Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*

Supporting Information

Molecular Simulations for Adsorption and Separation of Natural Gas in IRMOF-1 and Cu-BTC Metal-Organic Frameworks

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Figure 1s. IRMOF-1 as reported by Yaghi and co-workers[1, 2]. IRMOF-1 structure consists of a cubic array of $Zn_4O(CO_2)_6$ clusters connected by phenylene links. Each unit cell contains 8 Zn_4O tetrahedral clusters and 24 linker molecules. The linkage of the Zn_4O complexes is forced to alternate between linkers pointing outwards and inwards, resulting in a structure with two alternating type of cavities. Four small cavities of about 10.9 Å and four larger cavities of about 14.4 Å diameter[2]. Carbon atoms in blue; hydrogen in white; oxygen in red; zinc in grey.

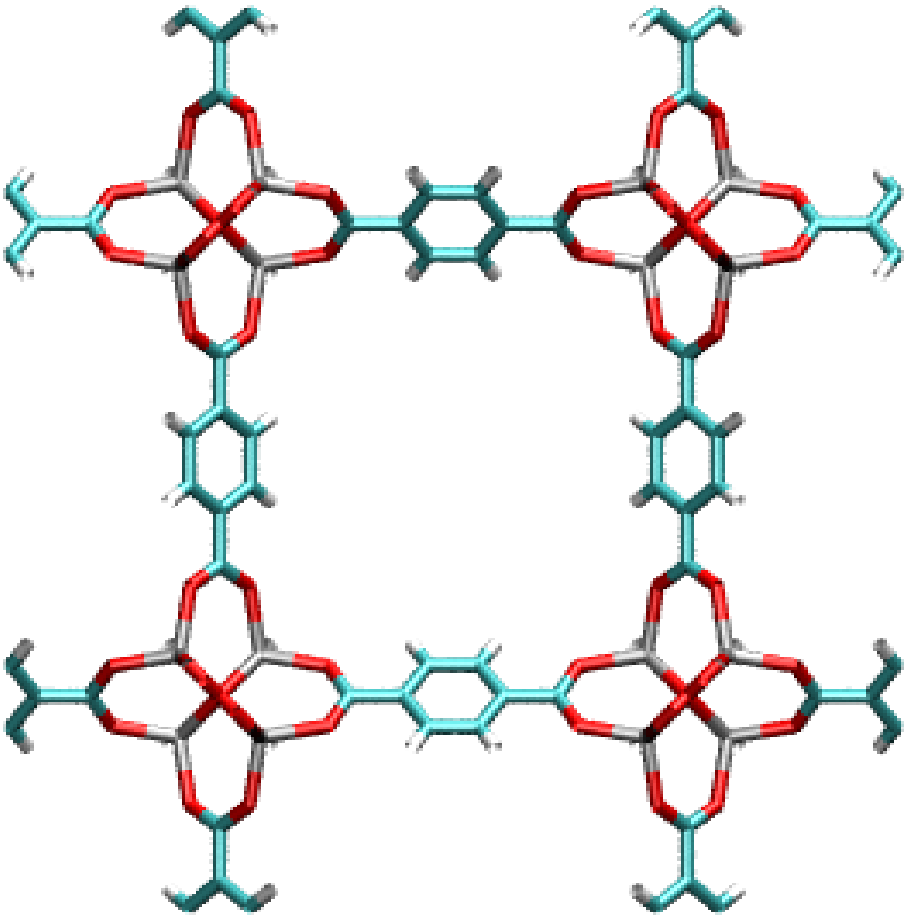


Figure 2s. Cu-BTC (BTC: benzene-1,3,5-tricarboxylate) as reported by Chui and co-workers[3], where the coordinated water molecules were removed. Cu-BTC structure consists of a metal coordination polymer based on copper as the metal centre and benzene-1,3,5-tricarboxylates as the linker molecule. It is formed by primary building blocks connected to form a face-centered cubic crystal framework, and secondary building blocks -octahedral units- forming tetrahedron-shaped pockets accessible for small molecules through the small windows. Carbon atoms in blue; hydrogen in white; oxygen in red; copper in green.

