Supporting information

A Cost-Effective and Innovative Detector for Iron Ions

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Due to the relatively large distance of the free water molecules from the primary structure, they were subtracted using a solvent mask for ease of mapping and to simplify the structure. Additionally, 1.1 water molecules were added to the molecular formula. This represents merely an estimate of the number of electrons computed from the solvent masking performed by the software. The molecular formula is $C_{30}H_{26.2}N_4O_{12.1}Zn_2$.

Table. S1 Crystallographic data and structure refinement

chemical formula	$C_{30}H_{24}N_4O_{11}Zn_2$	V/nm^3	2991.08(254)
relative molecular mass	747.27 g/mol	Z	4
Space group	P 1 21/c 1 (14)	ρ /g.cm^{-3}	1.659
crystal system	monoclinic crystal	absorption coefficientμ/mm^{-1}	1.674
a/ Å	22.1729(9)	F(000)	1520
b/ Å	8.4424(4)	R1, wR values (I > 2σ(I))	0.0583,0.1836
c/ Å	17.3538(6)	R1, wR values (all data)	0.0840,0.2049
α/°	90	The goodness of fit of F2.	1.048
β/°	112.96(0)	θ range	3.51-29.64
γ/°	90	Peak and pore with the maximum difference (e·nm^{-3})	2.971，-0.703

Table. S2 Bond lengths [Å] and angles [deg]

chemical bond	bond length /nm	chemical bond	bond length /nm
Zn1—O1	2.417(4)	Zn2—O6	2.000(3)
Zn1—N3	2.078(4)	Zn2—N4	2.031(4)
Zn1—O2	1.994(4)	Zn2—O1W	2.209(4)

chemical bond	bond angle /(°)	chemical bond	bond angle /(°)
O2—Zn1—N3	91.55(16)	O1—Zn1—C7	28.67(16)
O1—Zn1—O2	58.11(15)	O6—Zn2—N4	143.51(15)
N3—Zn1—O1	149.53(14)	O6—Zn2—O1W	94.11(15)
O2—Zn1—C7	29.45(17)	N4—Zn2—O1W	90.31(15)
N3—Zn1—C7	120.97(17)		

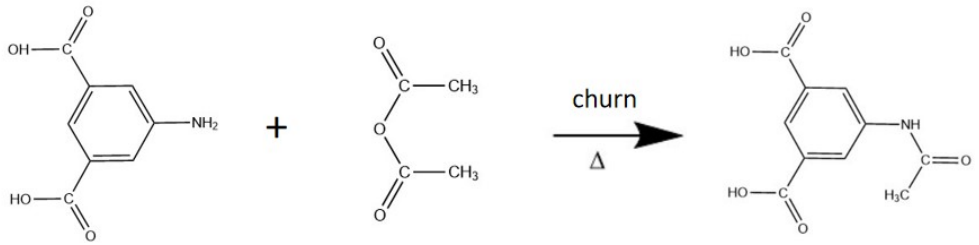

Fig. S1 Schematic diagram of the synthesis of H_2APA

In a 50 mL round bottom flask, 2.00 g of 5-amino-1,3-benzenedicarboxylic acid, 6 mL of acetic

anhydride and 6 drops of concentrated sulphuric acid were added respectively, and after initial mixing by shaking, a magnetic stirrer was added for stirring and the mixture was heated up to 90 ℃ in a water bath, and the reaction was carried out at 90 ℃ for 30 min, and then the reaction solution was quickly poured into 20 mL of cold distilled water and stirred to produce a precipitate, which was filtered and dried to give a white Solid (90% yield), that is, 5-acetamido-1,3-benzenedicarboxylic acid ligand (H_2APA).

