Supplementary Information

Eight semiconducting MOFs constructed with conjugated ligands and d-metals (Cd, Zn, Co, Ni) serve as functional materials for oxygen evolution reaction, photocatalytic degradation of dyes and photoluminescence

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The corresponding formula and calculation method

The Tafel plot can be calculated by the linear Tafel equation:

$$\eta = a \times \log(j) + b$$

where a is the Tafel slope, j and η are the catalytic current density and overpotential, respectively.

The electrochemically active surface area (ECSA) of the MOFs has the following relationship to the electric double layer capacitance:

$$EASA = C_{dl}/C_s$$

The electrochemical double layer capacitance (C_{dl}) is calculated by measuring the relevant CV curves at different scan rates (10 to 50 mV/s) in a non-Faraday region. The value of C_{dl} is the slope of the plot of capacitive current as a function of scan rate. The C_s is the specific capacitance of an atomically smooth surface of the material.

The turnover frequency (TOF) value has been measured via equation:

$$TOF = j \times A/(4 \times F \times m/M)$$

where j is the current density (A cm^{-2}) at a given overpotential, A is the loading area of the electrode (cm^2), F is Faraday constant = 96485 (C mol^{-1}) , m is the mass per square centimeter of the catalyst, and M is the molecular weight of the catalyst, respectively.

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According to the Kubelka-Munk function (F), the band gap can be calculated by the following equations:

$$F = (1- R)^2 /2R$$

$$(Fhv)^n = B(hv - Eg)$$

where R is the reflectance of an infinitely thick layer at a given wavelength, h is the Plank's constant, v is the frequency of light, Eg is the optical bandgap energy of the material, and factor B depends on the transition probability assumed to be as constant within the optical frequency range, $n = 2$ or1/2 represent the direct and indirect transition, respectively.

The degradation efficiency of MO is defined as follows:

$$\text{Degradation efficiency} = (1-(C_t/C_0)) \times 100\%$$

Where C_0 and C_t are the concentrations of MO solution when photocatalytic reaction at time 0 min and t min, respectively.

The graphs associated with the text

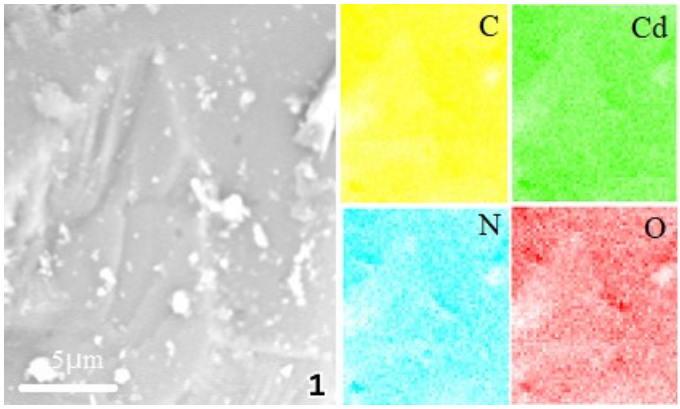

Fig. S1 EDS mapping images of MOF **1**.

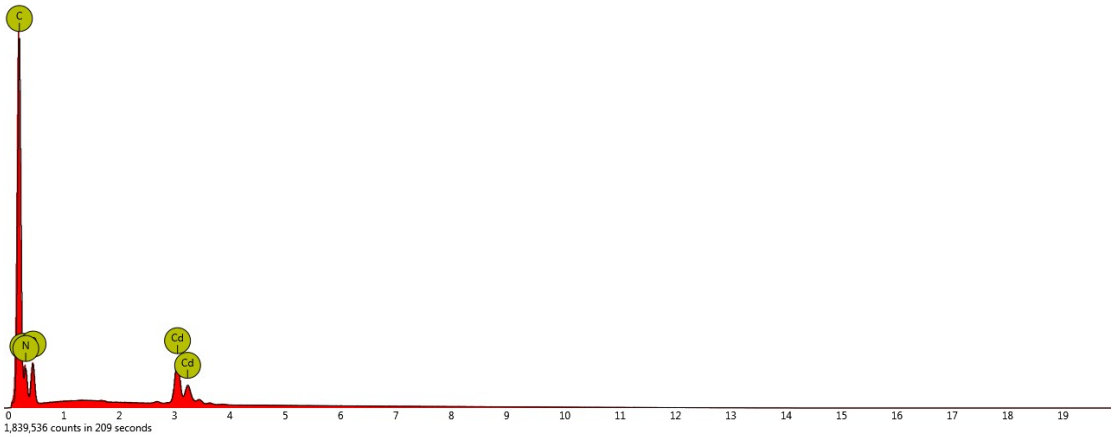

Fig. S2 EDX spectrum of MOF **1**.

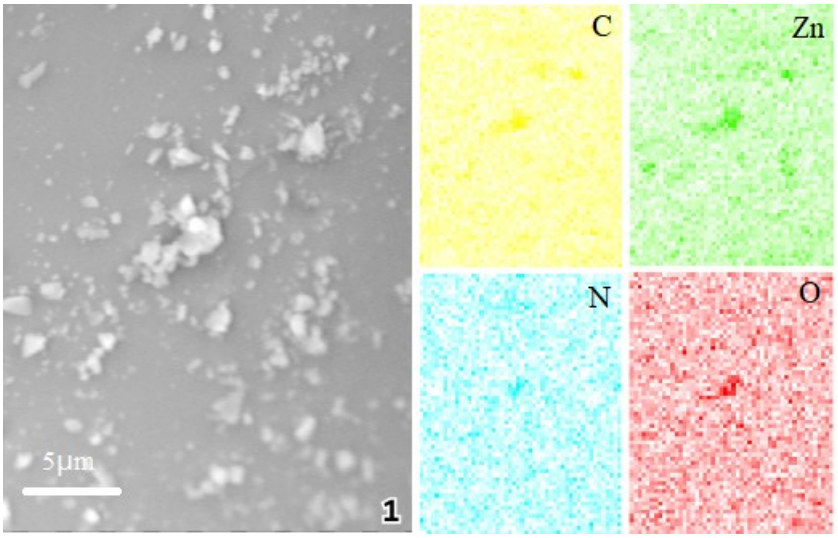

Fig. S3 EDS mapping images of MOF **2**.

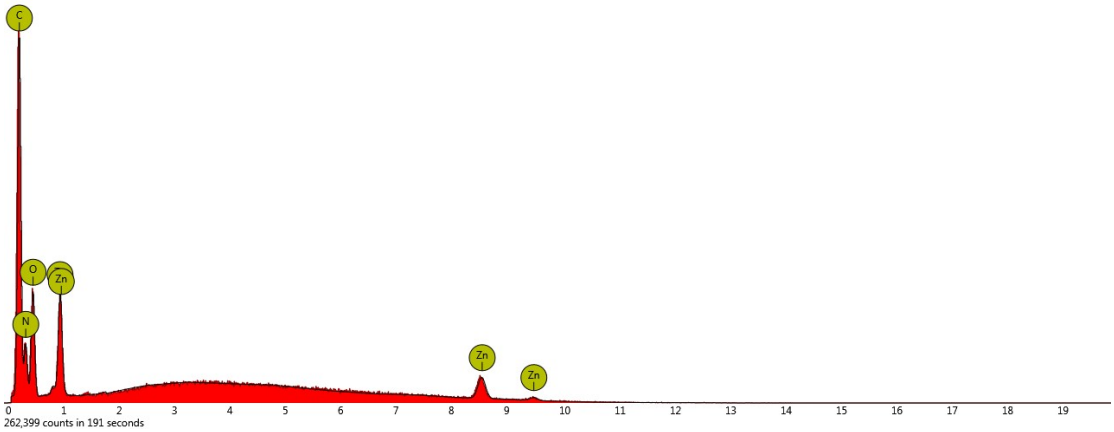

Fig. S4 EDX spectrum of MOF **2**.

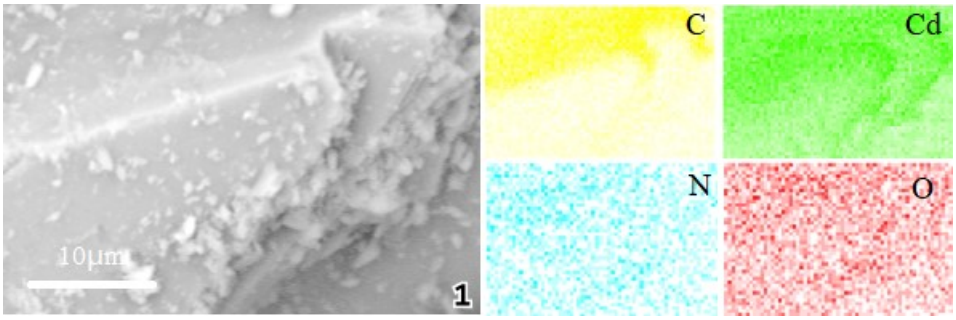

Fig. S5 EDS mapping images of MOF **3**.