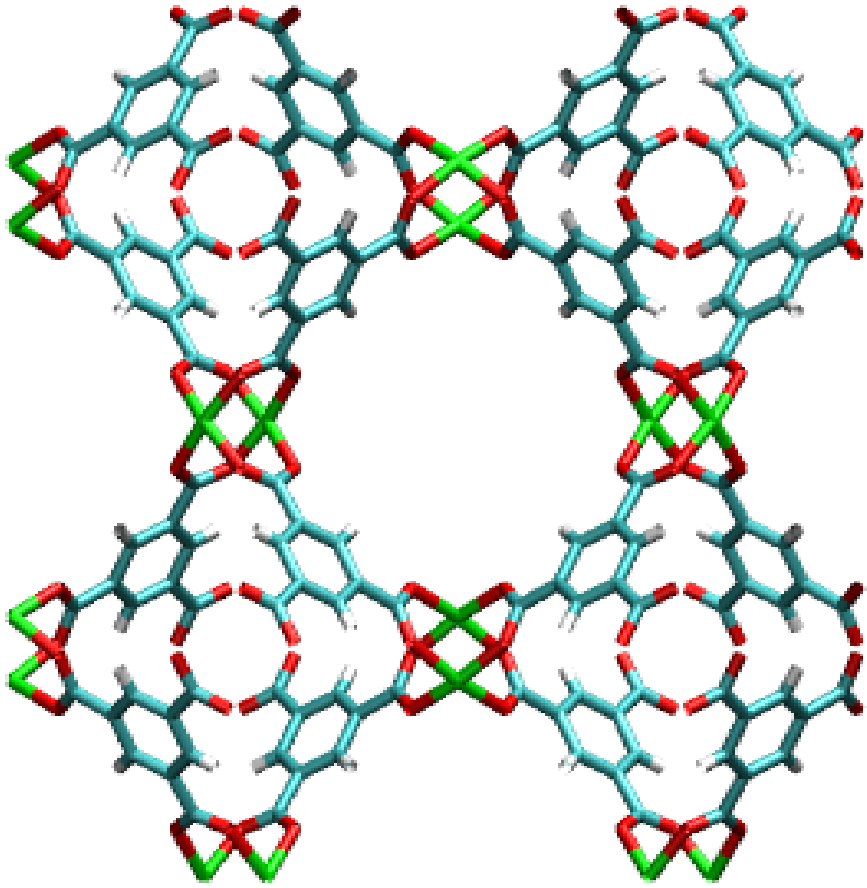
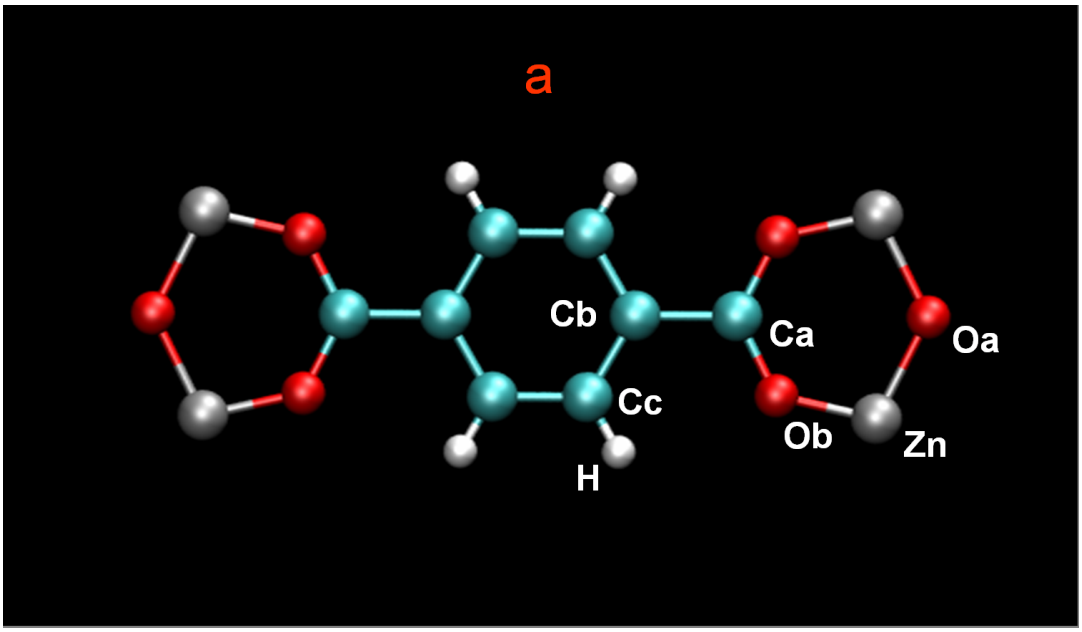


