Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Two 3D metal-organic frameworks of Cd(II): Modulation of structures and porous properties based on linker functionalities

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Table S1: Optimized cell parameters of MOF and percentage of error in volume with experimental volume using PBE, PBE-D2 and PBE-D3 methods. α and γ were not optimized as they were 90°.

Method	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	ΔV (%)
Experiment	16.36	16.00	12.10	111.40	2949.31	---
PBE	16.68	16.07	12.11	111.40	3022.66	2.49
PBE-D2	16.10	16.20	11.92	109.60	2929.20	-0.68
PBE-D3	16.16	16.23	11.92	109.60	2945.56	-0.13

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

Cd1-N1	2.282(2)	Cd1-N2	2.376(3)
Cd1-O1_b	2.546(2)	Cd1-O2_b	2.319(3)
Cd1-O3_g	2.314(2)	Cd1-O4_i	2.198(3)
N1-Cd1-N2	93.31(9)	O1_b-Cd1-N1	84.26(9)
O2_b-Cd1-N1	137.26(9)	O3_g-Cd1-N1	91.50(9)
O4_i-Cd1-N1	98.54(9)	O1_b-Cd1-N2	85.47(9)
O2_b-Cd1-N2	88.23(9)	O3_g-Cd1-N2	81.36(9)
O4_i-Cd1-N2	163.70(9)	O1_b-Cd1-O2_b	53.25(8)
O1_b-Cd1-O3_g	165.91(8)	O1_b-Cd1-O4_i	106.74(9)
O2_b-Cd1-O3_g	130.79(8)	O2_b-Cd1-O4_i	90.59(9)
O3_g-Cd1-O4_i	87.16(9)		

Symmetry codes: b = 1-x,-y,1-z; g = 1/2-x,1/2-y,1-z; i = 1/2+x,1/2-y,1/2+z

Table S3. Selected bond lengths (Å) and angles (°) for **2**

Cd1-O1	2.366(9)	Cd1-N1	2.285(10)
Cd1-O1_a	2.366(9)	Cd1-N1_a	2.285(10)
Cd1-O2_j	2.322(9)	Cd1-O2_l	2.322(9)
O1-Cd1-N1	146.9(3)	O1-Cd1-O1_a	55.5(3)
O1-Cd1-N1_a	91.4(3)	O1-Cd1-O2_j	99.84(19)
O1-Cd1-O2_l	99.84(19)	N1-Cd1-C6	119.2(2)
O1_a-Cd1-N1	91.4(3)	N1-Cd1-N1_a	121.7(4)
O2_j-Cd1-N1	84.60(11)	O2_l-Cd1-N1	84.60(11)
O1_a-Cd1-N1_a	146.9(3)	O1_a-Cd1-O2_j	99.84(19)
O1_a-Cd1-O2_l	99.84(19)	O2_j-Cd1-N1_a	84.60(11)
O2_l-Cd1-N1_a	84.60(11)	O2_j-Cd1-O2_l	157.7(3)

Symmetry codes: a = -x,1/2-y,z; j = -1/2+x,1/2-y,1-z

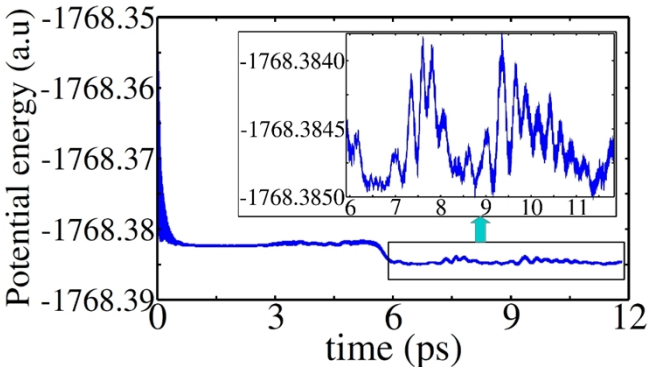

Fig. S1. Potential energy of the MOF with CO_2 molecule as a function of time.

