Electronic Supplementary Information (ESI)

Two-dimensional Cd_3-based metal–organic frameworks with halogen bonding sites for the uptake of I_2

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Table S1 A list of published I_2 adsorbents and MOF **2** as well as their adsorption capacities.

Materials	Solvent	Time (h)	Capacity (mg g^{-1})	Ref.
MIL-53-NH_2	cyclohexane	48	170	1
MIL-101-NH_2	cyclohexane	48	375	1
CAU-1	cyclohexane	48	300	1
ZIF-67@MCF	cyclohexane	10	1630	2
UiO-66-PYDC	cyclohexane	24	1250	3
Th-SINAP-8	cyclohexane	24	258	4
TMU-16-NH_2	n-hexane	0.5	450	5
ZIF-8	n-hexane	24	900	6
ZIF-A61	n-hexane	24	1140	7
MOF **2**	n-hexane	24	54.1	**This Work**

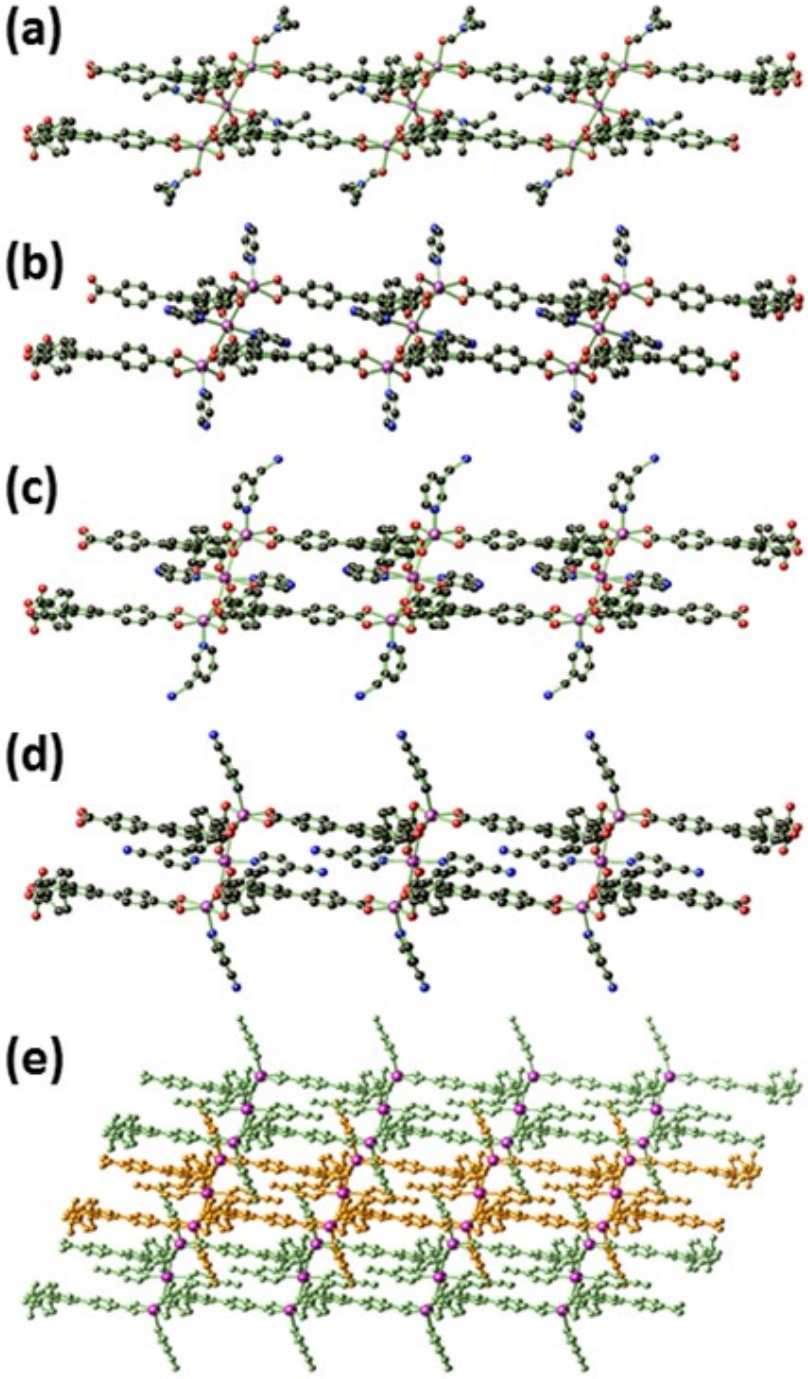


Fig. S1 The 2D structures of MOFs **1** (a), **2** (b), **3** (c), **4** (d), and a view of MOF **4** (e) showing three consecutive layers that highlight the four 4-PyCN ligands (two from adjacent layers and two coordinated from the same Cd^{2+} of the central layer) that are within the same pore of the central layer. All free solvates, disordered domains, and hydrogen atoms are omitted. The colors of the layers are distinguished by bamboo and orange for clarity.