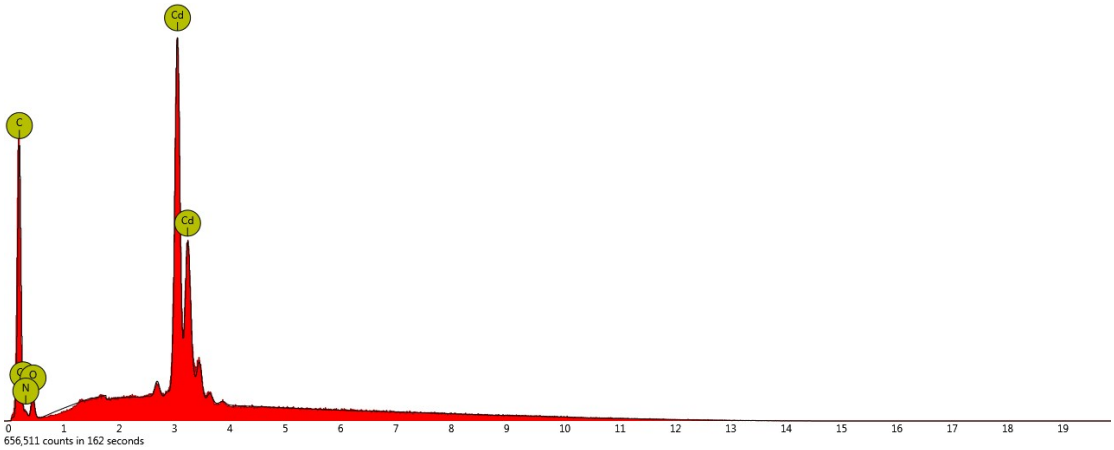

Fig. S6 EDX spectrum of MOF **3**.

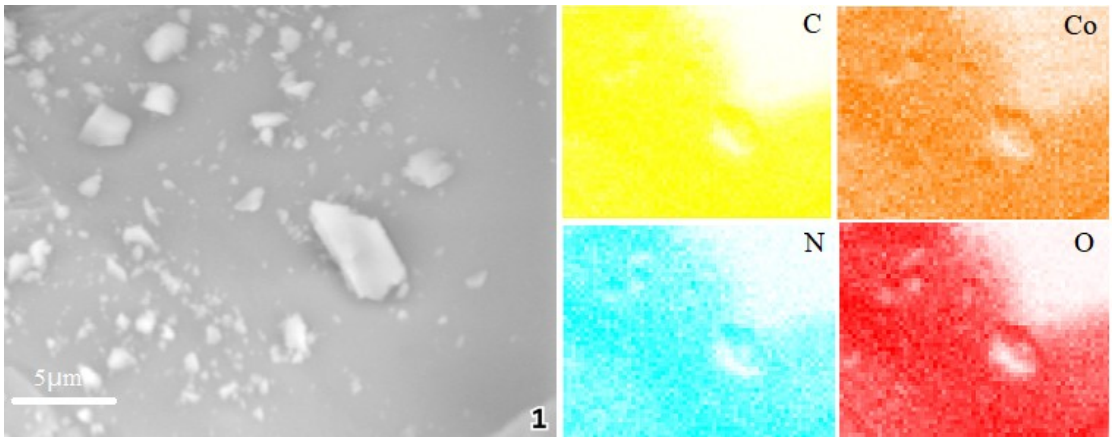

Fig. S7 EDS mapping images of MOF **4**.

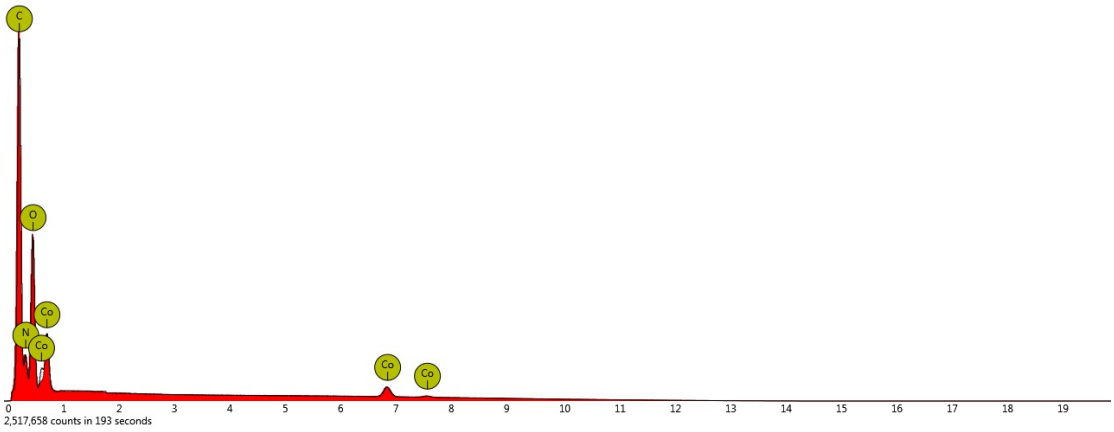

Fig. S8 EDX spectrum of MOF **4**.

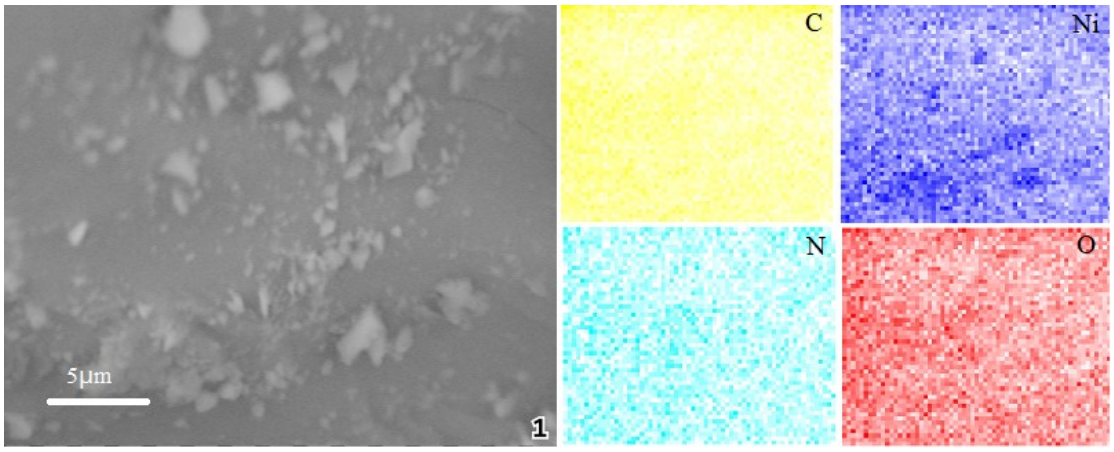

Fig. S9 EDS mapping images of MOF **5**.

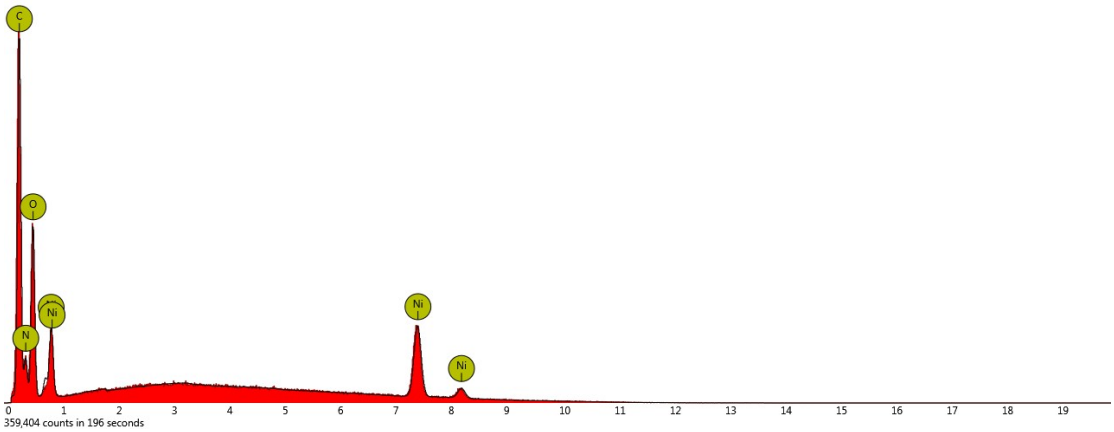

Fig. S10 EDX spectrum of MOF **5**.

