4-phenylene)-dipyridine; $H_2dcps = 4,4'$ -sulfon-ylidibenzoic acid; $H_2bdc = 1,4$ -dicarboxybenzene; $H_2oba = 4,4'$ -oxy-bisbenzoic acid; phen = 1,10-phenanthroline; $H_2L^2 = 6$ -methoxy-2,2'-sulfone-4,4'-dicarboxylic acid; 2,2'-bipy = 2,2'-bipyridine; $H_4L^3 = 1,1'$ -biphenyl]-2,3,3',5'-tetracarboxylic acid; $H_2L^4 = 9$ H-carbazolyl-3,6-dicarboxylic acid; 4,4'-bipy = 4,4'-bipyridine; bbibp = 4,4'-bis(benzimidaz-1-yl)biphenyl; $H_2L^5 = 4,4'$ -(4,4'-bipyridine-2,6-diyl)dibenzoic acid; $L^6 = 9,10$ -bis(N-benzimidazolyl)-anthracene; $L^7 = (9,10$ -bis(N-benzimidazolyl)-anthracene; $H_2bdc = terephthalic\ acid$; $H_3BTB = 1,3,5$ -tris(4-carboxyphenyl)benzene; $H_3btc = 1,3,5$ -benzenetricarboxylic acid; $H_2Br-bdc = bromo-terephthalic\ acid$; $L^8 = 1,3,4$ -trikisisoniacyl-2-deoxy- β -D-ribopyranose; $H_2NH_2-bdc = amino-terephthalic\ acid$; TPHC = [1,1':2',1"-terphenyl]-3,3",4,4',4",5'-hexacarboxylic acid; 1,4-H₂ndc = 1,4-naphthalenedicarboxylic acid; dpb = 1,4-bis(pyrid-4-yl)benzene; $H_2S-asba = 2$ -amino-5-sulfobenzoic acid; bimb = 1,4-bis(1H-imidazol-1-yl)butane; Htrz = 1H-1,2,3-triazole; $H_2HIP = 5$ -hydroxyisophthalic acid; $H_2hfipbb = 4,4'$ -(hexafluoroisopropylidene)bis(benzoic acid); $L^9 = 5,8$ -di(1H-imidazol-1-yl)quinoxaline; $H_5L^{10} = 2,5$ -bis(3',5'-dicarboxylphenyl)-benzoic acid; $L^{11} = 4,4'$ -(2,5-bis(methylthio)-1,4-phenylene)dipyridine; $H_2BPDC = 4,4'$ -biphenyldicarboxylic acid; $H_2SDBA = 4,4'$ -sulfonyldibenzoic acid; mtrb = 1,3-bis(1,2,4-triazole-4-ylmethyl)benzene; $H_2L^{12} = 5$ -(4-pyridylamino)isophthalic acid; $H_2DBTDC-O_2 = S,S$ -dioxodibenzothiophen-3,7-dicarboxylic acid; $HL^{13} = 4$ -(4-(2-chloroimidazo[1,2-a]pyridin-3-yl)-[2,30-bipyridin]-6-yl)benzoic acid; $H_2TBA = 4$ -(1H-tetrazol-5-yl)-benzoic acid; Hcptpy=4-(4-carboxyphenyl)-2,2':4",4"-terpyridine; $H_4L^{14} = 1$ -(3,5-dicarboxylatobenzyl)-3,5-pyrazole dicarboxylic acid; HEDP = 1-hydroxyethylidene diphosphonate; $H_5L^{15} = 2,4$ -di(3',5'-dicarboxylphenylbenzoic acid); 5-H₂AIP = 5-aminoisophthalic acid; $H_2ATA = 2$ -aminoterephthalic acid; $L^{16} = 3$ -pyridin-3-yl-N-[5-(3-pyridin-3-yl-acryloylamino)-naphthalen-1-yl]-acrylamide; $L^{17} = (E)$ -N'-(pyridin-4-ylmethylene)isonicotinohydrazide; $H_4bptc = 3,3',5,5'$ -biphenyltetra carboxylic acid; bpe = (E)-1,2-di(pyridin-4-yl)ethene; $L^{18} = 4,4'$ -((1,2-phenylenebis(methylene))bis(oxy))dibenzoic acid; $L^{19} = 5',5'''$ -bis(4-carboxyphenyl)-[1,1':3',1":4",1'''":3",1'''":quinquephenyl]-4,4'''-dicarboxylate; $L^{20} = 4,4',4'',4'''$ -(4,4'- (1,4-phenylene)bis(pyridine-6,4,2-triyl))-tetrabenoate; $H_2L^{21} = 2',3',5',6'$ -tetramethyl-[1,1':4',1"-terphenyl]-4,4"-dicarboxylic acid; BIMB = 4,4-bis(imidazol-1-ylmethyl)biphenyl; BIBP = 4,4-bis(imidazol-1-yl)diphenyl; $H_3cpt = 2$ -(2-carboxyphenoxy)terephthalic acid; $H_3L^{22} = 5$ -(6-carboxypyridin-2-yl)benzene-1,3-dicarboxylic acid; $H_2DHT = 2,5$ -dihydroxyterephthalic acid; BPP = 1,3-di(4-pyridyl)propane; Cz-3,6-bpy = 3,6-bis(pyridin-4-yl)-9H-carbazole; 4-tkpvb = 1,2,4,5-