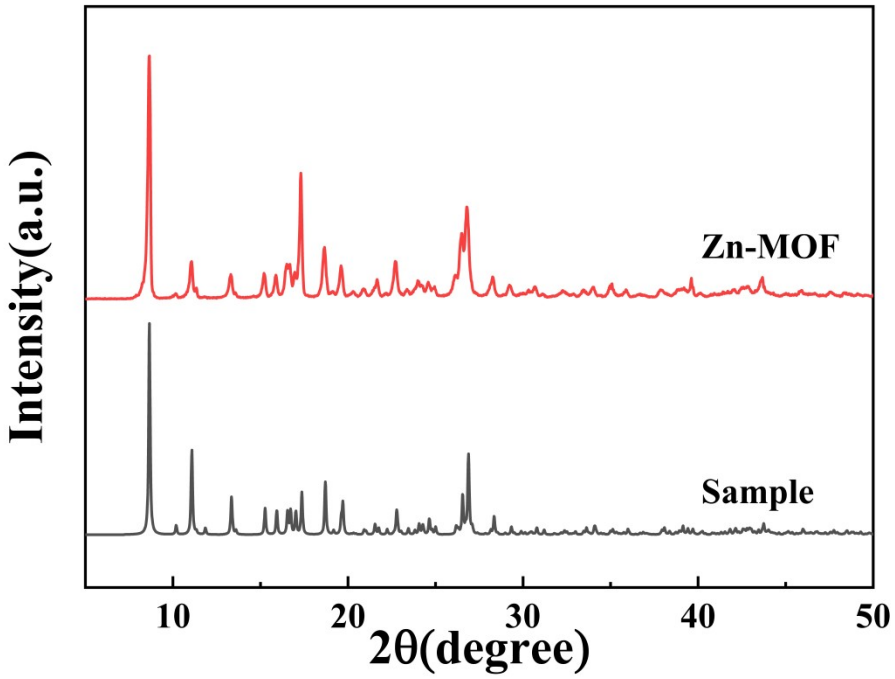

Fig. S2 XRD patterns of Zn-MOFs

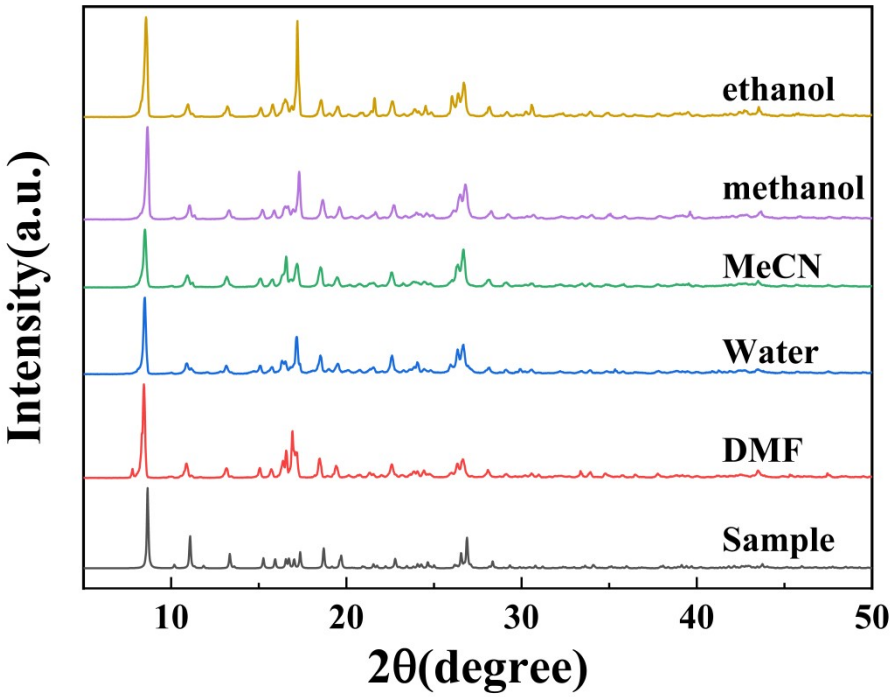

Fig. S3 XRD spectra of Zn-MOFs before and after immersion

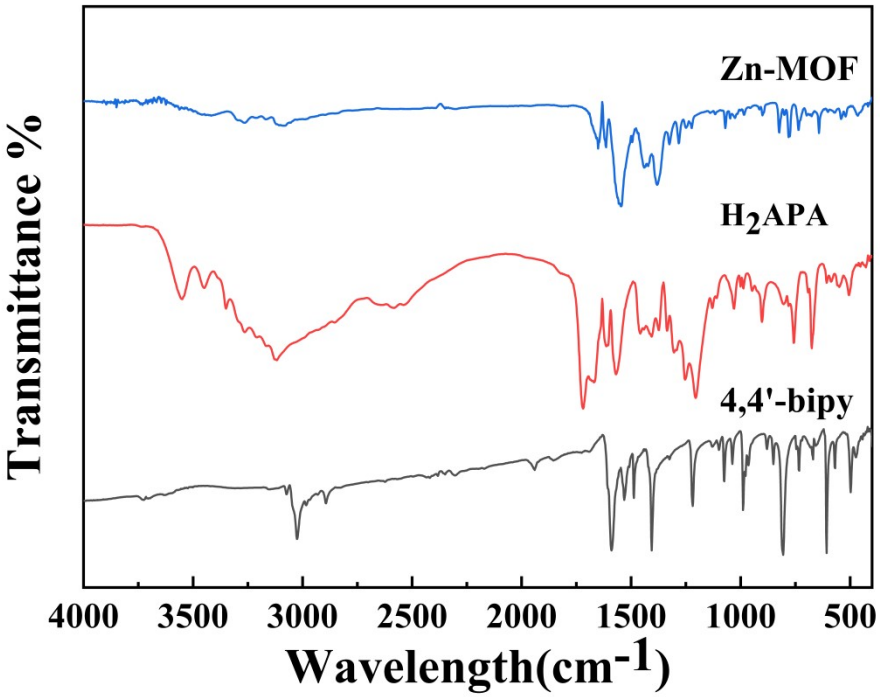

Fig. S4 Infrared spectra of ligands and complexes

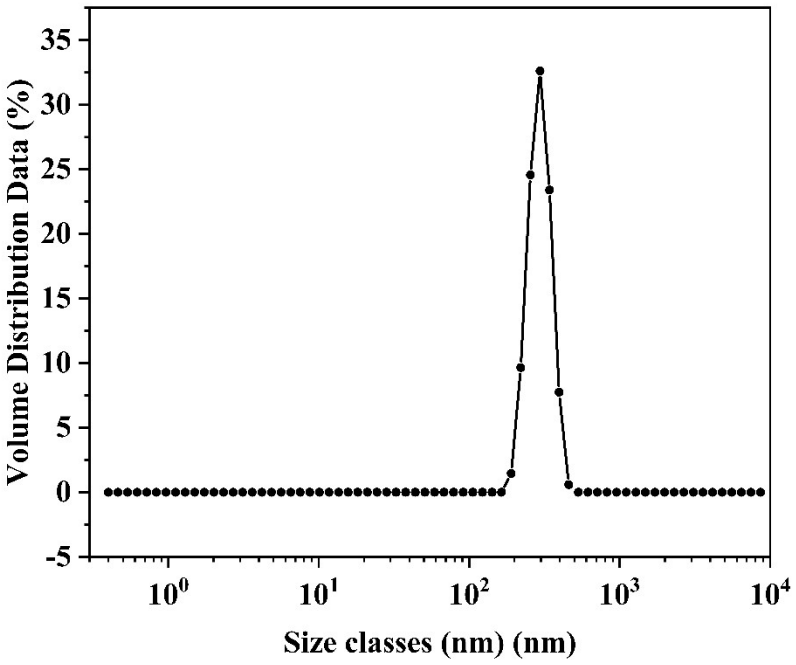

Fig. S5 The particle size distribution diagram in solution

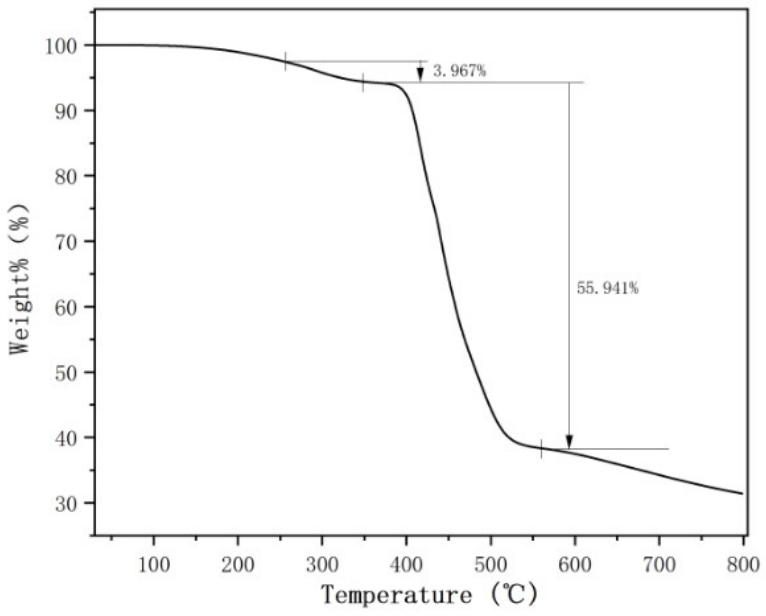

Fig. S6 Thermogravimetric carves of Zn-MOFs

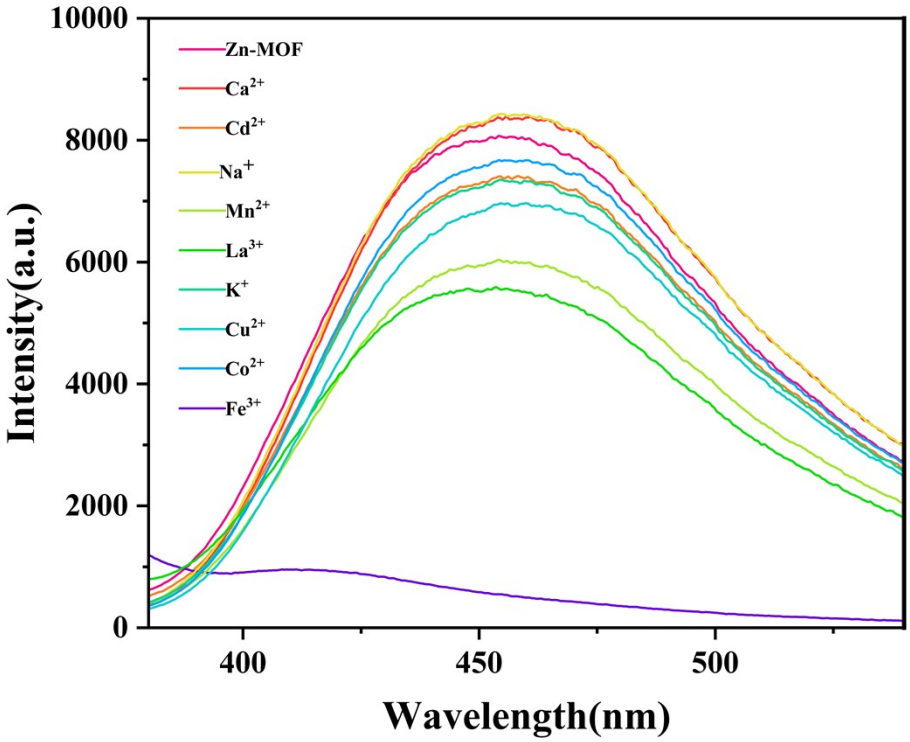