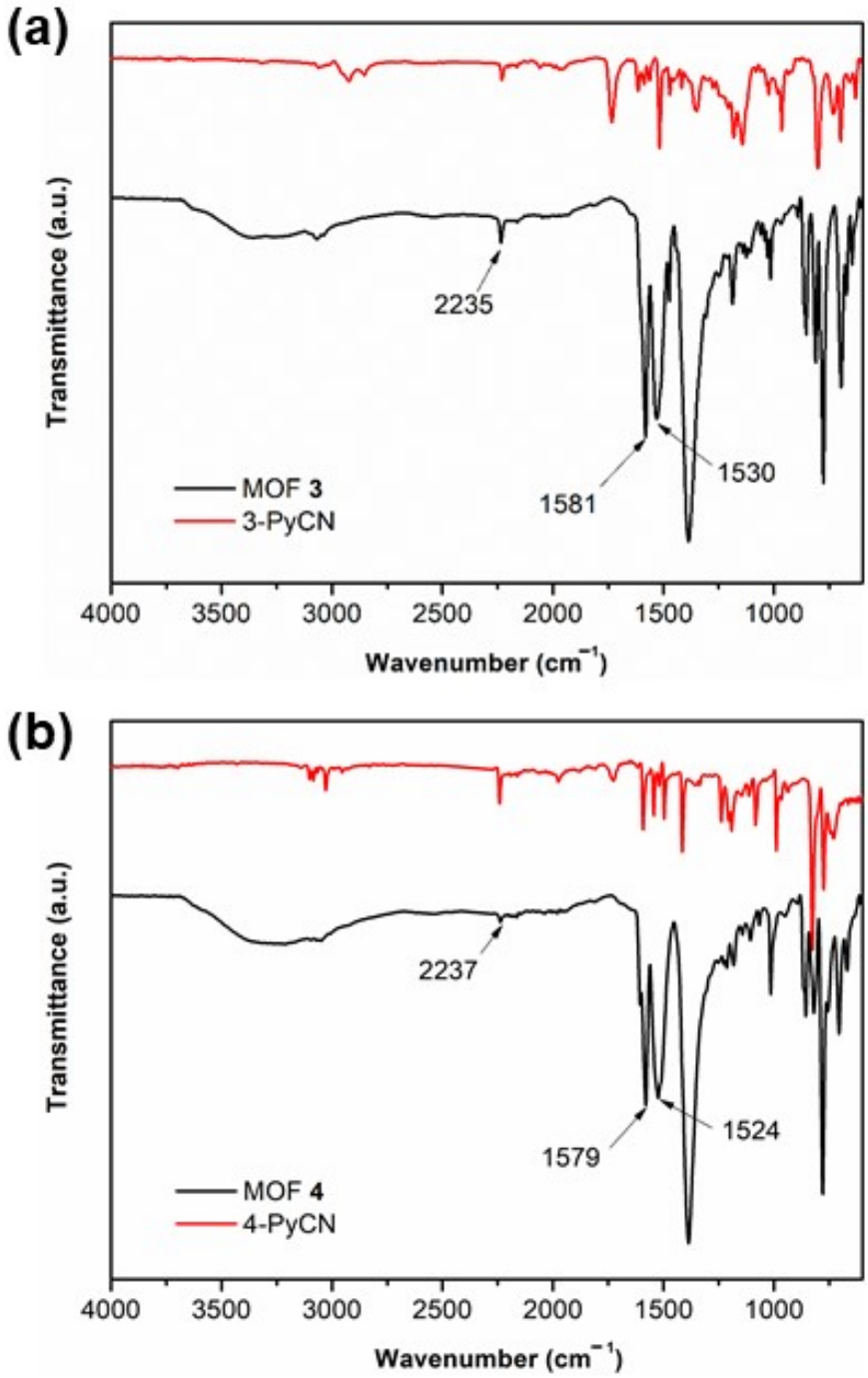
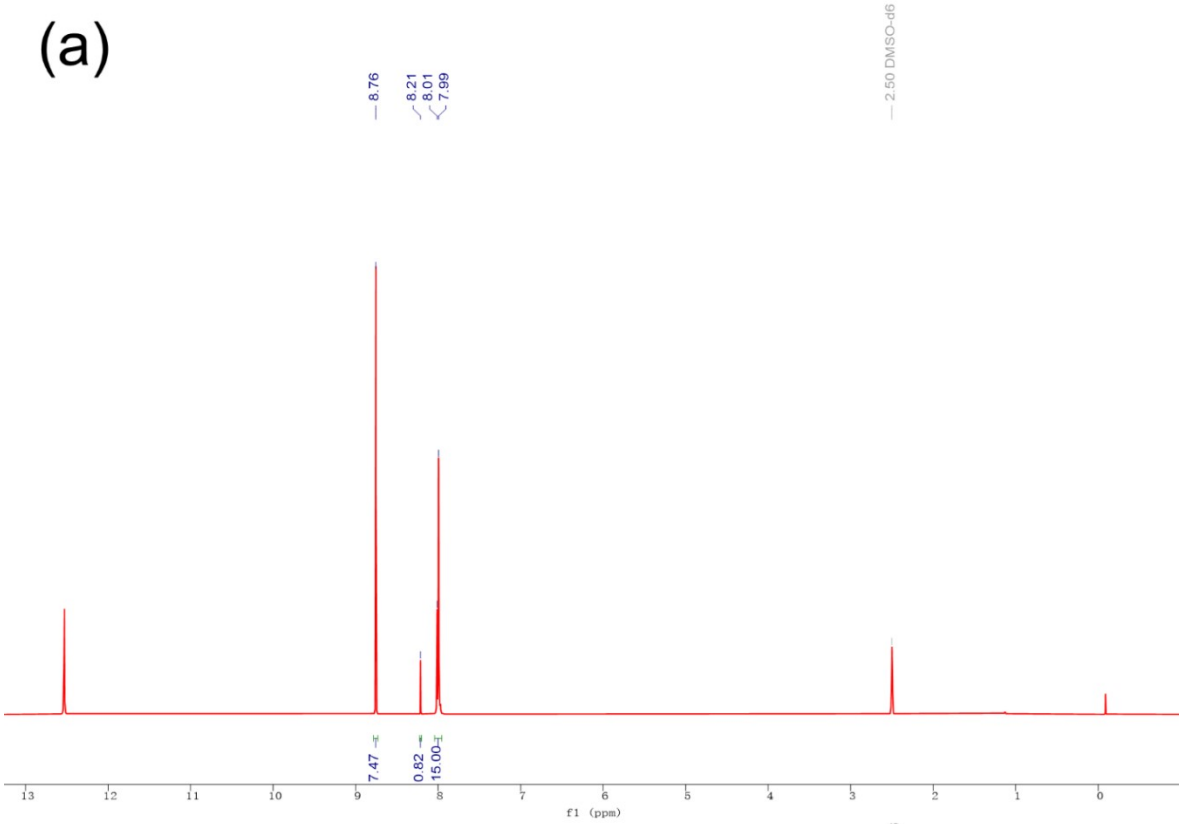