Figure 3s. The definitions of the crystallographically different atoms in the linker molecules for (a) IRMOF-1 and (b) Cu-BTC. The crystallographically different atoms are labeled; the other labels follow by symmetry.



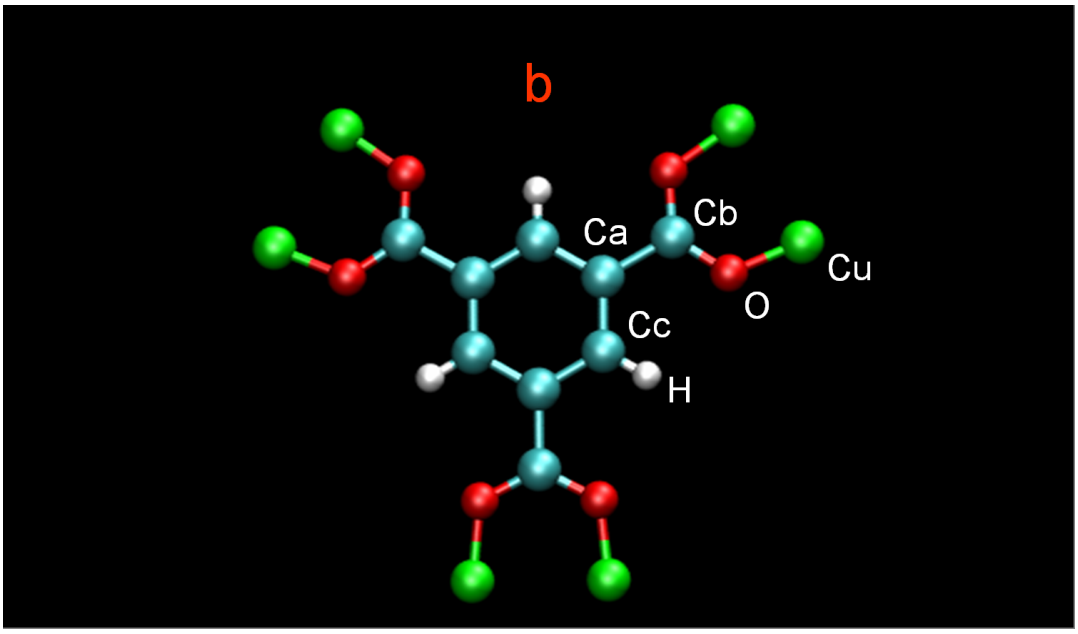


Figure 4s. Preferential adsorption sites in Cu-BTC labeled I, I', II, and III. Color spheres illustrate the positions of the different sites. Site I, region close to the Cu atoms of the framework (blue spheres); site II, centre of the octahedral side pockets (green sphere); site III, windows of the octahedral side pockets (yellow spheres); site I', centre of the big Cu-BTC cages (grey sphere).

