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Supporting information for article:

Using neutron powder diffraction and first-principles calculations to understand the working mechanisms of porous coordination polymer sorbent

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Table S1 Temperature-dependent unit cell parameters for guest-free $\text{Cu}_3(\text{cdm})_4$, determined using NPD.

T / K	a / Å	c / Å	V / Å
13	11.21463(30)	21.5714(10)	2712.99(16)
20	11.21651(30)	21.5632(10)	2712.87(16)
30	11.21694(29)	21.5596(10)	2712.62(16)
40	11.21743(29)	21.5565(9)	2712.48(15)
50	11.21741(29)	21.5579(10)	2712.63(16)
60	11.21618(30)	21.5602(10)	2712.33(16)
70	11.21462(29)	21.5662(9)	2712.33(15)
80	11.21342(29)	21.5712(10)	2712.38(16)
90	11.21206(30)	21.5769(10)	2712.44(16)
100	11.21038(30)	21.5846(10)	2712.60(16)
110	11.20865(31)	21.5916(10)	2712.63(17)
120	11.20724(33)	21.6002(11)	2713.03(18)
130	11.20476(33)	21.6099(11)	2713.05(18)
140	11.20252(34)	21.6207(11)	2713.31(18)
150	11.20015(32)	21.6318(11)	2713.57(17)
160	11.19699(33)	21.6454(11)	2713.74(18)
170	11.19443(32)	21.6569(11)	2713.94(18)
180	11.19204(32)	21.6677(11)	2714.14(18)
190	11.18962(32)	21.6800(11)	2714.50(17)
200	11.18721(33)	21.6903(12)	2714.62(18)
250	11.18133(32)	21.7207(11)	2715.57(18)
300	11.1710(4)	21.7730(13)	2717.06(21)
350	11.1545(4)	21.8514(15)	2718.83(23)

Table S2 Temperature-dependent unit cell parameters for guest-free $\text{Cu}_3(\text{cdm})_4 \cdot 1\text{CO}_2$, determined using NPD.

T / K	a / Å	c / Å	V / Å
15	11.2777(6)	21.3598(19)	2716.66(32)
20	11.2777(6)	21.3590(19)	2716.57(32)
30	11.2762(6)	21.3645(17)	2716.56(29)
40	11.2748(7)	21.3695(21)	2716.5(4)
50	11.2707(6)	21.3831(19)	2716.25(32)
60	11.2658(6)	21.4046(19)	2716.64(32)
70	11.2623(5)	21.4218(17)	2717.14(29)
80	11.2583(5)	21.4363(17)	2717.04(28)
90	11.2540(5)	21.4549(15)	2717.34(24)
100	11.2500(4)	21.4696(14)	2717.26(23)
110	11.2458(4)	21.4894(13)	2717.74(21)
120	11.2411(4)	21.5090(14)	2717.93(22)
130	11.2366(4)	21.5274(12)	2718.06(20)
140	11.2319(4)	21.5491(13)	2718.55(21)
150	11.2272(4)	21.5725(13)	2719.21(20)
160	11.22317(32)	21.5930(11)	2719.84(18)
170	11.21926(32)	21.6164(12)	2720.89(18)
180	11.2156(4)	21.6350(12)	2721.46(20)
190	11.2121(4)	21.6599(12)	2722.90(20)

Table S3 Temperature-dependent unit cell parameters for guest-free $\text{Cu}_3(\text{cdm})_4 \cdot 2\text{CO}_2$, determined using NPD.

T / K	a / Å	c / Å	V / Å³
15	11.2794(7)	21.3370(22)	2714.6(4)
20	11.2801(7)	21.3345(24)	2714.6(4)
30	11.2792(7)	21.3379(23)	2714.6(4)
40	11.2784(7)	21.3422(23)	2714.8(4)
50	11.2779(7)	21.3467(22)	2715.1(4)
60	11.2754(7)	21.3558(23)	2715.1(4)
70	11.2752(7)	21.3586(22)	2715.3(4)
80	11.2709(7)	21.3768(21)	2715.6(4)
90	11.2673(7)	21.3919(21)	2715.7(4)
100	11.2632(6)	21.4109(20)	2716.19(33)
110	11.2595(6)	21.4291(18)	2716.69(31)
120	11.2552(6)	21.4485(17)	2717.06(29)
130	11.2517(6)	21.4666(18)	2717.68(30)
140	11.2469(5)	21.4884(17)	2718.13(28)
150	11.2406(5)	21.5216(17)	2719.25(29)
160	11.2356(4)	21.5509(13)	2720.54(21)
170	11.2295(4)	21.5809(15)	2721.40(24)
180	11.2237(4)	21.6140(14)	2722.77(23)
190	11.21890(32)	21.6426(11)	2724.01(18)
200	11.21329(30)	21.6737(11)	2725.20(17)
250	11.1914(4)	21.7911(13)	2729.28(21)
300	11.1755(5)	21.8508(18)	2728.98(28)
350	11.1588(6)	21.9172(25)	2729.1(4)
350	11.1562(6)	21.9111(25)	2727.1(4)