tetrakis((E)-2-(pyridin-4-yl)vinyl)benzene; HBB = 3-bromobenzoic acid; H₂L²³ = 3-carboxy-1-(3'-carboxybenzyl)-2-oxidopyridinium; 1,4-bib = 1,4-bis(1H-imidazol-1-yl)benzene; H₂TPA-Cl₂ = 2,5-dichloro-terephthalic acid; H₄L²⁴ = 1-(3,5-dicarboxylatobenzyl)-3,5-pyrazole dicarboxylic acid; H₄bpta = 2,2',4,4'-biphenyltetracarboxylic acid; bpea = 1,2-bis(4-pyridyl)ethane; 3-bpah = N,N'-bis(3-pyridinecarboxamide)-1,2-cyclohexane; H₃cip = 5-(3-carboxybenzylamino)-isophthalic acid; H₃dttz = 4,5-di(1H-tetrazol-5-yl)-2H-1,2,3-triazole; Hdpa = 4,4'-dipyridylamine; bpa = 9,10-bis(4-pyridyl)anthracene; bztpy = 1,2,4,5-tetrakis(4-pyridyl)benzene; H₂TBTA = tetrabromoterephthalic acid; L²⁵ = 1,2-bis(benzimidazole-1-ylmethyl)benzene; L²⁶ = 1,3-bis(benzimidazole-1-ylmethyl)-benzene; L²⁷ = 1,4-bis(benzimidazole-1-ylmethyl)-benzene; Htpbpc = 4'-[4,2';6',4'']-terpyrindin-4'-biphenyl-4-carboxylic acid; H₂TBIP = 5-tert-butylisophthalic acid; L²⁸ = 1,3-bis(5,6-dimethylbenzimidazol-1-yl)propane; bpz = 2-(1H-pyrazol-3-yl)pyridine; H₅DDB = 3,5-di(2',4'-dicarboxylphenyl)benzoic acid; H₂IPA = isophthalic acid; L²⁹ = 3-pyridylcarboxaldehyde nicotinoylhydrazone; H₂L³⁰ = 5-(1H-1,2,4-triazol-1-yl)isophthalic acid; 4-tkpvb = 1,2,4,5-tetrakis(4-pyridylvinyl)benzene; 5-tert-H₂BIPA = 5-tert-butylisophthalic acid; BBI = 1,1'-(1,4-butanediyl)bis(imidazole); H₂L³¹ = benzo-(1,2;4,5)-bis(thiophene-2'-carboxylic acid; TPOM = tetrakis(4-pyridyloxymethylene)methane; H₂btz = 1,5-bis(5-tetrazolo)-3-oxapentane; H₃ttz = 1,2,3-tris-[2-(5-tetrazolo)-ethoxy]propane; H₃cpota = 2-(4-carboxyphenoxy)terephthalic acid; bib = 1,4-bis(imidazol-1-yl)benzene; H₅DDB = 3,5-di(2',4'-dicarboxylphenyl)benozoic acid; m-bimb = 1,3-bis(imidazol-1-ylmethyl)benzene; p-bimb = 1,4-bis(imidazol-1-ylmethyl)benzene; dpa = 9,10-di(4-pyridyl)anthracene; H₂cda = cyclohexane-1,4-dicarboxylic acid.