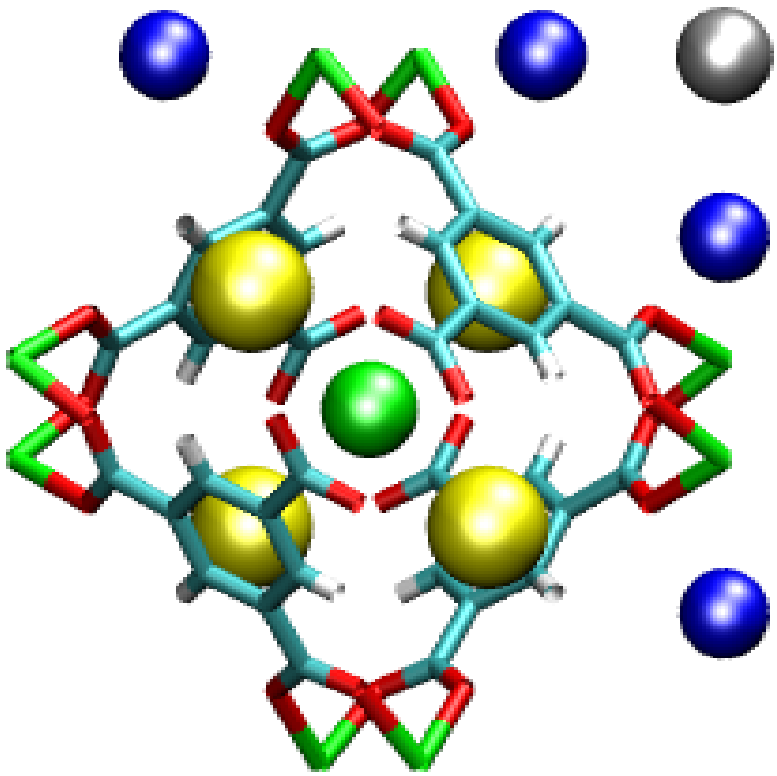


Figure 5s. Preferential adsorption sites in IRMOF-1. Color spheres illustrate the positions of the different sites. Site I, yellow; site II, red; site III, green; site IV, light blue; site V, dark blue; site VI, grey; site VII, white; site VIII, pink. Sites I and II are located in the large and small cages, respectively. Site III is located in the region that separates both types of cages. Sites IV and V are close to the linker molecules, above and beneath the center of the phenyl ring (site IV) and on the edges (site V) of it. Sites VI and VII form a layer above site IV, and site VIII is located at the center of the small cage, above site II and surrounded by site V

