Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

An excellent water-stable 3D Zn-MOF with 8-fold interpenetrated diamondiod topology showing "Turn-On/Turn-Off" luminescent detection of Al^{3+} and SNT in aqueous media

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Supplementary Figures

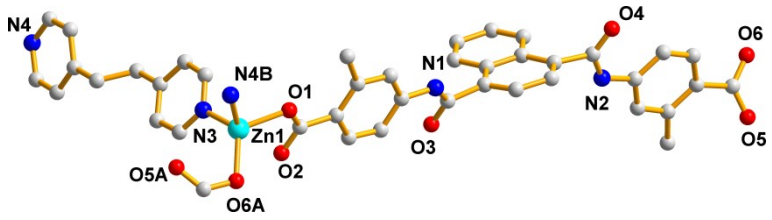

Fig. S1 Coordination environment of Zn(II) in **1**, the isolated H_2O molecules, isolated DMF molecule and H atoms are omitted for clarity. (A: x−3/2, −y+1/2, z−1/2; B: x−1/2, −y+3/2, z+1/2)

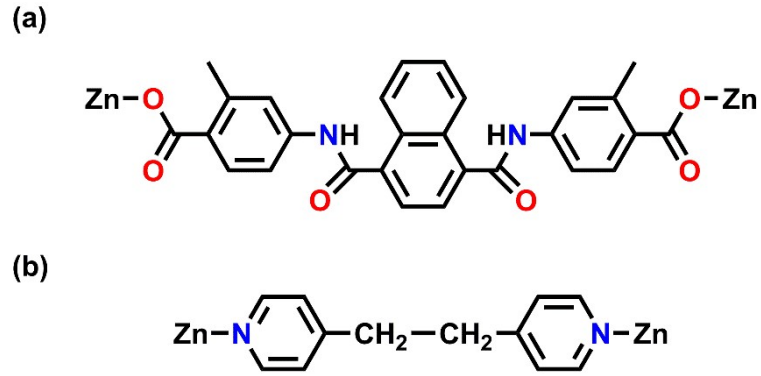

Fig. S2 (a) Coordination modes of carboxylate groups in L^{2-} ligand. (b) Coordination modes of N atoms in dpe ligand.

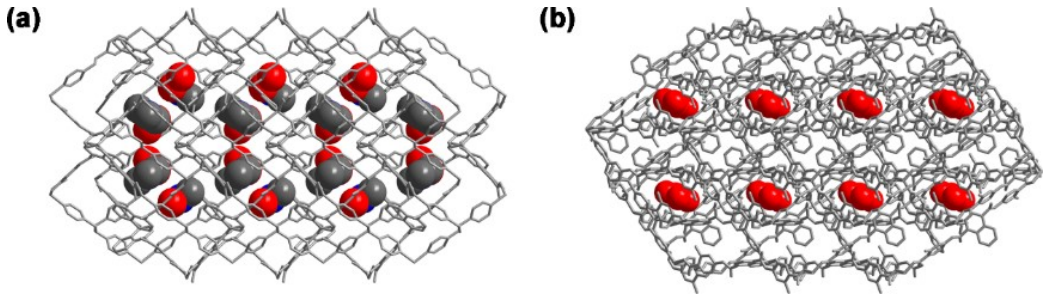

Fig. S3 Solvent molecules of DMF and H_2O in **1** are represented as space filling spheres along the [101] (a) and [0-11] (b) directions.

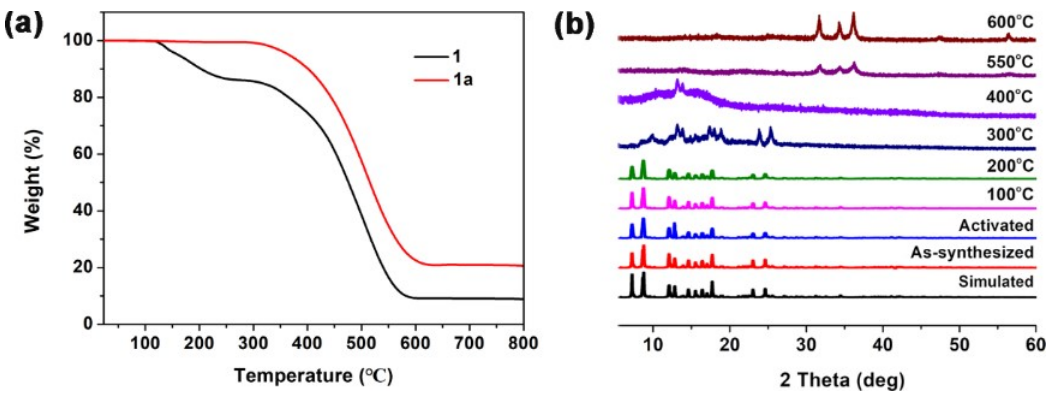

Fig. S4 (a) TGA curves of **1** and **1a**. (b) Variable-temperature PXRD patterns for **1**.