Fig. S7 Fluorescence Emission Spectrum Graph of Metal Ions

Table. S3 Price comparison of some MOFs that can quench Fe^{3+}

CCDC number	sample name	total price of metal salts/ $	total price of organicligands/ $	price of organic solvents/ $	cost of a 0.1 mmol sample/ $
2396827	Zn-MOF	5.77×10^{-4}	0.022	7.73×10^{-3}	0.03
1573428	$[Eu_2IJDMTDC)_3IJDEF)_4]\cdot DEF\cdot 6H_2O$	0.085	7.00	0.6750	7.76
1573429	$[Tb_2IJDMTDC)_3IJDEF)_4]\cdot DEF\cdot 6H_2O$	0.208	7.00	0.6750	8.00
1521670	$\{(Me_2NH_2)[Tb(OBA)_2](Hatz)(H_2O)_{1.5}\}_n$	0.220	0.016	0.0155	0.252
1565344	$\{[Eu_2(pdba)_3(H_2O)_3]\cdot 2H_2O\}_n$	0.0485	1.361	0.1156	1.525
1565345	$\{[Eu_3(pdba)_4(H_2O)_4]\cdot 5H_2O\}_n$	0.0485	1.362	0.1156	1.526
1509860	534-MOF-Tb	0.0988	5.968	0.8508	6.9176
1410772	$[(CH_3)_2NH_2]\cdot[Tb(bptc)]\cdot x(solvents)$	0.0274	0.551	0.3911	0.6175
1035886	Eu–BPDA	0.0436	0.0384	0.3265	0.4445
1965138	Eu-MOF	0.0582	0.0865	0	0.1447
1965139	Tb-MOF	0.2169	0.0865	0	0.3034
1056662	UiO-66-NH_2	0.5437	0.4686	0.0231	1.035
2217760	$\{[Ag(L)]ClO_4\cdot H_2O\}_n$	0.1842	6.0	0	6.1842