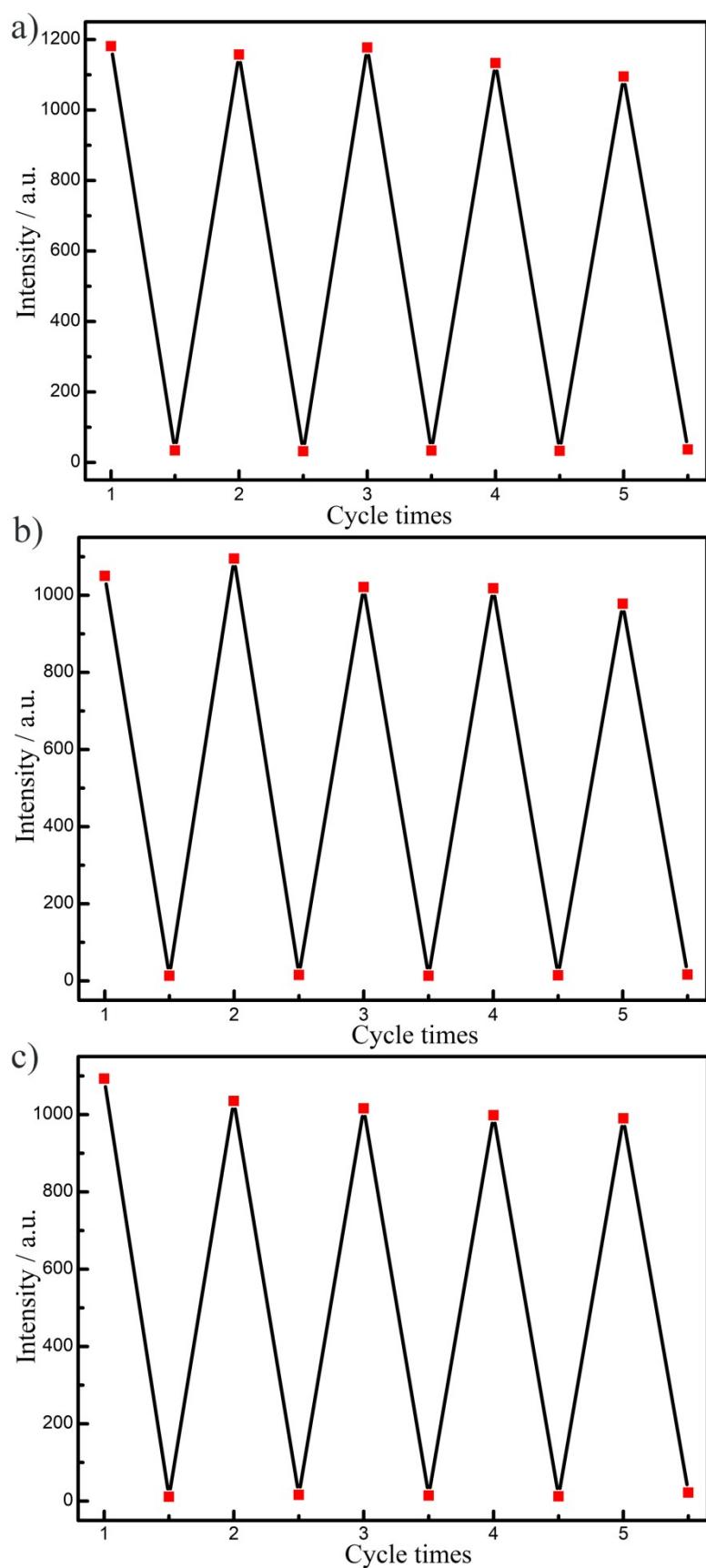


Fig. S7 The recyclable luminescence experiments of **1** towards sensing Fe^{3+} (a), $\text{Cr}_2\text{O}_7^{2-}$ (b), and CrO_4^{2-} (c), respectively.