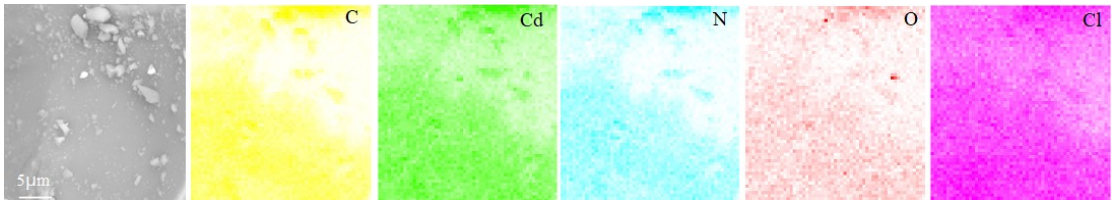

Fig. S11 EDS mapping images of MOF **6**.

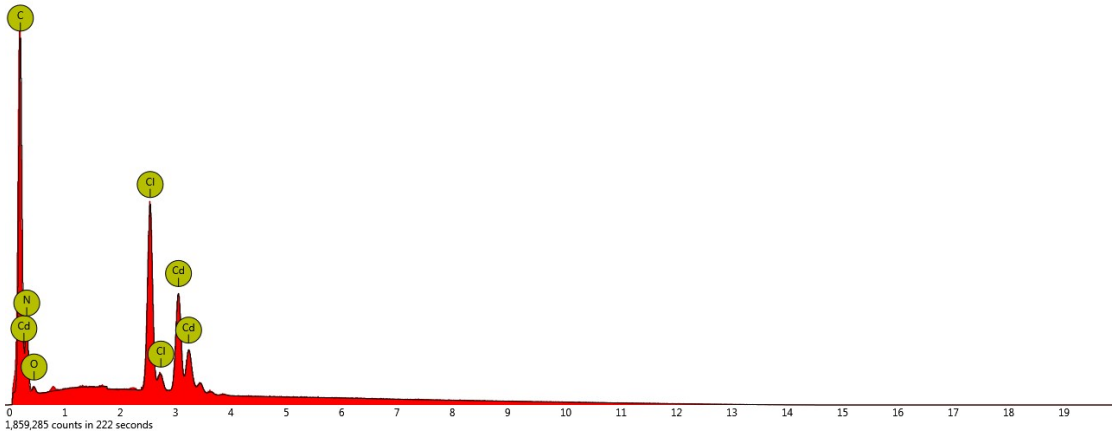

Fig. S12 EDX spectrum of MOF **6**.

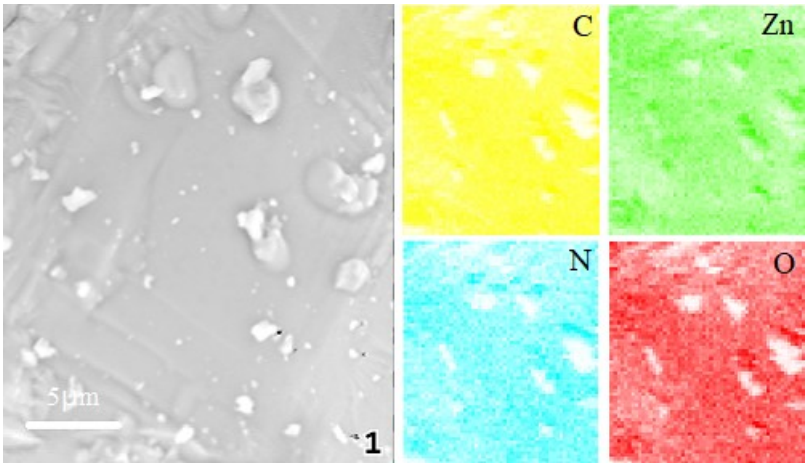

Fig. S13 EDS mapping images of MOF **7**.

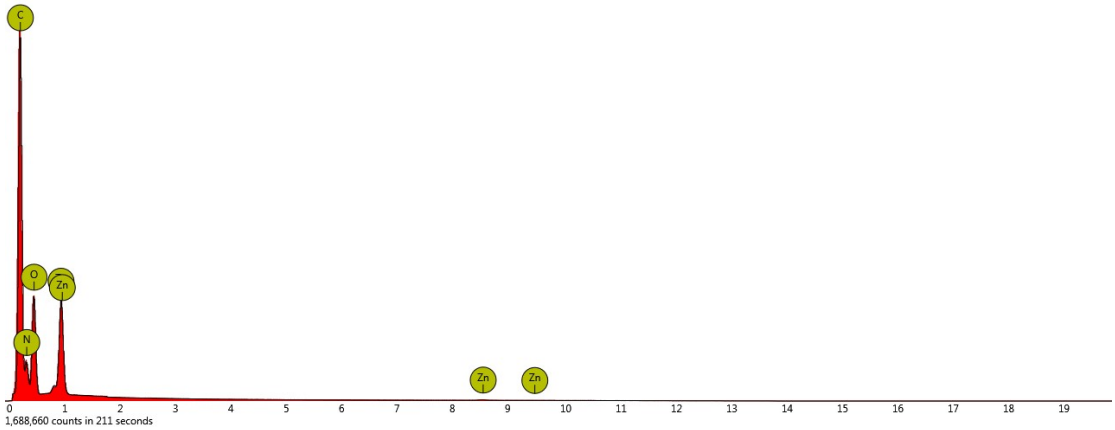

Fig. S14 EDX spectrum of MOF **7**.

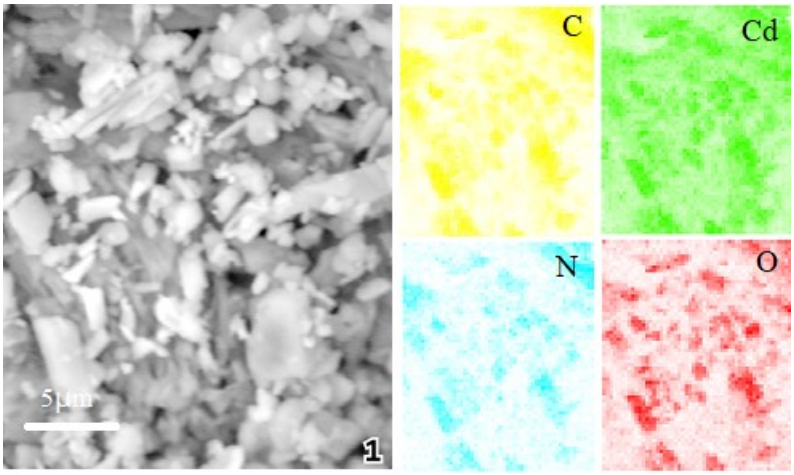

Fig. S15 EDS mapping images of MOF **8**.

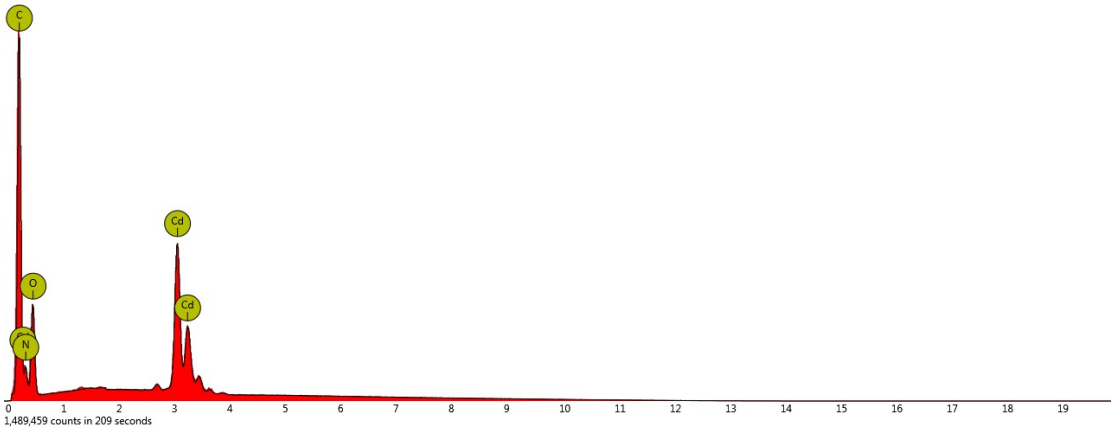

Fig. S16 EDX spectrum of MOF **8**.