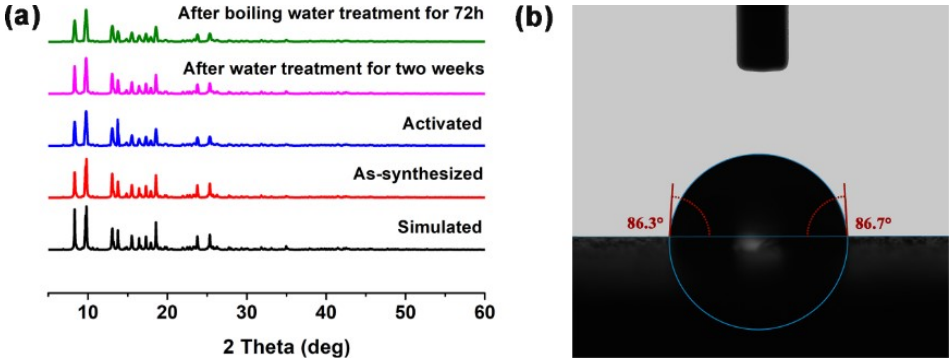

Fig. S5 (a) PXRD patterns of simulated, as-synthesized, activated, as well as **1a** after immersion in water and boiling water. (b) Water contact angle of **1a**.

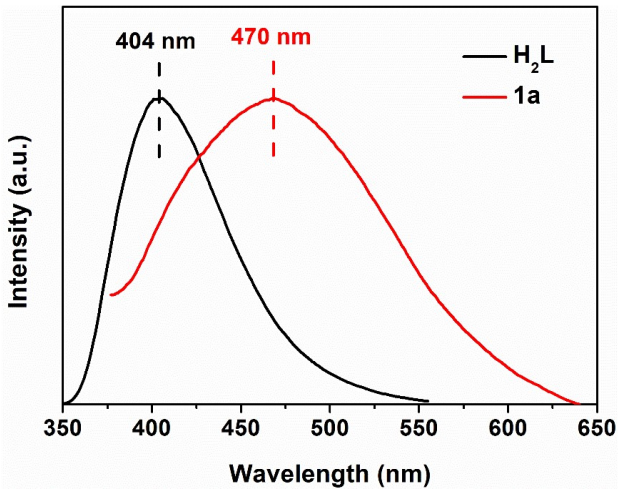

Fig. S6 The emission spectrum of H_2L ligand and **1a** dispersed in water at room temperature.

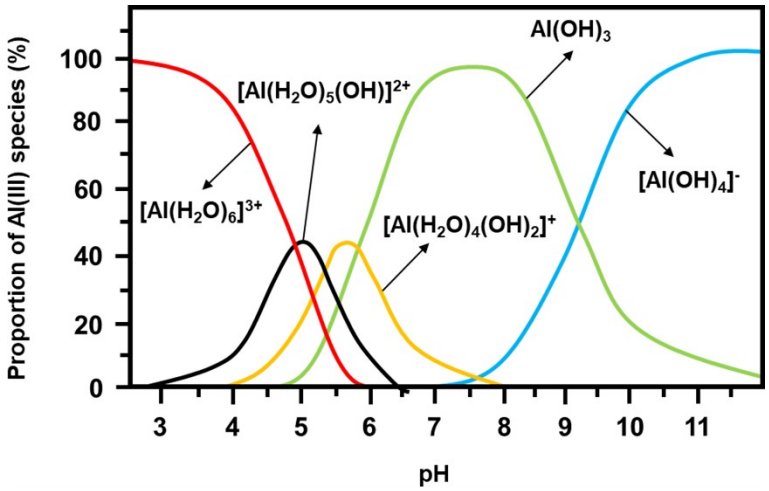

Fig. S7 The pH-dependence of various Al(III) species in aqueous solution.