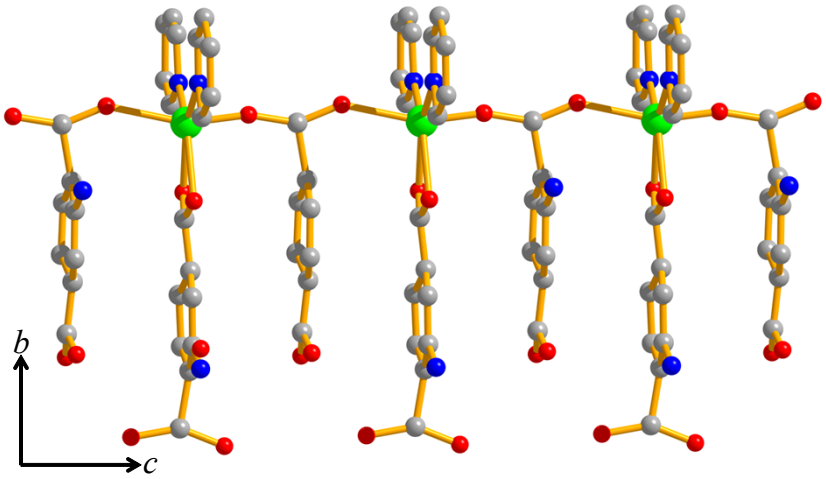

Fig. S2: 1D chain like structure in compound **2**.

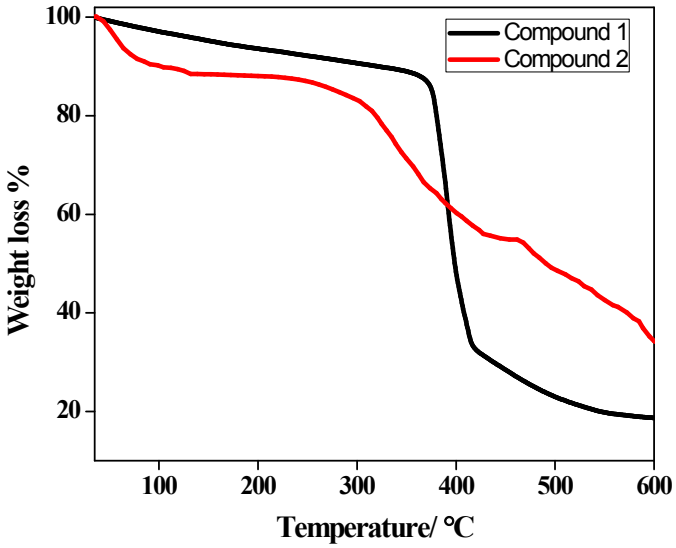

Fig. S3: TGA profiles of compound **1** and **2** in the temperature range 35-600 °C under N_2 atmosphere.

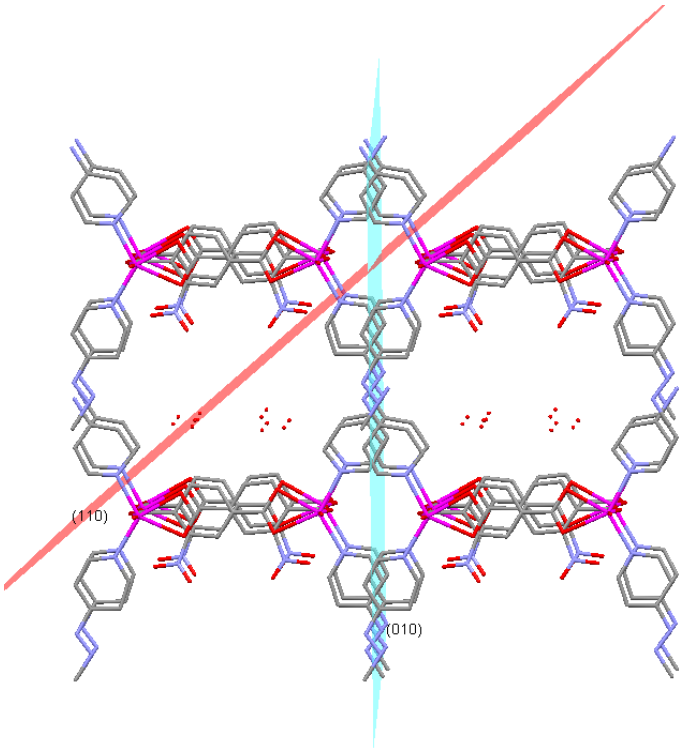

Fig. S4: View of 010 and 110 Braggs' planes in compound **2**.