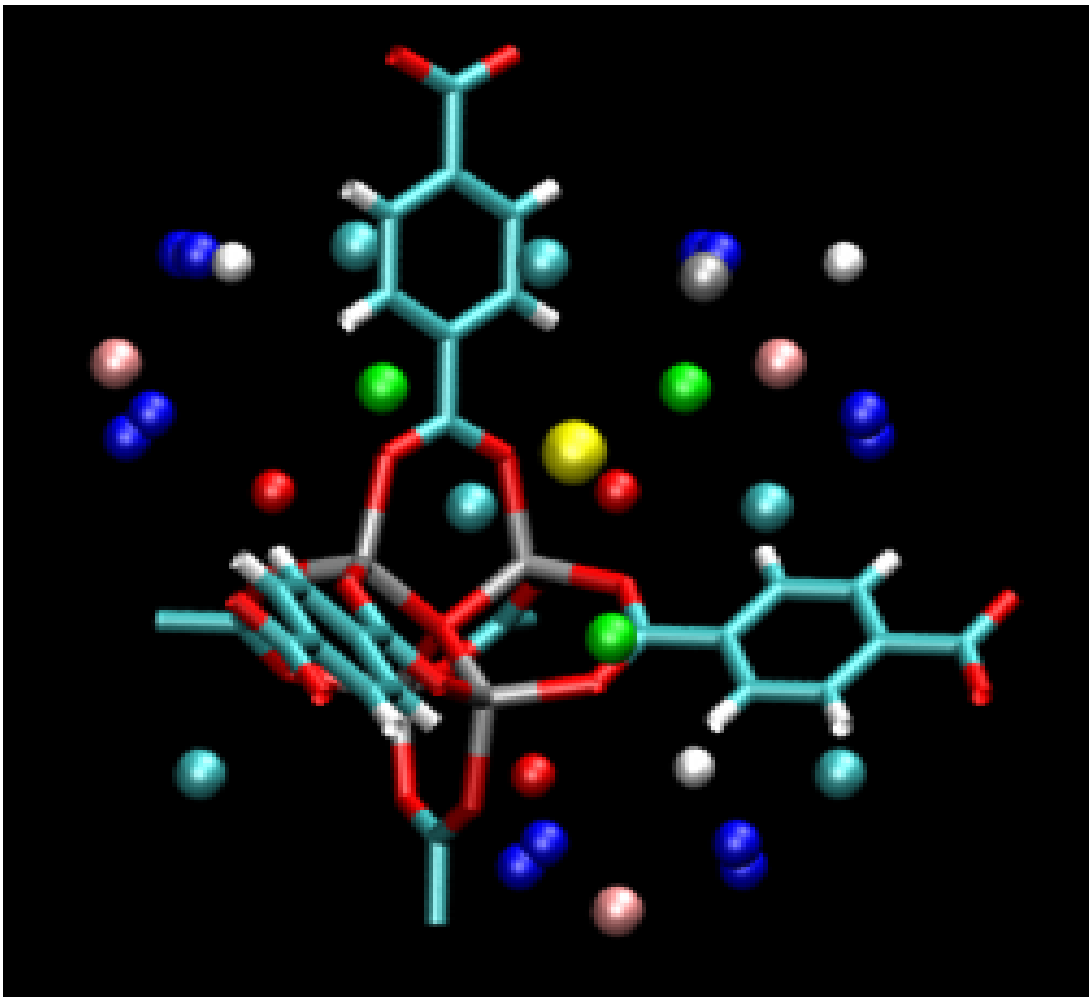


Figure 6sa. Adsorption isotherms of pure methane (triangles), ethane (squares), and propane (circles) in Cu-BTC (full symbols) and IRMOF-1 (open symbols) at 298 K.

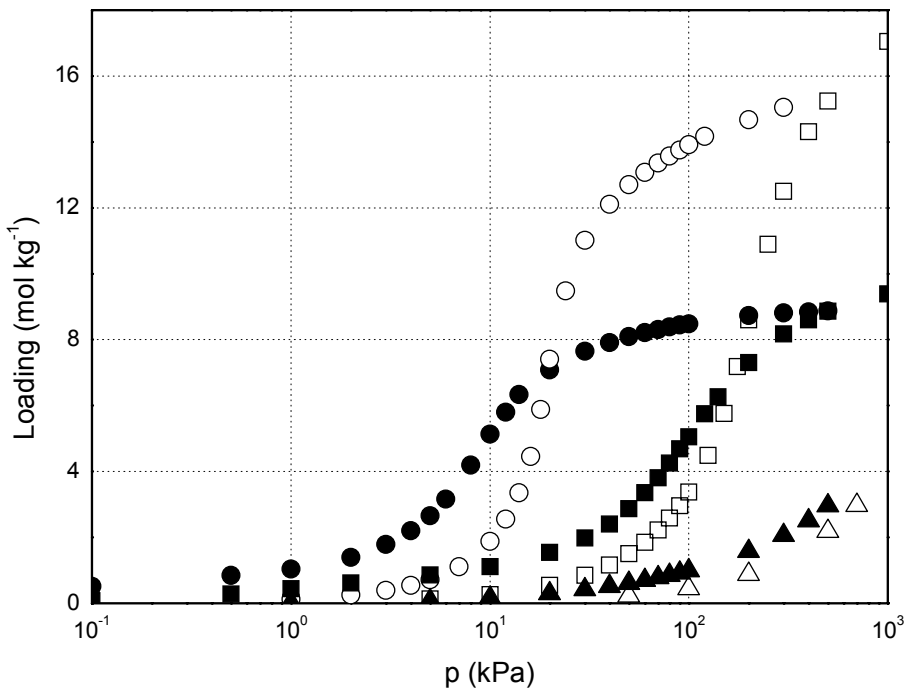


Figure 6sb. Adsorption isotherms of pure CO_2 (triangles) and N_2 (squares) in Cu-BTC (full symbols) and IRMOF-1 (open symbols) at 298 K.