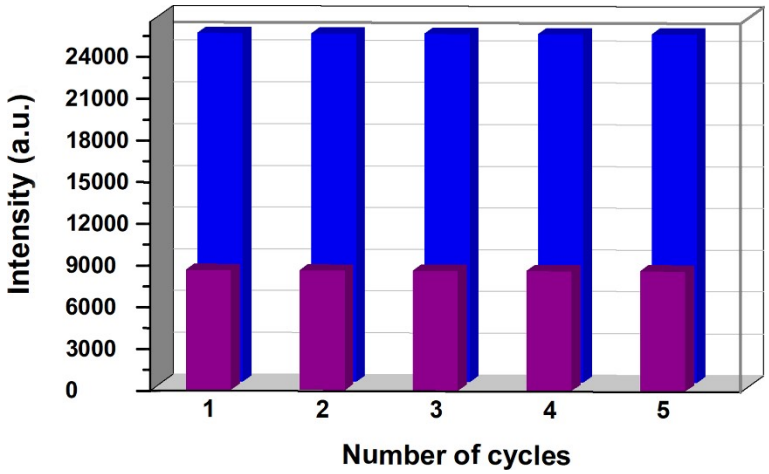

Fig. S8 Recyclability experiments of **1a** implemented with Al^{3+}.

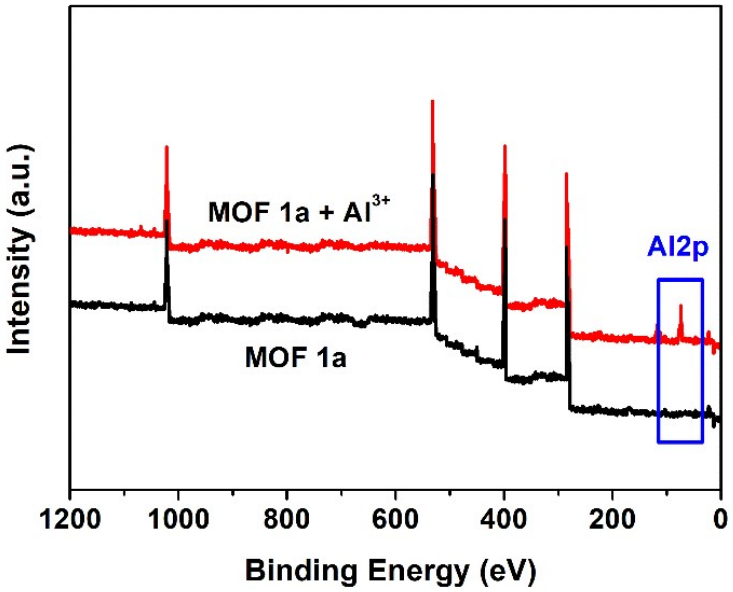

Fig. S9 XPS spectra of **1a** and **1a**+Al^{3+}.