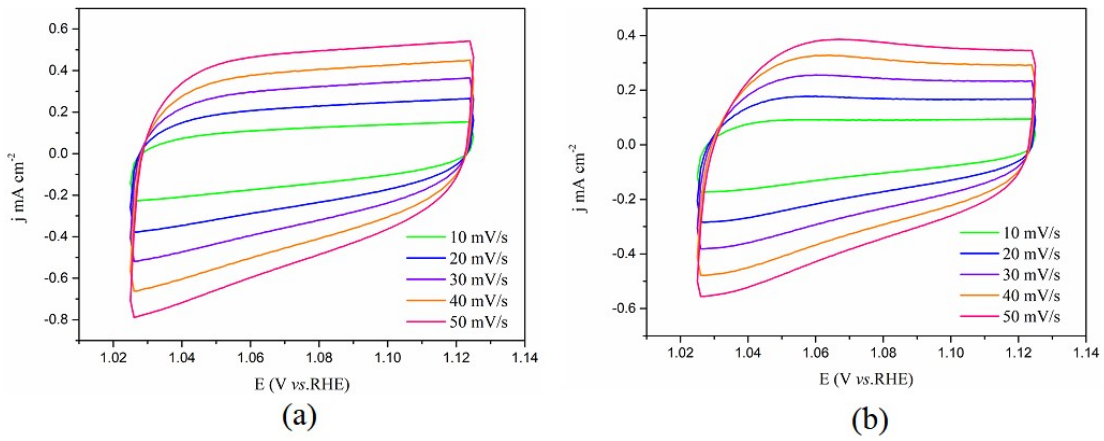

Fig. S17 Cyclic voltammetry (CV) curve in a non-Faraday region (a) Corresponds to MOF **4**. (b)

Corresponds to MOF **5**

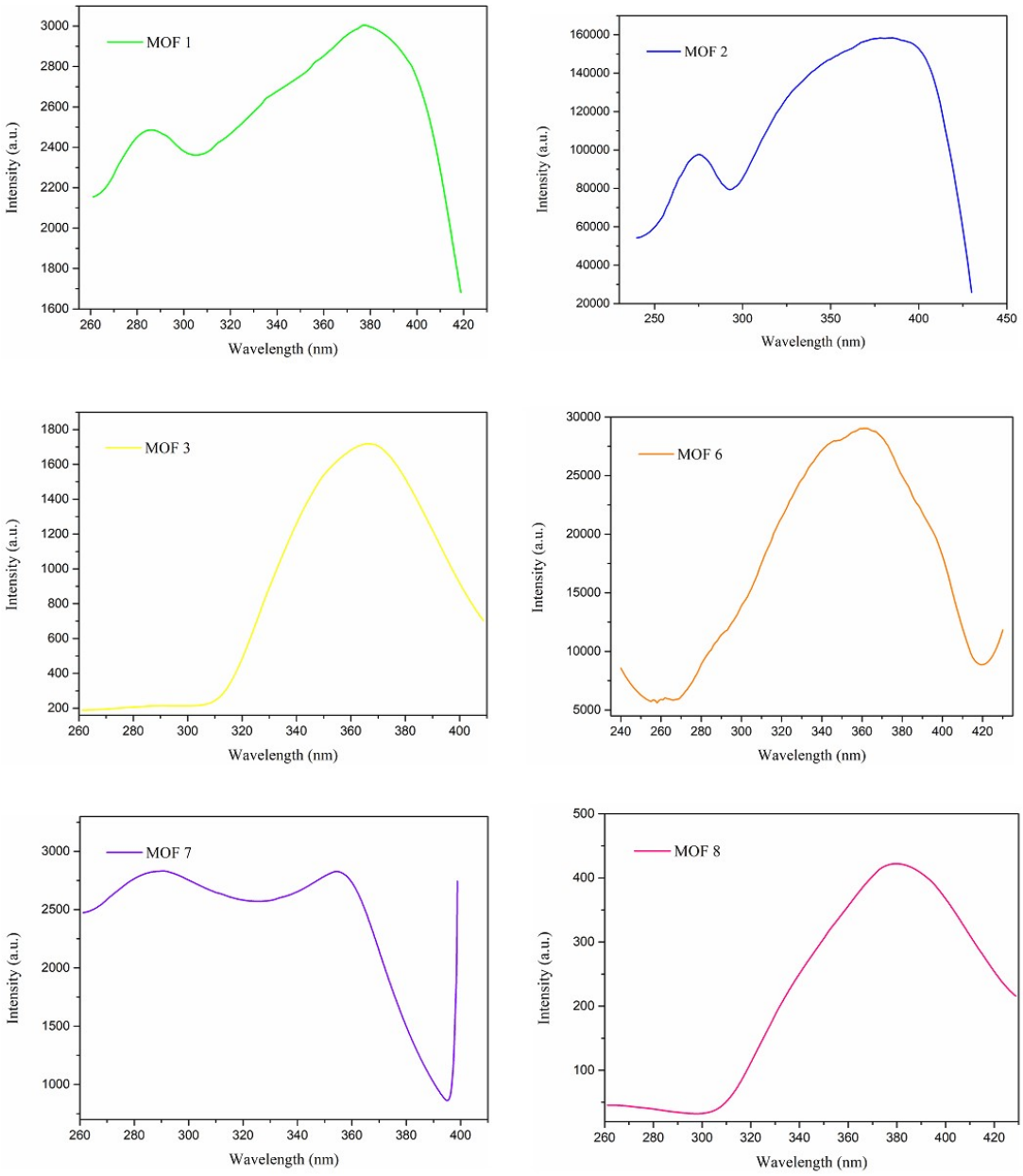

Fig. S18 Solid-state excitation spectra of Cd-based and Zn-based MOF.

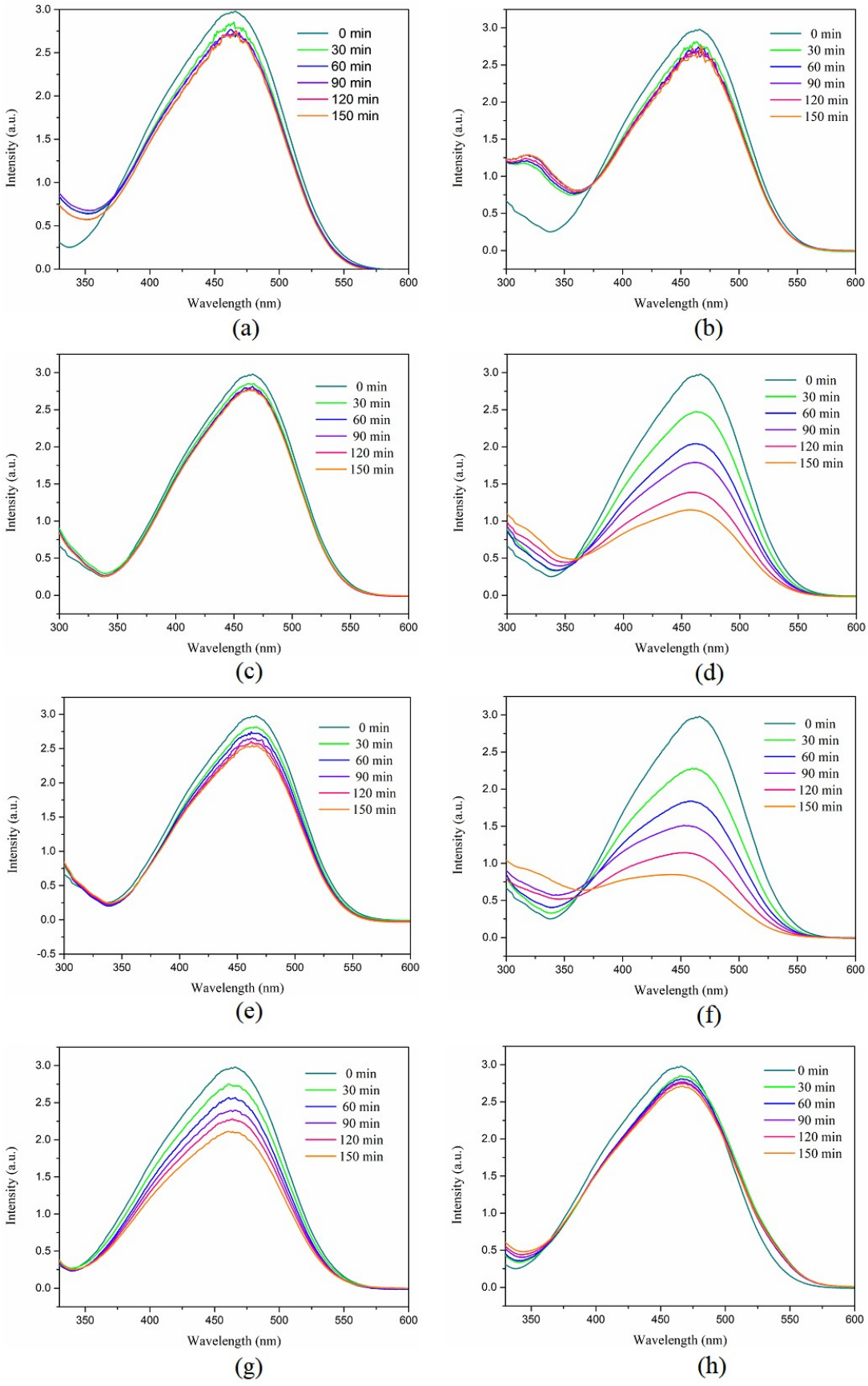

Fig. S19 Time-dependent UV-Vis absorption spectra of the MO solution with MOF as catalyst.