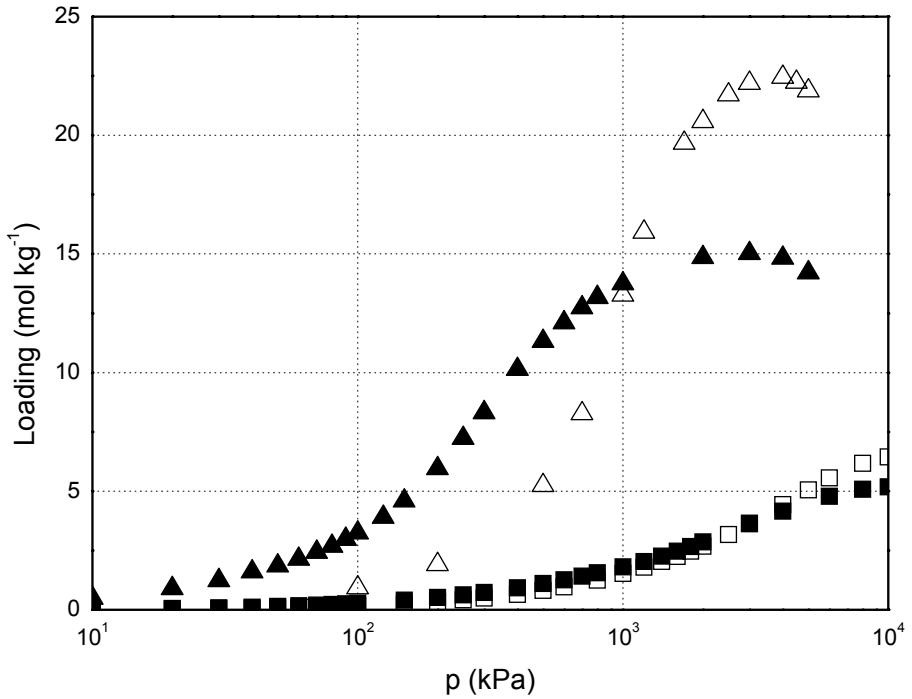


Figure 7s. Excess adsorption for the 10:90 mixture of CO_2 (triangles) and N_2 (squares) mixture in