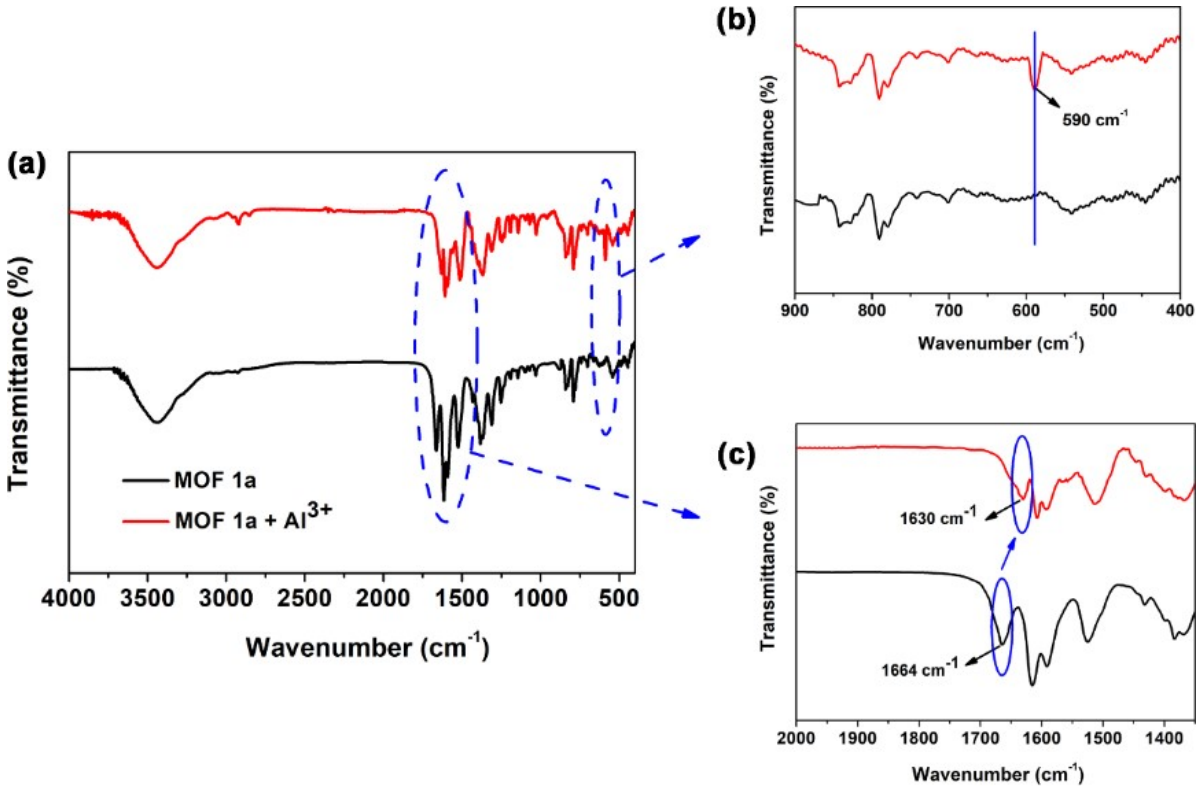

Fig. S10 IR spectra of **1a** and **1a**+Al^{3+}.

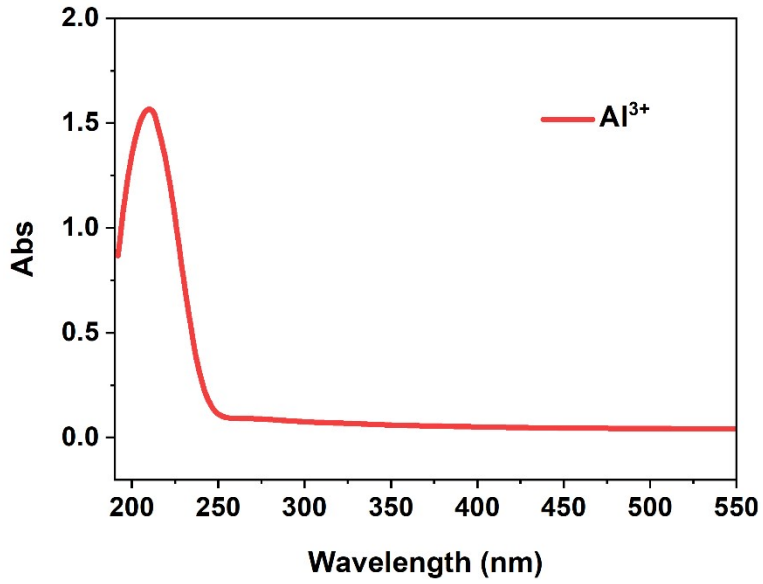

Fig. S11 Absorption spectra of Al^{3+} in the concentration of 10^{-5} mol·L^{-1} in aqueous solution.

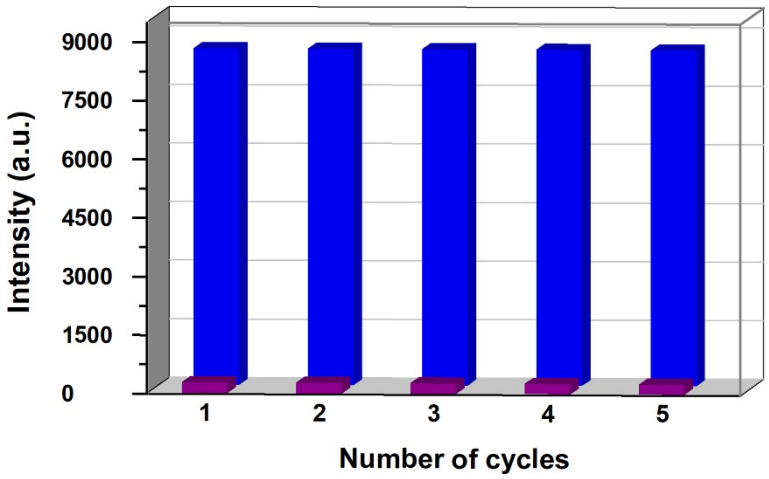

Fig. S12 Recyclability experiment of **1a** implemented with SNT.