(a-h) correspond to MOF **1-8.**

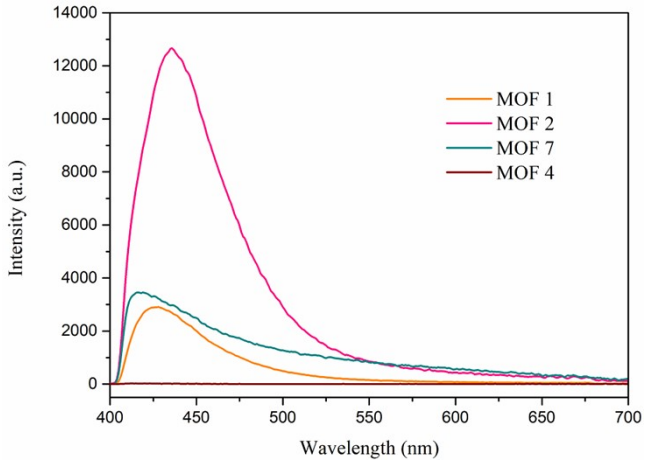

Fig. S20 Solid-state emission spectrum of 10 mg **1**, **2** and **7** excited by 360 nm light source.

The corresponding parameters of crystallographic data, selected bonds, angles and hydrogen bonds

Table S1 Crystallographic Data and Structural Refinements for MOF **1**-**8**

Identification code	MOF **1**	MOF **2**	MOF **3**	MOF**4**
Empirical formula	$C_{22}H_{19}CdN_5O_4$	$C_{33}H_{31}N_7O_9Zn_2$	$C_{22}H_{20}CdN_4O_5$	$C_{31}H_{36}Co_2N_4O_{14}$
Formula weight	529.82	800.39	532.82	806.50
Temperature/K	296.15	296.15	296.15	296.15
Wavelength	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	C2/c	$P2_1/m$	$P2_1/c$	C2/c
Unit cell dimensions	a=1.43795(11) nm, α= 90 º b=2.0139(15) nm, β=115.4160(10) º c=0.86813(7)nm , γ=90 º	a=0.89817(12) nm, α= 90 º b=2.1696(3) nm, β=114.994(2) º c=1.00342(14) nm, γ=90 º	a=0.59643(4) nm, α= 90 º b=2.16185(15) nm, β=90.4440(10) º c=1.63630(14) nm, γ=90 º	a=1.79346(12) nm, α= 90 º b=1.44912(9) nm, β=107.8950(10) º c=2.71194(17) nm, γ=90 º
Volume/nm^3	2.2904(3)	1.7722(4)	2.1098(3)	6.7072(7)
Z	4	2	4	8
Calculate density/g/m^3	1.567	1.500	1.677	1.597
Absorption coefficient/mm^{-1}	0.991	1.416	1.078	1.065
F(000)	1064.0	820.0	1072.0	3328.0
Crystal size/mm^3	0.11 × 0.1 × 0.09	0.11 × 0.1 × 0.08	0.11 × 0.1 × 0.08	0.11 × 0.1 × 0.07
Theta range for data collection	3.137 º to 25.01 º	2.502 º to 25.004 º	1.561 º to 25.007 º	1.844 º to 25.013 º
Index range	-17 ≤ h ≤ 17, -20 ≤ k ≤ 24, -10 ≤ l ≤ 10	-10 ≤ h ≤ 5, -25 ≤ k ≤ 25, -11 ≤ l ≤ 11	-7 ≤ h ≤ 7, -25 ≤ k ≤ 24, -15 ≤ l ≤ 19	-21 ≤ h ≤ 21, -12≤ k ≤ 17, -31 ≤ l ≤ 32
Reflections collected	5775	9071	10595	16918
Independent reflection	2022 [R(int)= 0.0155, R(sigma) = 0.0162]	3204 [R(int) = 0.0254, R(sigma) = 0.0299]	3699 [R(int) = 0.0162, R(sigma) = 0.0174]	5908 [R(int) = 0.0355, R(sigma) = 0.0493]
Completeness to theta	99.8% (25.010 º)	99.9% (25.004 º)	99.8% (25.007 º)	99.9% (25.008 º)
Max. and min.	0.598 and 0.746	0.502 and 0.746	0.587 and 0.746	0.628 and 0.746

transmission				
Goodness-of-fit on F^2	1.123	1.299	1.141	1.064
Final R indices[I>2σ(I)]	R_1= 0.0340, wR_2= 0.1033	R_1 = 0.0619, wR_2 = 0.1311	R_1 = 0.0467, wR_2 = 0.1087	R_1 = 0.0325, wR_2 = 0.0789
R indexes (all data)	R_1= 0.0373, wR_2= 0.1094	R_1 = 0.0726, wR_2 = 0.1352	R_1 = 0.0527, wR_2 = 0.1127	R_1 = 0.0455, wR_2 = 0.0931
Largest diff. peak and hole/e·nm^{-3}	1150 and -370	780 and -450	1260 and -650	340and -320
CCDC number	2183697	2183698	2183700	2183703

Identification code	MOF **5**	MOF **6**	MOF **7**	MOF **8**
Empirical formula	$C_{31}H_{35}N_4Ni_2O_{14}$	$C_{28}H_{28}CdCl_2N_8$	$C_{15}H_{14}N_4O_3Zn$	$C_6H_{12}CdO_{10}$
Formula weight	805.05	659.88	363.67	356.56
Temperature/K	296.15	296.15	296.15	296.15
Wavelength	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	C2/c	P-1	$P2_1/c$	P-1
Unit cell dimensions	a=1.7789(9) nm, α= 90 º b=1.4391(8) nm, β=108.934(10) º c=2.7261(17) nm, γ=90 º	a=0.78796(10) nm, α= 106.732(2) º b=0.88579(11) nm, β=91.035(2) º c=1.10989(13) nm, γ=107.410(2) º	a=1.11555(9) nm, α= 90 º b=8.5094(7) nm, β=103.2480(10) º c=1.79223(15) nm, γ=90 º	a=0.6724(4) nm, α= 62.77 º b=0.9949(6)(11) nm, β=71.873(5) º c=0.9949(6)(13)nm, γ=71.873(5) º
Volume/nm^3	6.601(6)	0.70326(15)	1.6560(2)	0.5511(5)
Z	8	1	4	2
Calculate density/g/m^3	1.620	1.558	1.459	2.149
Absorption coefficient/mm^{-1}	1.218	1.000	1.502	2.026
F(000)	3336.0	334.0	744.0	352.0
Crystal size/mm^3	0.09 × 0.08 × 0.07	0.11 × 0.08 × 0.05	0.11 × 0.1 × 0.09	0.11 × 0.1 × 0.08
Theta range for data collection	0.79 º to 25.009 º	1.929 º to 25.002 º	1.875 º to 25.009 º	2.575 º to 24.998 º
Index range	-19 ≤ h ≤ 21, -17≤ k ≤ 16, -32 ≤ l ≤ 28	-9 ≤ h ≤ 9, -10 ≤ k ≤ 10, -9 ≤ l ≤ 13	-13 ≤ h ≤ 8, -10 ≤ k ≤ 10, -21 ≤ l ≤ 20	-7 ≤ h ≤ 7, -11 ≤ k ≤ 11, -11 ≤ l ≤ 9
Reflections collected	16424	3629	8221	2675
Independent reflection	5800 [R(int) = 0.0808,	2470 [R(int) = 0.0245,	2922 [R(int) = 0.0242,	1897[R(int) = 0.0342,