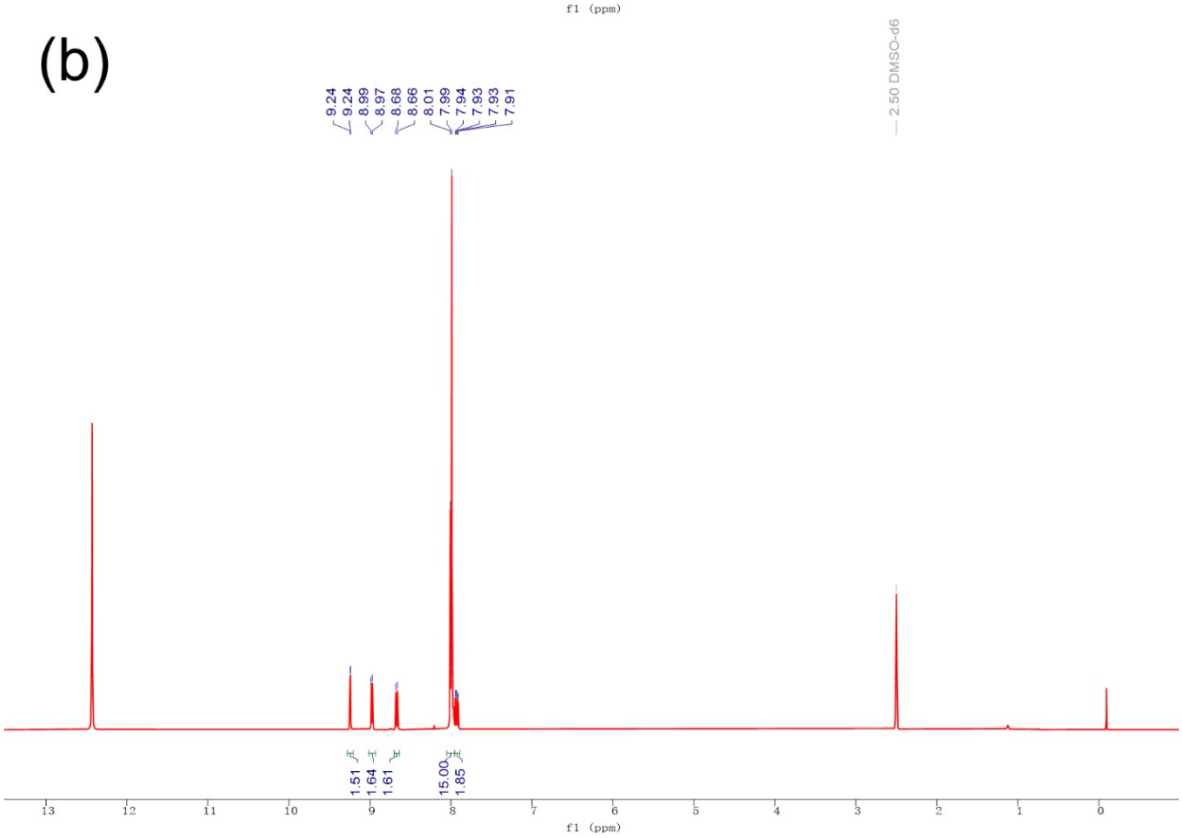