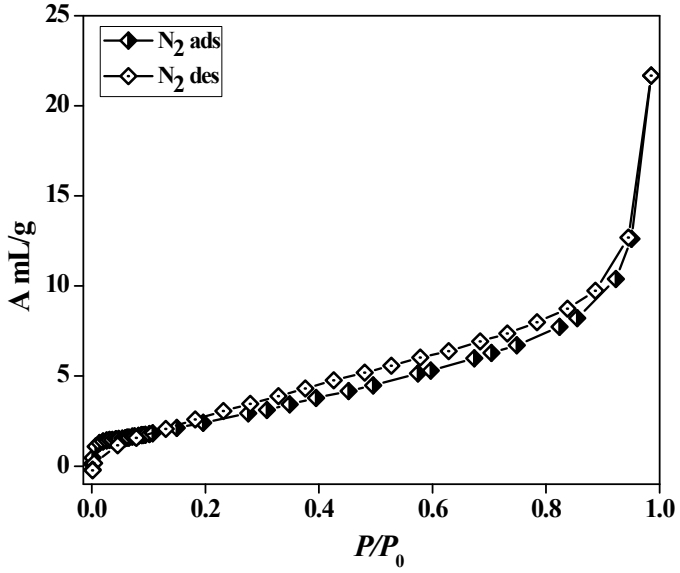

Fig. S5: N_2 adsorption profiles at 77 K for **2′**.

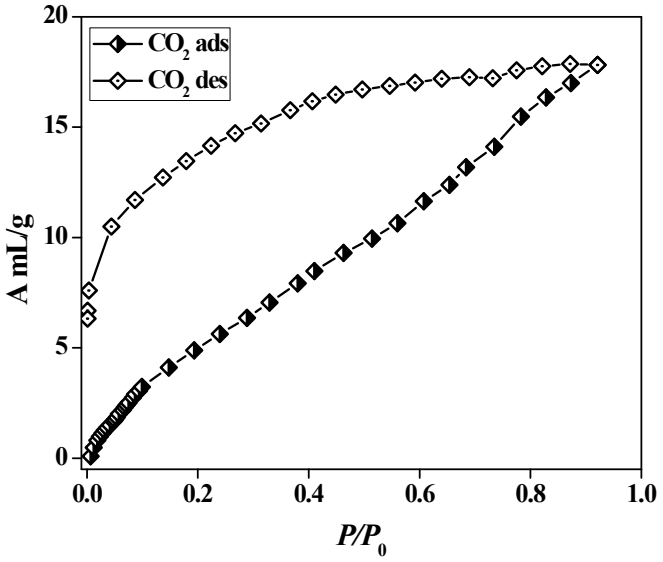

Fig. S6: CO_2 adsorption profiles at 195 K for **2′**.

Indexing result of the powder pattern of the compound 1 after heating at 80 ˚C

Cell parameters : a = 16.7227 Å, b = 16.5213 Å, c = 12.7736 Å , β = 110.563 °, V = 2849.938 Å^3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OBS	2TH-CALC	D-OBS	FREE PARAM.
0	0	1	.005182	.005192	-.000011	8.256	8.264	10.7011	0
0	2	0	.007340	.007346	-.000007	9.829	9.834	8.9912	0
1	0	1		.007428			9.888		
2	1	0		.007526			9.954		
-2	0	1	.009256	.009255	.000001	11.042	11.041	8.0066	0
1	1	1		.009265			11.047		
-2	1	1	.011124	.011092	.000032	12.108	12.091	7.3036	0
2	0	1		.012509			12.843		
0	2	1	.012557	.012539	.000019	12.868	12.859	6.8740	0
3	2	0	.020098	.020148	-.000050	16.300	16.321	5.4336	0
-2	0	2	.023197	.023206	-.000009	17.521	17.524	5.0576	0
1	3	1	.024024	.023958	.000066	17.833	17.808	4.9698	0
4	2	0	.030124	.030105	.000019	19.990	19.984	4.4382	0
3	3	1		.036963			22.169		
-4	0	2	.037024	.037021	.000003	22.188	22.187	4.0033	0
2	2	2		.037058			22.198		
-1	3	2		.037095			22.209		
3	1	2		.040287			23.158		
1	3	2	.040403	.040348	.000056	23.192	23.175	3.8322	0
2	4	1	.041908	.041894	.000014	23.626	23.622	3.7628	0
5	0	1		.044819			24.445		
-3	4	1	.044948	.044940	.000008	24.480	24.478	3.6333	0
1	5	0	.047332	.047338	-.000005	25.131	25.133	3.5406	0
0	5	1	.051070	.051108	-.000038	26.122	26.132	3.4086	0
6	0	0		.051206			26.157		