Cu-BTC (full symbols) and IRMOF-1 (open symbols) at 298 K.

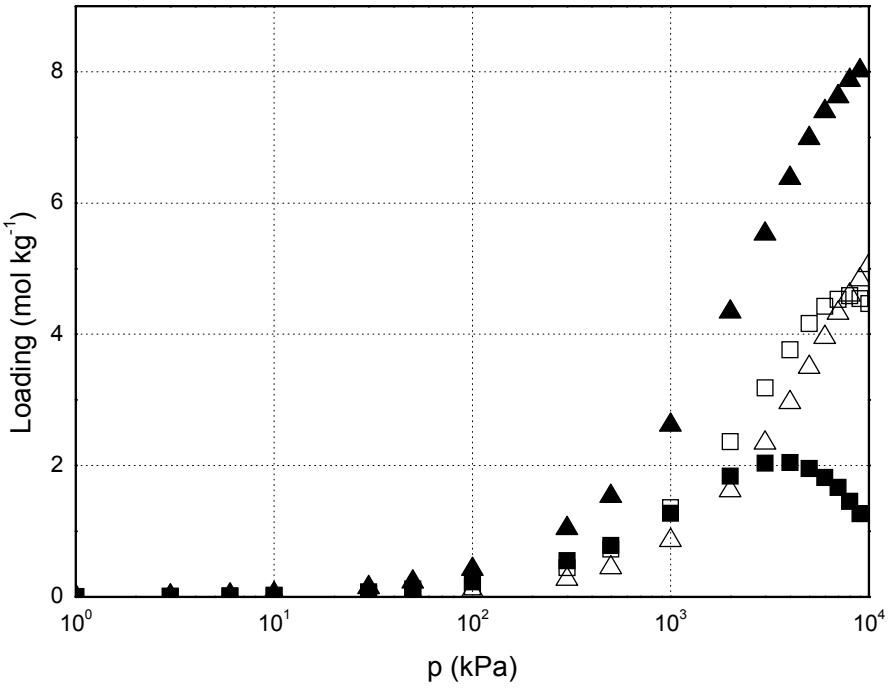
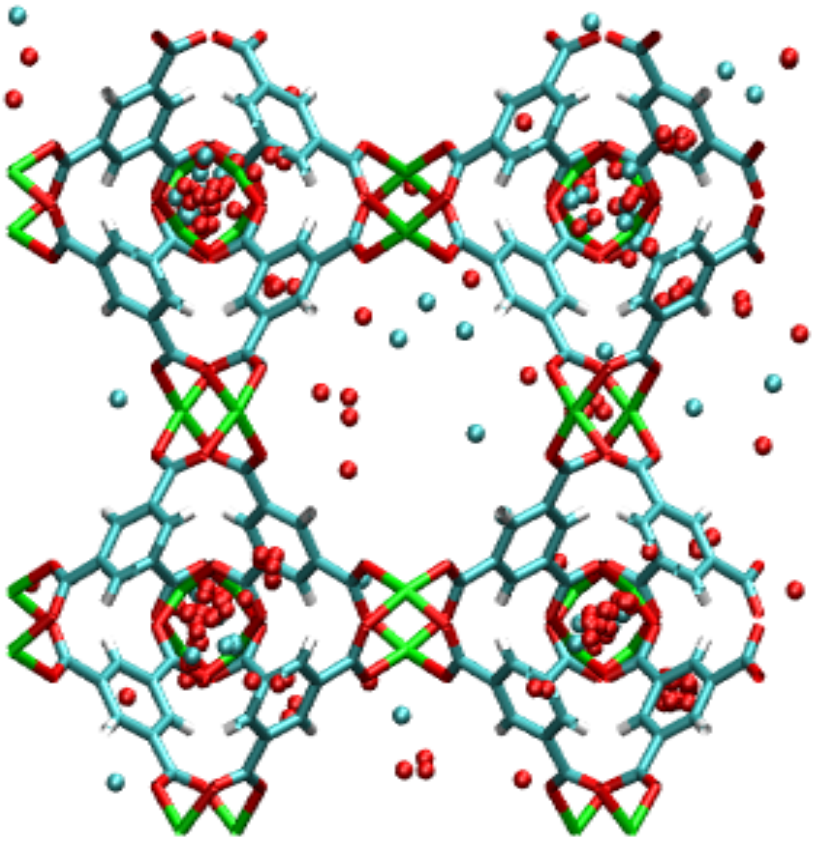