Fig. S2 Fourier-transform infrared (FT-IR) spectra of MOF **3** (a, black), 3-PyCN (a, red), MOF **4** (b, black), and 4-PyCN (b, red).

(a)


8.76
8.21
8.01
7.99
2.50 DMSO-d6
7.47
0.82
15.00
f1 (ppm)

(b)


9.24
9.24
8.99
8.97
8.68
8.66
8.01
7.99
7.94
7.93
7.93
7.91
2.50 DMSO-d6
1.51
1.64
1.61
15.00
1.85
f1 (ppm)

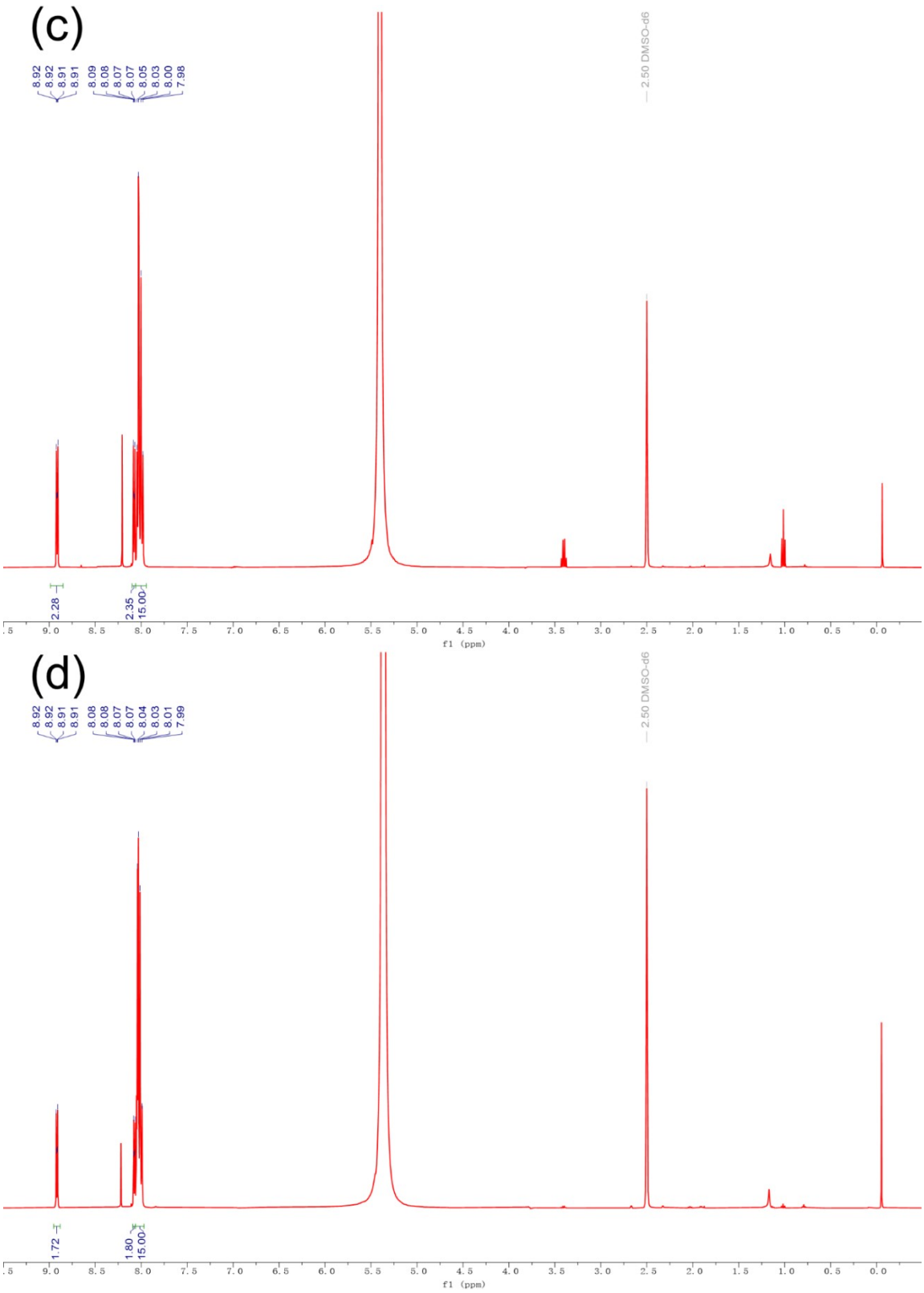