	R(sigma) = 0.1036]	R(sigma) = 0.0503]	R(sigma) = 0.0285]	R(sigma) = 0.0591]
Completeness to theta	99.4% (25.009 º)	99.5% (25.002º)	100% (25.009 º)	98.4% (24.998º)
Max. and min. transmission	0.417 and 0.746	0.670 and 0.746	0.848 and 0.874	0.451 and 0.746
Goodness-of-fit on F^2	1.003	1.088	1.149	1.097
Final R indices[I>2σ(I)]	R_1 = 0.0747, wR_2 = 0.2008	R_1 = 0.0322, wR_2 = 0.0752	R_1 = 0.0333, wR_2 = 0.1118	R_1 = 0.0449, wR_2 = 0.1130
R indexes (all data)	R_1 = 0.0948, wR_2 = 0.2260	R_1 = 0.0394, wR_2 = 0.0951	R_1 = 0.0466, wR_2 = 0.1268	R_1 = 0.0480, wR_2 = 0.1149
Largest diff. peak and hole/e·nm^{-3}	1270 and -2130	400 and -430	310 and -360	2080 and -2090
CCDC number	2183702	2183699	2183704	2183701

Table S2 Selected Bond lengths (nm) and Angles (°) for MOF **1**

Parameter	Value	Parameter	Value
Cd(1)−O(1)	0.2409(3)	Cd(1)−O(2)#1	0.2340(3)
Cd(1)−O(1)#1	0.2409(3)	Cd(1)−N(1)	0.2269(3)
Cd(1)−O(2)	0.2340(3)	Cd(1)−N(1)#1	0.2269(3)
O(1)−Cd(1)−O(1)	109.24(18)	N(1)#1−Cd(1)−O(1)#1	87.00(12)
O(1)#1−Cd(1)−C(1)	27.30(12)	N(1)−Cd(1)−O(1)	87.00(12)
O(1)−Cd(1)−C(1)	27.30(12)	N(1)#1−Cd(1)−O(1)	142.38(12)
O(1)−Cd(1)−C(1)	105.19(12)	N(1)−Cd(1)−O(1)#1	142.37(12)
O(1)#1−Cd(1)−C(1)	105.20(12)	N(1)#1−Cd(1)−O(2)#1	121.13(12)
O(2)−Cd(1)−O(1)	54.55(11)	N(1)−Cd(1)−O(2)#1	91.34(12)
O(2)#1−Cd(1)−O(1)#1	54.55(11)	N(1)−Cd(1)−O(2)	121.13(12)
O(2)#1−Cd(1)−O(1)	95.17(11)	N(1)#1−Cd(1)−O(2)	91.34(12)
O(2)−Cd(1)−O(1)#1	95.17(11)	N(1)#1−Cd(1)−(N1)	100.59(17)
O(2)−Cd(1)−O(2)#1	129.95(16)	N(1)#1−Cd(1)−C(1)	116.78(12)
O(2)#1−Cd(1)−C(1)	115.51(12)	N(1)−Cd(1)−C(1)	103.92(12)
O(2)−Cd(1)−C(1)	27.34(11)	N(1)#1−Cd(1)−C(1)#1	103.92(12)
O(2)−Cd(1)−C(1)#1	115.51(12)	N(1)−Cd(1)−C(1)#1	116.78(12)
O(2)#1−Cd(1)−C(1)#1	27.34(11)	C(1)−Cd(1)−C(1)	114.49(16)

Symmetry code: #1 = 1-x, +y, 1/2-z.

Table S3 Selected Bond lengths (nm) and Angles (°) for MOF **2**

Parameter	Value	Parameter	Value
Zn(1)−O(1)#1	0.1960(4)	Zn(1)−N(1)	0.1997(4)
Zn(1)−O(2)	0.1978(3)	O(1)−Zn(1)#1	0.1960(4)
Zn(1)−O(3)	0.1925(4)		

O(1)#1−Zn(1)−O(2)	114.51(18)	O(3)−Zn(1)−O(1)#1	113.79(18)
O(1)#1−Zn(1)−N(1)	103.08(17)	O(3)−Zn(1)−O(2)	101.92(18)
O(2)−Zn(1)−N(1)	98.67(17)	O(3)−Zn(1)−N(1)	124.3(2)

Symmetry code: #1 = 2-x, 1-y, 1-z.

Table S4 Selected Bond lengths (nm) and Angles (°) for MOF **3**

Parameter	Value	Parameter	Value
Cd(1)−O(1)#1	0.2528(4)	Cd(1)−N(1)#2	0.2258(4)
Cd(1)−O(1W)	0.2354(3)	Cd(1)−N(4)	0.2269(5)
Cd(1)−O(2)#1	0.2418(4)	O(1)−Cd(1)#3	0.2527(4)
Cd(1)−O(3)	0.2357(4)	O(2)−Cd(1)#3	0.2418(4)
Cd(1)−O(4)	0.2616(4)	N(2)−Cd(1)#4	0.2258(4)
O(1)#1−Cd(1)−O(4)	88.12(12)	N(1)#2−Cd(1)−O(1W)	89.89(15)
O(1W)−Cd(1)−O(1)#1	137.70(12)	N(1)#2−Cd(1)−O(2)#1	86.23(16)
O(1W)−Cd(1)−O(2)#1	85.04(13)	N(1)#2−Cd(1)−O(3)	97.63(15)
O(1W)−Cd(1)−O(3)	82.07(13)	N(1)#2−Cd(1)−O(4)	93.62(14)
O(1W)−Cd(1)−O(4)	134.12(12)	N(1)#2−Cd(1)−N(4)	176.79(19)
O(2)#1−Cd(1)−O(1)#1	52.85(12)	N(4)−Cd(1)−O(1)#1	94.60(17)
O(2)#1−Cd(1)−O(4)	140.83(12)	N(4)−Cd(1)−O(1W)	89.08(16)
O(3)−Cd(1)−O(1)#1	140.22(13)	N(4)−Cd(1)−O(2)#1	90.65(19)
O(3)−Cd(1)−O(2)#1	166.53(13)	N(4)−Cd(1)−O(3)	85.24(18)
O(3)−Cd(1)−O(4)	52.11(12)	N(4)−Cd(1)−O(4)	89.28(18)
N(1)#2−Cd(1)−O(1)#1	84.13(16)		

Symmetry code: #1 = 1-x, -1/2+y, 1/2-z; #2 = 2-x, -1/2+y, 1/2-z; #3=1-x, 1/2+y, 1/2-z; #4 = 2-x, 1/2+Y, 1/2-z.

Table S5 Selected Bond lengths (nm) and Angles (°) for MOF **4**

Parameter	Value	Parameter	Value
Co(1)−O(1W)#1	0.21676(19)	Co(2)−O(2W)	0.2080(2)
Co(1)−O(2)#1	0.21267(18)	Co(2)−O(4)#3	0.20946(19)
Co(1)−O(3)#1	0.20294(19)	Co(2)−O(6)	0.21503(19)
Co(1)−O(5W)	0.2079(2)	Co(2)−N(4)	0.2105(2)
Co(1)−O(8)	0.21325(18)	O(1W)−Co(1)#3	0.21675(19)
Co(1)−N(1)#2	0.2111(2)	O(2)−Co(1)#3	0.21267(18)
Co(2)−O(1)	0.20365(19)	O(4)−Co(1)#1	0.20947(19)
Co(2)−O(1W)	0.21592(19)	N(4)−Co(1)#4	0.2111(2)
O(2)#1−Co(1)−O(1W)#1	91.97(7)	O(1)−Co(2)−O(1W)	90.82(8)
O(2)#1−Co(1)−O(8)	177.93(7)	O(1)−Co(2)−O(2W)	176.92(9)
O(3)−Co(1)−O(1W)#1	90.96(7)	O(1)−Co(2)−O(4)#3	93.05(8)
O(3)−Co(1)−O(2)#1	91.50(8)	O(1)−Co(2)−O(6)	86.85(8)
O(3)−Co(1)−O(5W)	178.43(9)	O(1)−Co(2)−N(4)	88.68(8)
O(3)−Co(1)−O(8)	89.57(8)	O(2W)−Co(2)−O(1W)	89.41(9)
O(3)−Co(1)−N(1)#2	88.76(8)	O(2W)−Co(2)−O(4)#3	83.88(8)

O(5W)−Co(1)−O(1W)#1	87.77(8)	O(2W)−Co(2)−O(6)	96.22(8)
O(5W)−Co(1)−O(2)#1	89.46(8)	O(2W)−Co(2)−N(4)	91.32(9)
O(5W)−Co(1)−O(8)	89.52(8)	O(4)#3−Co(2)−O(1W)	93.14(8)
O(5W)−Co(1)−N(1)#2	92.50(9)	O(4)#3−Co(2)−O(6)	178.57(8)
O(8)−Co(1)−O(1W)#1	89.79(7)	O(4)#3−Co(2)−N(4)	91.08(8)
N(1)#2−Co(1)−O(1W)#1	178.99(8)	O(6)−Co(2)−O(1W)	88.29(7)
N(1)#2−Co(1)−O(2)#1	89.01(8)	N(4)−Co(2)−O(1W)	175.77(8)
N(1)#2−Co(1)−O(8)	89.24(8)	N(4)−Co(2)−O(6)	87.49(8)

Symmetry code: #1 = 1/2-x, -1/2+y, 1/2-z; #2 = 3/2-x, -1/2+y, 1/2-z; #3 = 1/2-x, 1/2+y, 1/2-z; #4 = 3/2-x, 1/2+Y, 1/2-z.