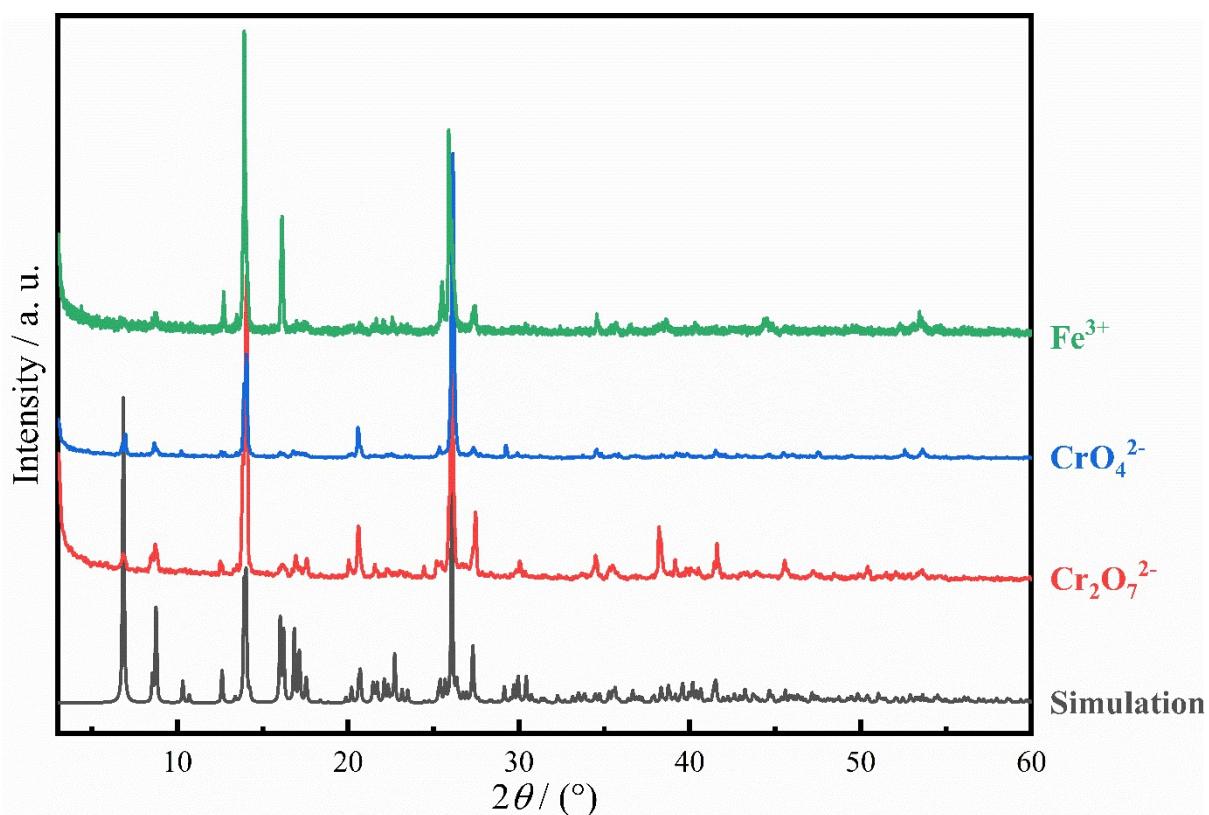


Fig. S8 The PXRD spectra for the simulation and sample of **1** immersed into the aqueous of Fe^{3+} , $\text{Cr}_2\text{O}_7^{2-}$ and CrO_4^{2-} for one week.