Fig. S3 ^{1}H NMR spectra of MOFs **2** (a), **3** (b), **4**_30min (c), and **4**_120min (d) in DMSO-d_6 + 10% D_2SO_4 mix solvent. MOF **4**_30min and **4**_120min denote MOF **4** immersed into $CHCl_3$ for 30 min and 120 min, respectively.

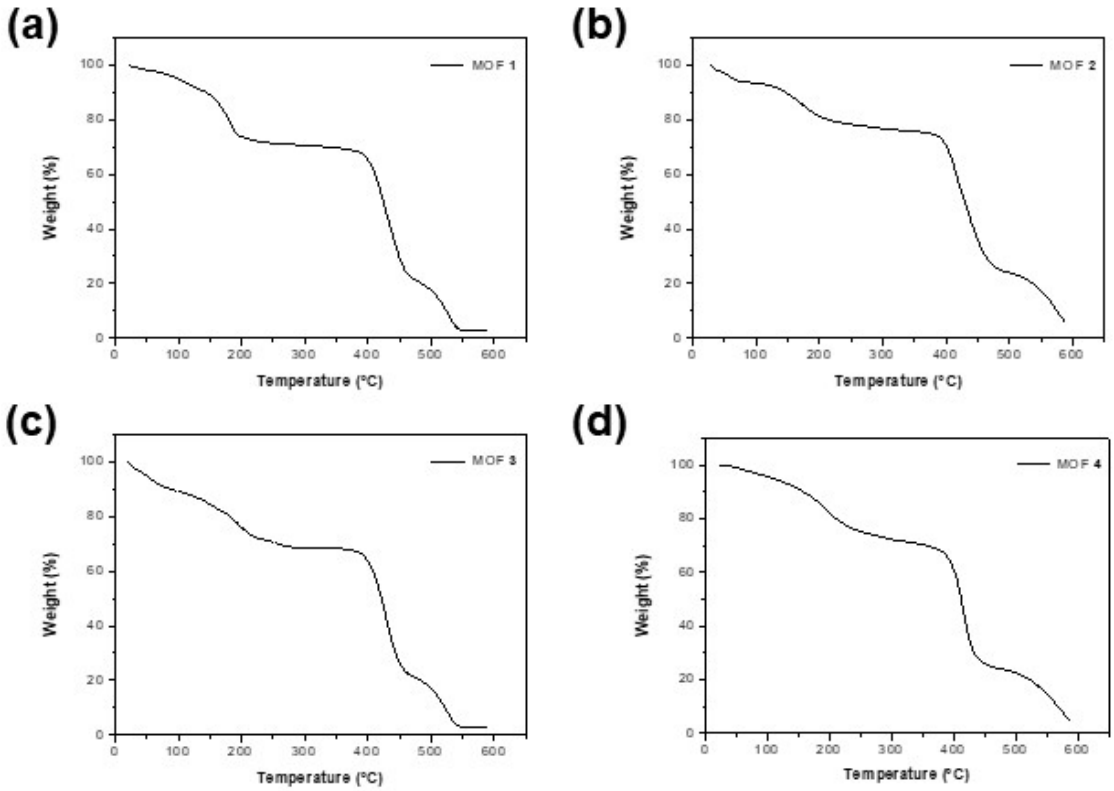


Fig. S4 Thermogravimetric analysis (TGA) curves of MOFs **1** (a), **2** (b), **3** (c), and **4** (d).