Table S6 Selected Bond lengths (nm) and Angles (°) for MOF **5**

Parameter	Value	Parameter	Value
Ni(1)−O(1W)	0.2042(5)	Ni(2)−O(2W)	0.2100(4)
Ni(1)−O(4)	0.2007(5)	Ni(2)−O(3)	0.2078(4)
Ni(1)−O(6)#1	0.2056(5)	Ni(2)−O(5)#1	0.2012(4)
Ni(1)−O(8)	0.2102(5)	Ni(2)−O(9)	0.2069(5)
Ni(1)−O(9)	0.2152(4)	Ni(2)−N(3)	0.2027(6)
Ni(1)−N(2)	0.2077(5)	O(5)−Ni(2)#2	0.2012(4)
Ni(2)−O(1)	0.2112(4)	O(6)−Ni(1)#1	0.2057(5)
O(1W)−Ni(1)−O(6)#1	84.1(2)	O(2W)−Ni(2)−O(1)	87.79(17)
O(1W)−Ni(1)−O(8)	97.0(2)	O(3)−Ni(2)−O(1)	177.34(15)
O(1W)−Ni(1)−O(9)	89.03(18)	O(3)−Ni(2)−O(2W)	90.39(17)
O(1W)−Ni(1)−N(2)	91.5(2)	O(5)#1−Ni(2)−O(1)	90.04(18)
O(4)−Ni(1)−O(1W)	176.0(2)	O(5)#1−Ni(2)−O(2W)	177.0(2)
O(4)−Ni(1)−O(6)#1	92.0(2)	O(5)#1−Ni(2)−O(3)	91.85(18)
O(4)−Ni(1)−O(8)	86.9(2)	O(5)#1−Ni(2)−O(9)	90.70(18)
O(4)−Ni(1)−O(9)	91.82(17)	O(5)#1−Ni(2)−N(3)	88.6(2)
O(4)−Ni(1)−N(2)	87.9(2)	O(9)−Ni(2)−O(1)	90.40(17)
O(6)#1−Ni(1)−O(8)	177.25(17)	O(9)−Ni(2)−O(2W)	87.29(19)
O(6)#1−Ni(1)−O(9)	93.70(16)	O(9)−Ni(2)−O(3)	91.45(17)
O(6)#1−Ni(1)−N(2)	89.88(19)	N(3)−Ni(2)−O(1)	88.3(2)
O(8)−Ni(1)−Ni(1)−O(9)	88.85(16)	N(3)−Ni(2)−O(2W)	93.4(2)
Ni(2)−Ni(1)−O(9)	87.57(19)	N(3)−Ni(2)−O(3)	89.8(2)
Ni(2)−Ni(1)−O(8)	176.42(19)	N(3)−Ni(2)−O(9)	178.53(19)

Symmetry code: #1 = 1/2-x, 1/2+y, 1/2-z; #2 = 1/2-x, -1/2+y, 1/2-z.

Table S7 Selected Bond lengths (nm) and Angles (°) for MOF **6**

Parameter	Value	Parameter	Value
Cd(1)−Cl(1)#1	0.26499(10)	Cd(1)−N(4)#2	0.2374(3)
Cd(1)−Cl(1)	0.26499(10)	Cd(1)−N(4)#3	0.2374(3)
Cd(1)−N(1)	0.2354(3)	N(4)−Cl(1)#4	0.2374(3)
Cd(1)−N(1)#1	0.2354(3)		

Cl(1)−Cd(1)−Cl(1)#1	180.0	N(1)−Cd(1)−N(4)#2	91.61(11)
N(1)#1−Cd(1)−Cl(1)#1	91.90(8)	N(1)#1−Cd(1)−N(4)#3	91.61(11)
N(1)−Cd(1)−Cl(1)	91.90(8)	N(4)#3−Cd(1)−Cl(1)#1	86.73(8)
N(1)−Cd(1)−Cl(1)#1	88.10(8)	N(4)#2−Cd(1)−Cl(1)	86.73(8)
N(1)#1−Cd(1)−Cl(1)	88.10(8)	N(4)#2−Cd(1)−Cl(1)#1	93.27(8)
N(1)−Cd(1)−N(1)#1	180.00(15)	N(4)#3−Cd(1)−Cl(1)	93.27(8)
N(1)#1−Cd(1)−N(4)#2	88.39(11)	N(4)#2−Cd(1)−N(4)#3	180.0
N(1)−Cd(1)−N(4)#3	88.39(11)		

Symmetry code: #1 = 1-x, 1-y, 2-z; #2 = 1-x, 1-y, 1-z; #3 = +x,+y, 1+z; #4 = +x, +y, -1+z.

Table S8 Selected Bond lengths (nm) and Angles (°) for MOF **7**

Parameter	Value	Parameter	Value
Zn(1)−O(3)	0.1964(2)	Zn(1)−N(4)#2	0.2004(3)
Zn(1)−O(2)#1	0.1975(3)	O(2)−Zn(1)#3	0.1975(3)
Zn(1)−N(1)	0.1999(3)	N(4)−Zn(1)#4	0.2004(3)
O(3)−Zn(1)−O(2)#1	101.59(10)	O(2)#1−Zn(1)−N(1)#1	112.59(11)
O(3)−Zn(1)−O(1)	108.67(11)	O(2)#1−Zn(1)−N(4)#2	110.22(12)
O(3)−Zn(1)−N(4)#2	101.34(10)	N(1)−Zn(1)−N(4)#2	120.13(12)

Symmetry code: #1 = 2-x, -1/2+y, 3/2-z; #2 = 1+x, 1/2-y, 1/2+z; #3 = 2-x, 1/2+y, 3/2-z; #4 = -1+x, 1/2-y, -1/2+z.

TableS9 Selected Bond lengths (nm) and Angles (°) for MOF **8**

Parameter	Value	Parameter	Value
Cd(1)−O(2)	0.2273(4)	Cd(1)−O(4)#1	0.2382(4)
Cd(1)−O(1W)	0.2285(4)	Cd(1)−O(2W)	0.2321(4)
Cd(1)−O(3W)	0.2277(5)	O(5)−Cd(1)#1	0.2421(4)
Cd(1)−O(1)	0.2585(4)	O(4)−Cd(1)#1	0.2382(4)
Cd(1)−O(5)#1	0.2421(4)		
O(2)−Cd(1)−O(1W)	89.25(14)	O(3W)−Cd(1)−O(1)	84.85(15)
O(2)−Cd(1)−O(3W)	89.13(15)	O(3W)−Cd(1)−O(5)#1	97.45(15)
O(2)−Cd(1)−O(1)	53.32(13)	O(3W)−Cd(1)−O(4)#1	92.05(16)
O(2)−Cd(1)−O(5)#1	83.90(13)	O(3W)−Cd(1)−O(2W)	95.23(15)
O(2)−Cd(1)−O(4)#1	138.12(14)	O(5)#1−Cd(1)−O(1)	137.18(12)
O(2)−Cd(1)−O(2W)	135.27(14)	O(4)#1−Cd(1)−O(1)	168.25(13)
O(1W)−Cd(1)−O(1)	90.66(15)	O(4)#1−Cd(1)−O(5)#1	54.44(13)
O(1W)−Cd(1)−O(5)#1	86.76(15)	O(2W)−Cd(1)−O(1)	82.70(14)
O(1W)−Cd(1)−O(4)#1	92.10(16)	O(2W)−Cd(1)−O(5)#1	138.95(15)
O(1W)−Cd(1)−O(2W)	82.84(15)	O(2W)−Cd(1)−O(4)#1	86.30(15)
O(3W)−Cd(1)−O(1W)	175.31(14)		

Symmetry code: #1 = 1+x, 1+y, +z.