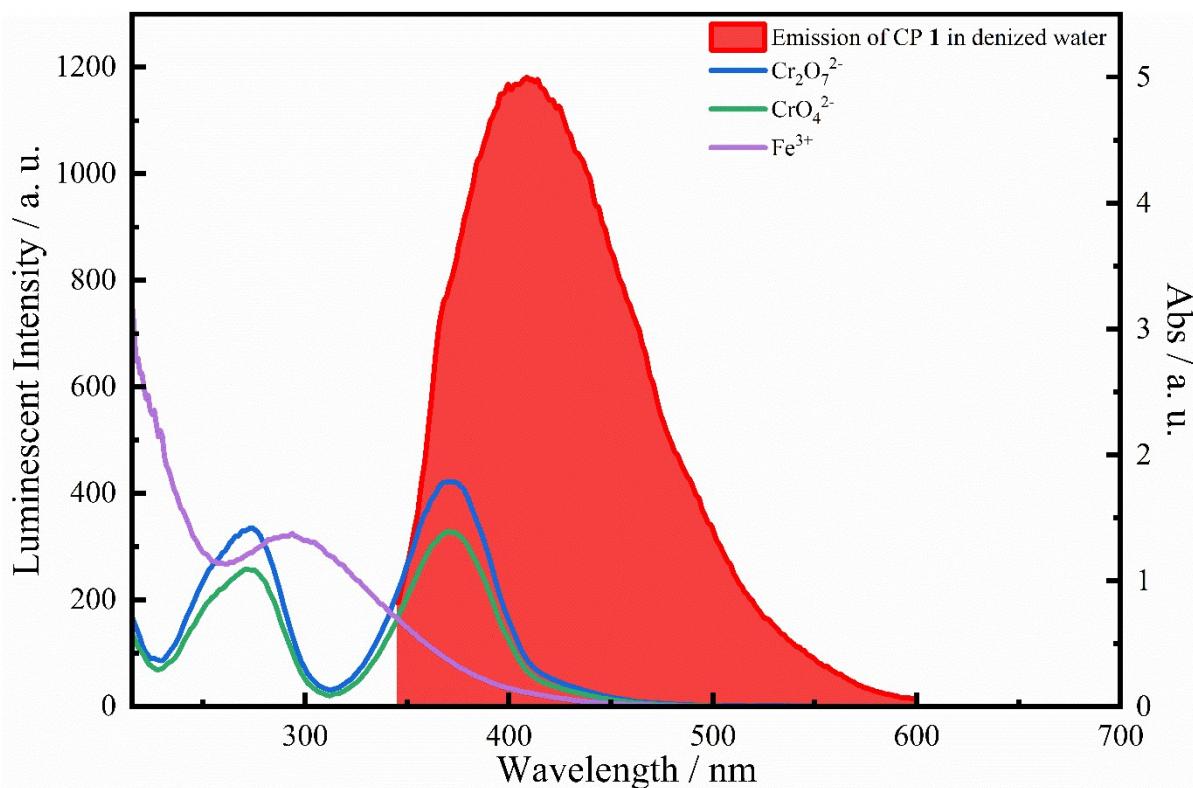


Fig. S9 The emission spectra of **1** in deionized water and the UV-vis spectra of the aqueous of Fe^{3+} , $\text{Cr}_2\text{O}_7^{2-}$ and CrO_4^{2-} .