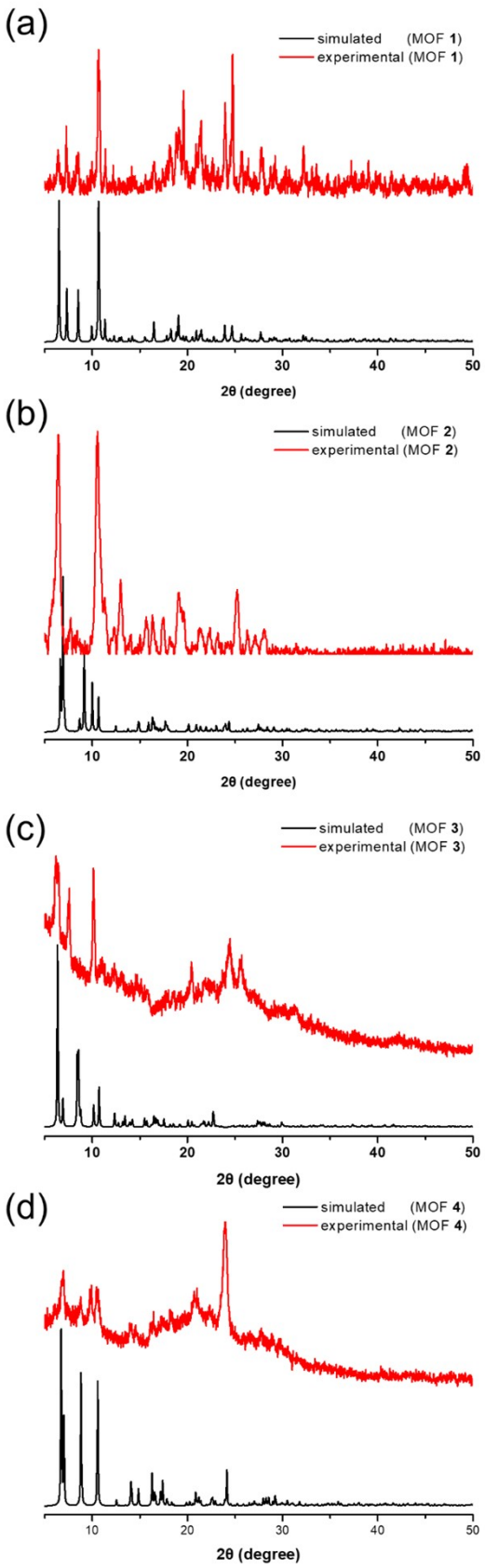


Fig. S5 A comparison of experimental (red) and simulated (black) powder X-ray diffraction (PXRD) patterns of MOFs **1** (a), **2** (b), **3** (c), and **4** (d).