Table S10 Hydrogen-bonding Geometry of MOF **1** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
C5-H5···N3#1	0.0931(4)	0.2961(10)	0.3616(11)	153.3(4)
C12-H12···O1#2	0.0930(4)	0.2714(8)	0.3422(14)	133.6(4)
N3-H3B···O2#3	0.0866(9)	0.2536(3)	0.3240(9)	139.1(7)

Symmetry code: #1 = +x, +y, -1/2z; #2 = 1/2-x, 3/2-y, -z; #3 = -1/2+x, -1/2-y, 1/2+z.

Table S11 Hydrogen-bonding Geometry of MOF **2** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
C6-H6···N4#1	0.0930(7)	0.272(4)	0.364(4)	175.3(7)
N3-H3A···O4#2	0.0859(13)	0.2017(8)	0.2772(16)	146.0(9)
C8-H8A···O4#3	0.0970(8)	0.2778(6)	0.3629(10)	146.8(4)
N4-H4B···O3	0.0860(3)	0.2002(5)	0.2590(3)	125.0(2)
C7-H7···N3	0.0930(6)	0.2769(4)	0.3565(6)	144.2(3)
N3-H3B···O1	0.0860(9)	0.1907(4)	0.2558(12)	131.4(10)
C18-H18···O2	0.0960(3)	0.27893)	0.365(3)	112.9(14)

Symmetry code: #1 = 1-x, 1-y, 1-z; #2 = +x, +y, -1+z; #3 = 2-x, 1-y, 2-z.

Table S12 Hydrogen-bonding Geometry of MOF **3** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
O1W-	0.0879(4)	0.1972(4)	0.2790(5)	154.4(4)
O1W-H1WB···O1#2	0.0878(4)	0.1925(4)	0.2764(5)	158.5(3)
C12-H12B···O3#3	0.0969(8)	0.2605(3)	0.3567(9)	171.9(5)
C19-H12A···O2#4	0.0970(8)	0.2632(5)	0.3555(9)	159.0(6)

Symmetry code: #1 = 1+x, +y, +z; #2 = 2-x, -1/2+y, 1/2-z; #3 = +x, 3/2-y, 1/2+z; #4 = 1+x, 3/2-y, 1/2+z.

Table S13 Hydrogen-bonding Geometry of MOF **4** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
O1W-H1WA···O5	0.088(3)	0.184(3)	0.2693(3)	163(3)
O1W-H1WB···O7#1	0.086(3)	0.175(2)	0.2602(3)	171(3)
O2W-H1WA···O3W	0.085(2)	0.191(2)	0.2757(4)	175(4)
O2W-H1WB···O7#2	0.0865(3)	0.185(3)	0.2687(3)	167(4)
O3W-	0.0890(5)	0.2070(6)	0.2918(3)	159(5)
O3W-H3WB···O7#1	0.0880(5)	0.2080(5)	0.2905(4)	156(4)
O4W-H1W···O9#2	0.088(4)	0.215(5)	0.3008(4)	166(6)
O4W-H1WB···O3W	0.088(7)	0.202(7)	0.2888(6)	169(5)
O5W-H1WA···O9	0.085(2)	0.198(2)	0.2817(3)	171(3)
O5W-H1WB···O5#4	0.085(3)	0.196(3)	0.2772(3)	160(3)
O9-H9···O2#3	0.0820(3)	0.1978(2)	0.2793(4)	171.9(2)

C3-H3···O4W	0.0930(3)	0.2578(3)	0.3503(4)	172.8(2)
C12-H12···O4W#5	0.0930(3)	0.2545(3)	0.3440(4)	161.7(2)

Symmetry code: #1 = 1/2-x, 1/2+y, 1/2-z; #2 = 1/2-x, 3/2+y, 1/2-z; #3 = 1-x, 2-y, 1-z; #4 = +x, 1-y, -1/2+z; #5 = -1/2x, 1/2+y, -+z.

Table S14 Hydrogen-bonding Geometry of MOF **5** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
O1W-H1WA···O4W	0.0854(5)	0.1915(6)	0.2751(8)	165.5(4)
O2W-H2WA···O10#1	0.0960(5)	0.2027(9)	0.2771(10)	132.8(3)
O2W-H2WB···O7#1	0.0961(5)	0.2031(4)	0.2792(5)	134.7(3)
O3W-	0.0850(7)	0.2169(6)	0.2889(8)	142.2(6)
O3W-H1WB···O10	0.0849(9)	0.2101(9)	0.2933(13)	166.7(5)
O4W-H4WA···O2	0.0850(6)	0.2319(5)	0.2935(7)	129.6(5)
O4W-H4WA···O7	0.0849(7)	0.2095(5)	0.2884(9)	154.3(5)
O9-H9···O7	0.086(3)	0.183(2)	0.2669(7)	164(3)
O10-H10···O3	0.0821(7)	0.2051(4)	0.2829(7)	158.2(6)
C7-H7···O3W	0.0931(6)	0.2668(6)	0.3466(9)	144.1(14)
C9-H9···O3W	0.0930(7)	0.2508(7)	0.3406(10)	162.1(4)
C24-H24···O3W#4	0.0930(7)	0.2521(7)	0.3447(10)	173.5(4)

Symmetry code: #1 = - x, 1-y, -z; #2 = -1/2+x, -1/2+y, +z; #3 = 1/2-x, 3/2-y, -z; #4 = 1/2+x, 3/2+y, +z.

Table S15 Hydrogen-bonding Geometry of MOF **6** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
C3-H3···Cl1#1	0.0930(4)	0.2855(11)	0.3683(5)	148.9(3)
C4-H4B···Cl1#1	0.0970(5)	0.2894(10)	0.3800(4)	156.0(3)
C11-H11B···Cl1#2	0.0970(4)	0.2487(11)	0.3640(4)	157.5(3)
C11-H11A···Cl1#3	0.0970(5)	0.2855(12)	0.3792(5)	162.6(3)
C11-H11A···Cl1#4	0.0930(4)	0.2837(12)	0.3430(5)	122.7(3)

Symmetry code: #1 = 1+x, +y, +z; #2 = 1-x, -y, 1-z; #3 = -1/2+x, -1/2-y, 1/2+z; #4 = 1-x, 1-y, 1-z.

Table S16 Hydrogen-bonding Geometry of MOF **7** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A
C3-H3···O2#1	0.0930(32)	0.2346(25)	0.3204(41)	153.1(218)
C10-H10···O1#2	0.0930(37)	0.2603(31)	0.3458(47)	152.9(221)
C12-H12···O1#3	0.0930(37)	0.2580(31)	0.3412(47)	149.2(231)

Symmetry code: #1 = +x, -1+y, +z; #2 = 1-x, -1/2+y, 3/2-z; #3 = -1/2+x, -1/2-y, 1/2+z.

Table S17 Hydrogen-bonding Geometry of MOF **8** (nm and °)

D-H···A	D-H	H···A	[D···A]	∠D-H···A

O1W-	0.0877(4)	0.1895(4)	0.2711(5)	153.9(3)
O1W-H1WB···O2#2	0.0878(3)	0.1997(5)	0.2813(6)	154.2(3)
O2W-	0.0880(6)	0.2114(6)	0.2944(8)	156.8(3)
O2W-H2WB···O1#4	0.0879(4)	0.1949(4)	0.2804(6)	163.8(3)
O3W-H3WA···O4W	0.0589(4)	0.1985(5)	0.2831(6)	168.2(5)
O3W-H3WB···O5#5	0.0984(5)	0.1817(4)	0.2770(6)	162.1(4)
O4W-H4WA···O1#4	0.0850(8)	0.2264(6)	0.2906(9)	132.4(4)
O5W-H5WA···O4W	0.0850(7)	0.1964(7)	0.2785(10)	162.1(4)
O5W-H5WB···O1#6	0.0850(7)	0.2169(7)	0.2915(10)	146.4(3)
C3-H3···O5W#5	0.0929(7)	0.2657(7)	0.3526(10)	155.9(3)
C4-H4···O3W#5	0.0930(5)	0.2588(5)	0.3344(7)	138.7(4)

Symmetry code: #1 = -1+x, 1+y, +z; #2 = -x, 2-y, 1-z; #3 = -1+x, +y, +z; #4 = 1-x, 2-y, -z; #5 = 1-x, 1-y, 1-z; #6 = +x,-1+y,+z.