Supplementary Tables

Table S1. Crystal data and structure refinement parameters for **1**.

Empirical formula	$C_{43}H_{45}N_5O_{10}Zn$
Formula weight	857.25
Temperature (K)	298(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	12.811 (1)
b (Å)	19.034 (2)
c (Å)	17.420 (2)
β (°)	91.017 (2)
Volume (Å^3)	4247.0 (7)
Z	4
Calculated density (mg·m^{-3})	1.341
Absorption coefficient (mm^{-1})	0.641
F(000)	1792
Crystal size (mm)	0.42 × 0.26 × 0.10
Theta range for data collection (°)	2.4385 to 21.593
Limiting indices	-15≤h≤12, -22≤k≤17, -20≤l≤18
Reflections collected/unique	19558/7426[Rint = 0.084]
Completeness to ϑ = 25.02°	99.1%
Data/restraints/parameters	7426/0/536
Goodness-of-fit on F^2	1.073
Final *R* indices [$I>2\sigma(I)$]	R_1= 0.065, wR_2= 0.109

Table S2. Selected bond lengths (Å) and angles (°) for **1**.

Bond lengths			
Zn1—O1	1.973 (3)	Zn1—O6A	1.962 (3)
Zn1—N3	2.013 (4)	Zn1—N4B	2.044 (3)
Bond angles			
O6A—Zn1—O1	115.49 (13)	O1—Zn1—N4B	96.44 (15)
O6A—Zn1—N3	121.11 (16)	N3—Zn1—N4B	106.44 (14)
O1—Zn1—N3	107.46 (14)	O6A—Zn1—N4B	106.62 (13)

Symmetry codes: A: x−3/2, −y+1/2, z−1/2; B: x−1/2, −y+3/2, z+1/2; C: x+3/2, −y+1/2, z+1/2.

Table S3. The LOD comparison of **1a** and some reported MOF sensors toward Al^{3+}.

MOFs	Analyte	LOD (ppb)	Ref.
UiO-66-NH_2-SA	Al^{3+}	930.7	S1
Zn(DMA)(TBA)	Al^{3+}	262.7	S2
NUM-2	Al^{3+}	100.0	S3
[Co(OBA)$(DATZ)_{0.5}(H_2O)$]	Al^{3+}	57.5	S4
MOF **1a**	Al^{3+}	41.9	This work

Table S4. HOMO and LUMO energies for the selected antibiotics by DFT calculations.

Analytes	HOMO (ev)	LUMO (ev)
SNT	-8.198	-1.171
AZM	-4.080	-0.850
ROX	-4.710	-0.850
SDZ	-7.564	0.016
SMX	-7.599	0.126
SMZ	-7.507	0.218
GEN	-6.330	1.360

Table S5. Al^{3+} and SNT determination in tap water, Dongchang Lake and Yellow River.

Samples	Analyte	Added [μM]	Found [μM]	Recovery [%]	RSD [%]
Tap water	Al^{3+}	0	not detected	—	—
		20	20.48	102.4	2.1
		40	37.46	93.7	1.9
	SNT	0	not detected	—	—
		20	20.98	104.9	4.2
		40	38.13	95.3	2.6
Dongchang Lake	Al^{3+}	0	not detected	—	—
		20	21.51	107.6	2.8
		40	38.8	97.0	1.5
	SNT	0	not detected	—	—
		20	21.18	105.9	4.8
		40	38.46	96.2	2.9
Yellow River	Al^{3+}	0	not detected	—	—
		20	20.51	102.6	3.0
		40	37.80	107.6	1.1
	SNT	0	not detected	—	—
		20	20.85	104.2	2.7
		40	39.80	99.5	2.2

References

S1. S. Y. Zhu and B. Yan, *Dalton Trans.*, 2018, **47**, 1674-1681.

S2. X. Zhang, X. Luo, N. X. Zhang, J. Wu and Y. Q. Huang, *Inorg. Chem. Front.*, 2017, **4**, 1888-1894.

S3. M. H. Yu, T. L. Hu and X. H. Bu, *Inorg. Chem. Front.*, 2017, **4**, 256-260.

S4. D. K. Singha and P. Mahata, *Inorg. Chem.*, 2015, **54**, 6373-6379.