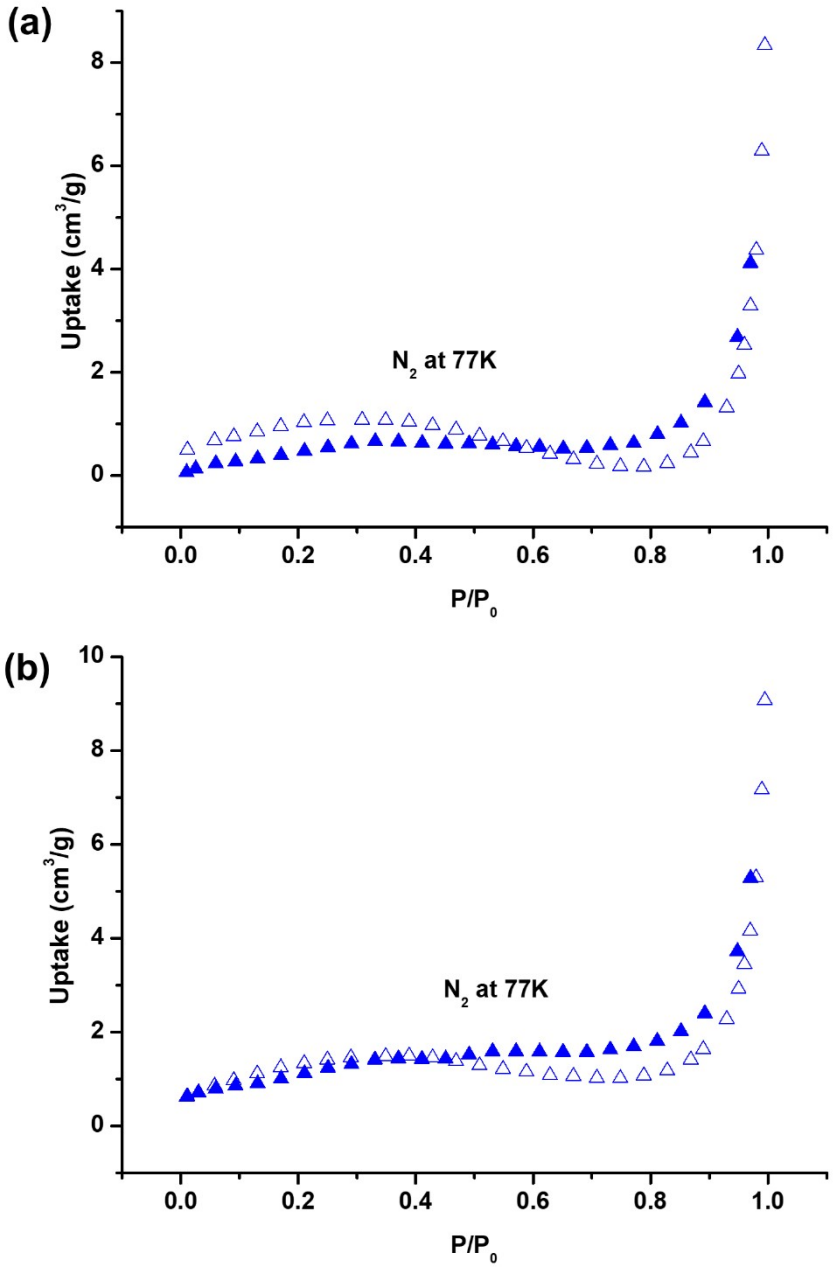


Fig. S6 N_2 (77 K) sorption isotherms of MOFs **3** (a) and **4** (b). The blue solid triangles indicate desorption and the blue hallowed triangles indicate adsorption. P_0 is the saturated vapor pressure of the adsorbates at the measurement temperatures.