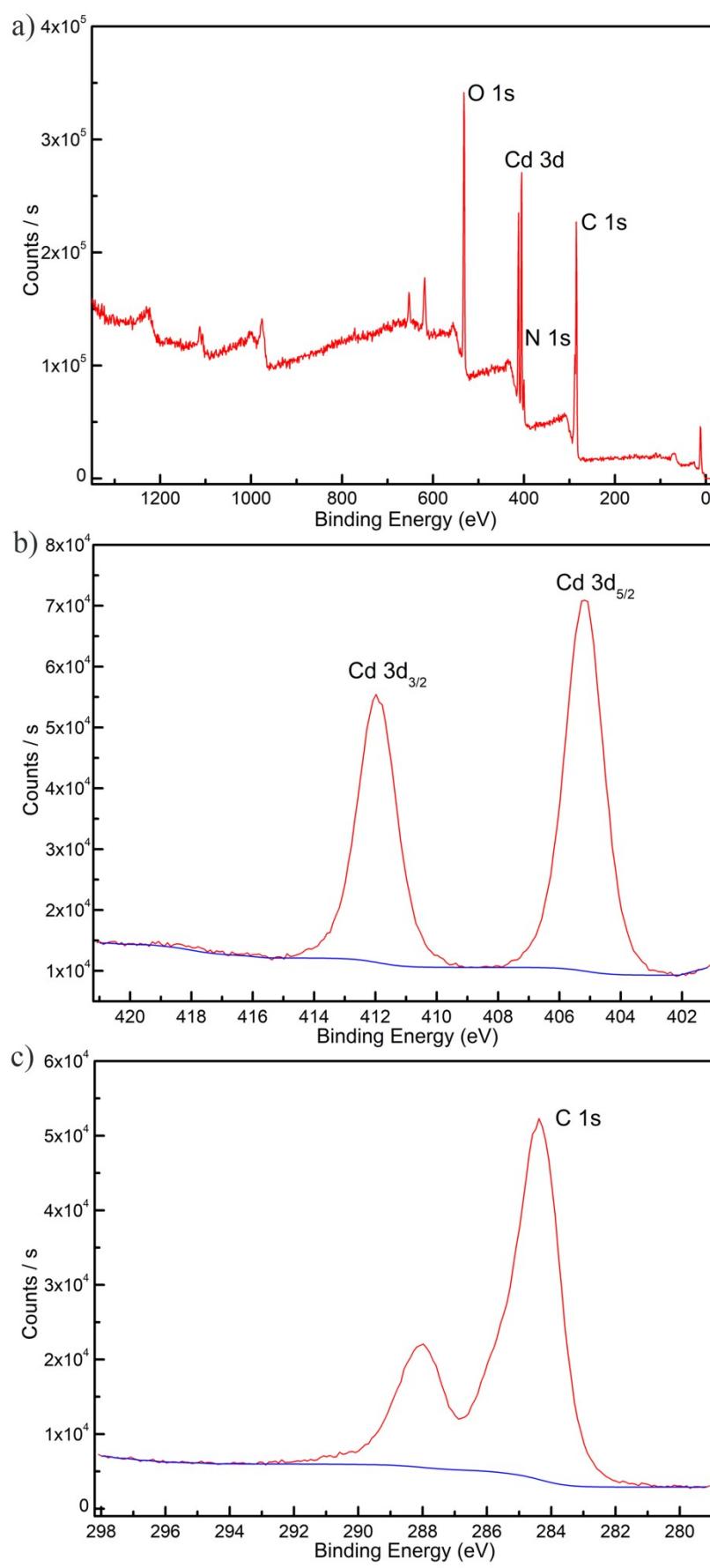


Fig. S10 The XPS spectrum of **1** (a), XPS spectra of **1** for Cd 3d (b) and C 1s (c).

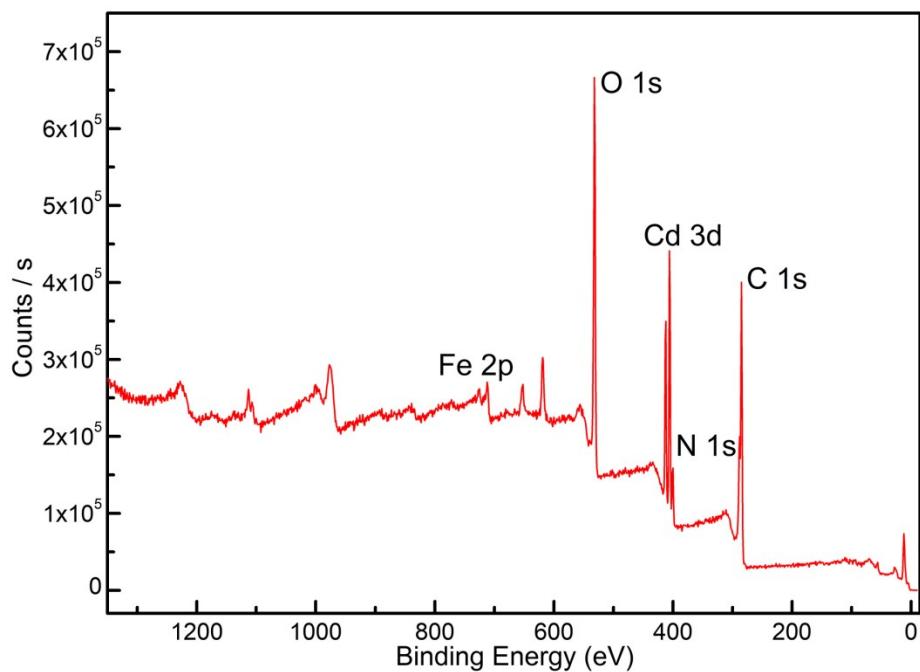


Fig. S11 The XPS spectrum of **1** after detection of Fe^{3+} ion.

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