NUMBER OF OBS. LINES = 15
NUMBER OF CALC. LINES = 25
M(15)= 10 AV.EPS.= .0000225
F 15 = 15.(.008682, 118)

Indexing result of the powder pattern of the compound 2 after heating at 120 ˚C

Cell parameters : a = 6.7227 Å, b = 9.5213 Å, c = 24.7736 Å , V = 2349.938 Å^3

2-TH EXP	D EXP.	1/D**2 EXP	H	K	L	2-TH CAL	D CAL.	1/D**2 CAL	D(2-TH)	(-D(D)	D(1/D**2)	MAX. DEV.	REF.	T-MERIT
7.1194	12.40648	.006497	BASE	0	1	0	7.1774	12.30634	.006603	-.0580	.810	.106E-03	.733E-04	2
14.3745	6.15686	.026380	BASE	0	2	0	14.3832	6.15317	.026412	-.0087	.060	.316E-04	.146E-03	9
15.0130	5.89642	.028762	BASE	1	1	4	15.0010	5.90110	.028717	.0120	-.079	-.457E-04	.153E-03	64
18.1514	4.88338	.041933	BASE	1	2	0	18.2039	4.86942	.042174	-.0525	.286	.241E-03	.184E-03	14
18.5726	4.77356	.043885		1	2	2	18.5464	4.78026	.043762	.0262	-.140	-.123E-03	.188E-03	25
19.0481	4.65546	.046140		0	2	7	18.9906	4.66944	.045864	.0575	-.300	-.276E-03	.192E-03	266
7	20.1894	4.39479	.051775		1	2	5	20.2530	4.38114	.052098	-.0636	.311	.323E-03	.203E-03	127
8	21.4801	4.13354	.058527		0	2	9	21.4876	4.13212	.058567	-.0075	.034	.403E-04	.216E-03	510

9	23.1376	3.84104	.067780	1	2	8	23.1031	3.84671	.067581	.0345	-.147	-.199E-03	.232E-03	386
10	23.7490	3.74352	.071357	2	1	2	23.7290	3.74663	.071239	.0200	-.083	-.118E-03	.237E-03	26
11	24.9989	3.55911	.078943	1	3	3	24.9697	3.56321	.078762	.0292	-.115	-.182E-03	.249E-03	69
12	25.4880	3.49191	.082011	1	2	10	25.4660	3.49489	.081872	.0220	-.085	-.139E-03	.254E-03	690
13	26.4798	3.36333	.088402	2	0	8	26.4879	3.36233	.088455	-.0081	.030	.529E-04	.263E-03	379
14	27.4716	3.24412	.095018	2	1	8	27.4774	3.24345	.095058	-.0058	.021	.393E-04	.272E-03	388
15	28.2188	3.15989	.100151	1	1	14	28.2219	3.15956	.100172	-.0031	.011	.213E-04	.279E-03	1698
16	28.7758	3.09998	.104059	0	2	14	28.7984	3.09760	.104219	-.0226	.077	.160E-03	.284E-03	1713

NUMBER OF LINES

INPUT DATA = 16

CALCULATED = 16

MEAN ABSOLUTE DISCREPANCIES

<Q> = .106E-03

<DELTA(2-THETA)> = .237E-01

MAX. ERROR ACCEPTED (DEG. 2-THETA) = .4500E-01

LOUER, D. & LOUER, M. (1972). J. APPL. CRYST. 5, 271-275.
BOULTIF, A. & LOUER, D. (1991). J. APPL. CRYST. 24, 987-993.