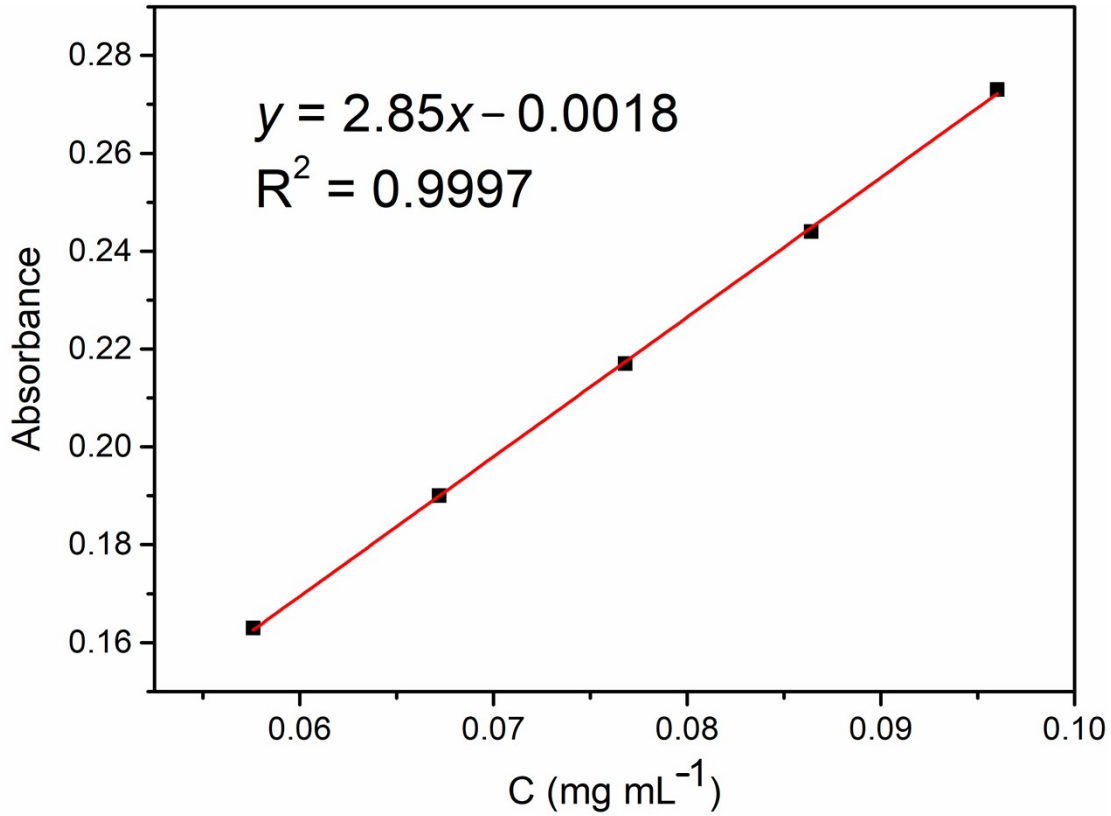


Fig. S7 Standard ultraviolet-visible spectroscopic (UV-Vis) curve of I_2/n-hexane solution.

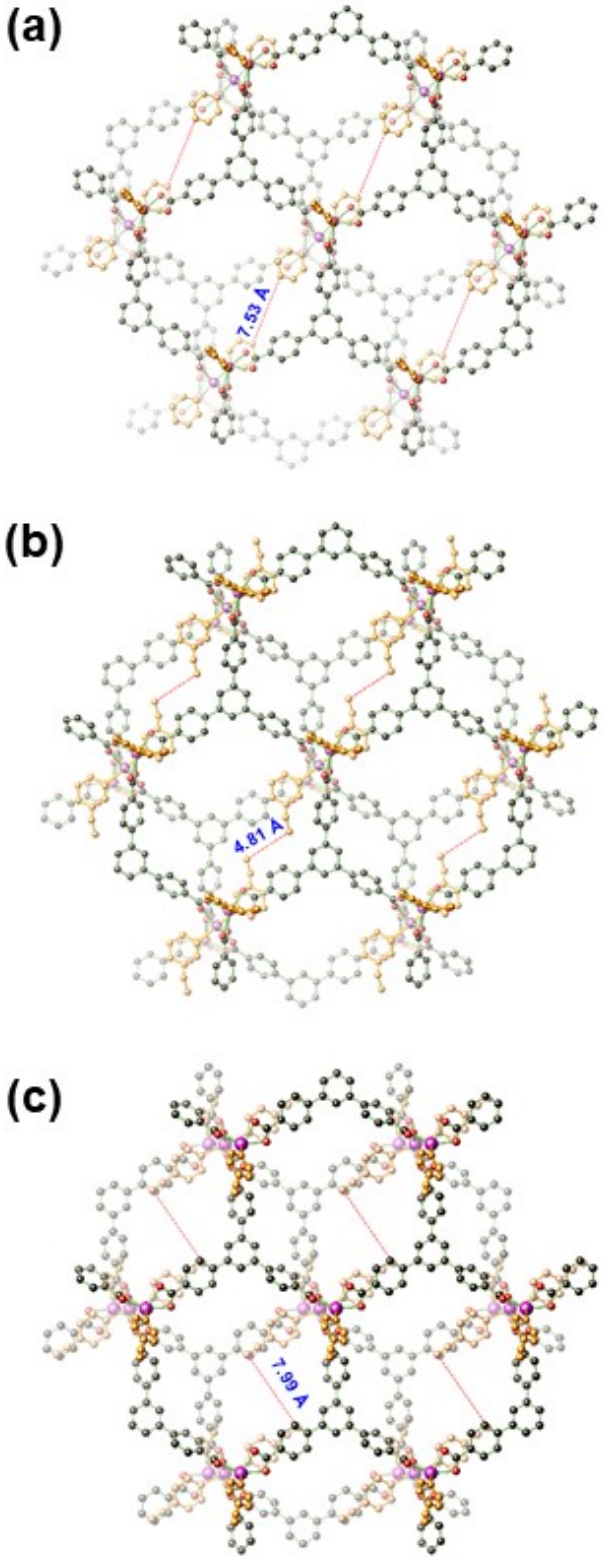


Fig. S8 Structures of MOFs **2** (a), **3** (b), and **4** (c) showing the proximate in-plane N···N separations. All free and coordinated solvates and hydrogen atoms are omitted. Color codes: Cd (dark magenta), O (red), C (black).

References

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