2217761	$\{[Ag(L)]NO_3\cdot H_2O\}_n$	0.0617	6.0	0	6.0617
2217762	$\{[Ag(L)]BF_4\cdot H_2O\}_n$	0.2202	6.0	0	6.2202
1916377	$\{[Cd(5\text{-}Brp)(dpa)]\cdot 0.5DMF\cdot H_2O\}_n$	0.0144	0.2282	2.884×10^{-4}	0.2429
1916379	$[Cd(5\text{-}Brp)(bpp)(H_2O)]n$	0.0144	0.1818	5.047×10^{-4}	0.1967
2076041	Tb-MOF	0.1445	0.2971	0.0232	0.4648
1905642	$[Cd_{0.5}(TBC)]_n$	0.1442	0.3954	0.2692	0.6790
1974695	Tb-MOF-A	0.2189	0.2173	0	0.4362
1846840	$[Tb_2(2,3'\text{-}oba)_3(phen)_2]_n$	0.2169	0.0882	0	0.3051

Solely the price parameters of chemical reagents are incorporated into consideration. The price details of all chemical reagents can be procured from Aladdin Reagents. In the realm of chemical synthesis, the computational process is predicated on the hypothesis of an ideal reaction, while the expenditure on electricity and water is omitted from the scope of consideration.

Table. S4 Comparison of LOD Values of Some MOFs that Can quench Fe^{3+}

CCDC number	sample name	LOD/mol·L^{-1}
2396827	Zn-MOF	5.619×10^{-6}
2354330	CUST-761	2.98×10^{-4}
1509860	534-MOF-Tb	1.3×10^{-4}
1410772	$[(CH_3)_2NH_2]\cdot[Tb(bptc)]\cdot x(solvents)$	1.8×10^{-4}
1974695	Tb-MOF-A	1.27×10^{-5}
1846840	$[Tb_2(2,3'\text{-}oba)_3(phen)_2]_n$	7.93×10^{-6}
2217760	$\{[Ag(L)]ClO_4\cdot H_2O\}_n$	11.46×10^{-6}
2217761	$\{[Ag(L)]NO_3\cdot H_2O\}_n$	15.83×10^{-6}
2217762	$\{[Ag(L)]BF_4\cdot H_2O\}_n$	15.44×10^{-6}
1521670	$\{(Me_2NH_2)[Tb(OBA)_2](Hatz)(H_2O)_{1.5}\}_n$	10^{-6}
2213445	$\{[Cd(ttc)(H_2O)]\cdot H_2O\}_n$.	5.34×10^{-8}
1873450	$[[Tb(Cmdcp)(H_2O)_3]_2(NO_3)_2\cdot 5H_2O]_n$	4.0×10^{-6}
1899278	Eu-CP	5.0×10^{-7}
1818852	$[Eu_2L(1,3\text{-}bdc)_3]\cdot 5H_2O$	2.3×10^{-5}
1884067	$[Eu_2(ppda)_2(npdc)(H_2O)]\cdot H_2O$	1.66×10^{-5}
1821918	$[Eu(IMS1)_2]Cl\cdot 4H_2O$	2.3×10^{-5}
1035886	$[[Eu(bpda)_{1.5}]\cdot H_2O]_n$	0.9×10^{-6}
1538770	$\{[Zn(ATA)(L)]\}_n\cdot xH_2O$	3.76×10^{-6}
1538771	$\{[Cd(ATA)(L)]\}_n\cdot xH_2O$	1.77×10^{-6}
1542239	$\{[Zn(DPTMIA)]\cdot(H_2O)_2(DMF)_{0.5}\}_n$	1.09×10^{-3}
1840235	$\{[Cd_3(HL)_2(H_2O)_3]\cdot 3H_2O\cdot 2CH_3CN\}_n$	9.06×10^{-5}

Upon examination of the comparison table, it becomes manifestly evident that our Zn-MOF material exhibits a remarkably lower limit of detection (LOD) value with respect to Fe^{3+}. When juxtaposed

with the preponderant majority of MOFs, it conspicuously showcases a more preponderant advantage in the domain of LOD. This distinctive characteristic endows it with the capacity to effectuate a more exquisitely sensitive and highly accurate detection of Fe^{3+}.

Notes and references

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