Figure 8s. Center-of-mass distributions of CO_2 (red) and methane (blue) molecules adsorbed in Cu-BTC at 298 K. a) low pressure (2 kPa); b) high pressure ($5 \cdot 10^3$kPa). The equilibrium snapshots are taken from two independent simulations (pure component adsorption) and combined into one figure. Snapshots were taken every 5000 steps in a simulation of one million MC steps at low pressure, and every 200000 steps in a simulation of four million MC steps at high pressure. At low pressures, methane and CO_2 preferentially adsorb in the small octahedral cages. At higher pressures, and once the octahedral cages are partially filled, the molecules adsorb in the windows (Site III) and in the big cage (Site I'). Site I remains empty for both molecules over the entire range of pressures.



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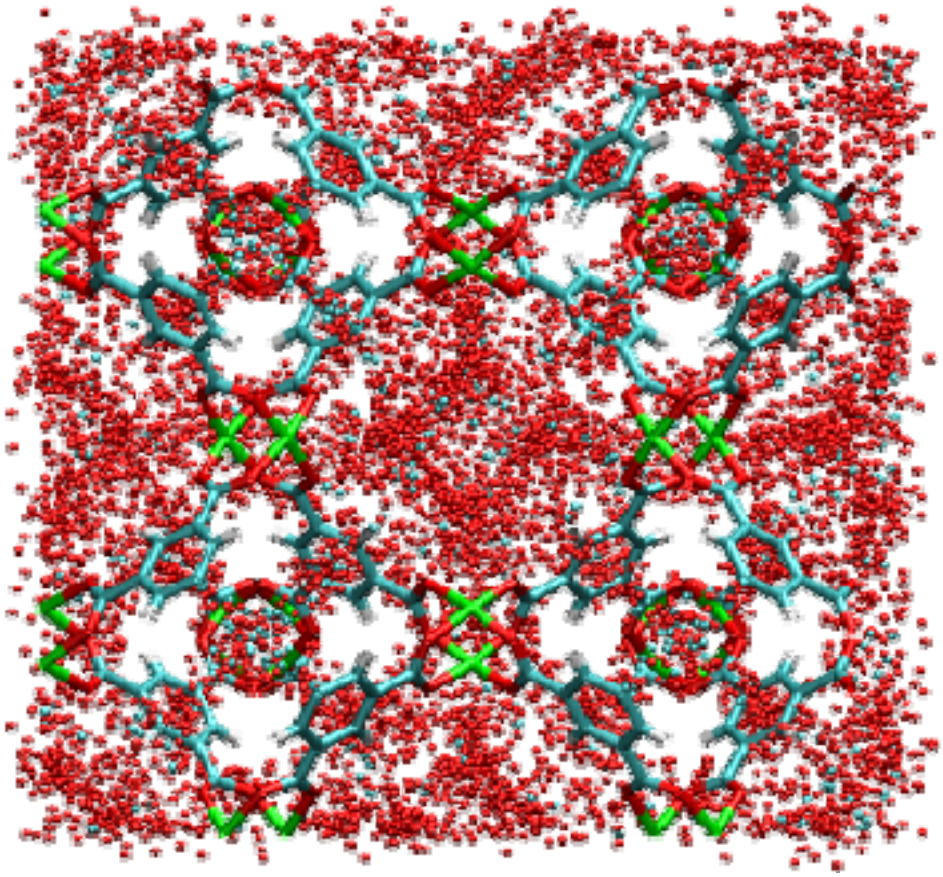

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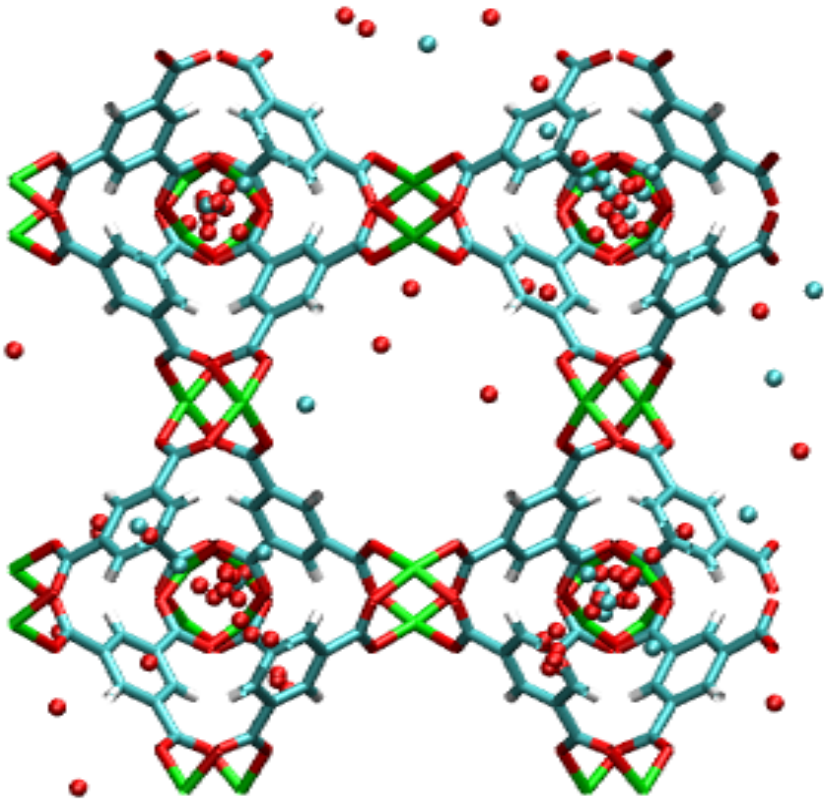
Figure 9s. Center-of-mass distributions of CO_2 (red) and methane (blue) molecules adsorbed in Cu-BTC at 298 K a) low pressure (2kPa); b) high pressure ($5 \cdot 10^3$kPa). The equilibrium snapshots are taken from one single simulation (50:50 mixture adsorption). Snapshots were taken every 5000 steps in a simulation of one million MC steps at low pressure, and every 200000 steps in a simulation of four million MC steps at high pressure.

At low pressure, methane preferentially adsorbs in the octahedral cages displacing an important fraction of CO_2 molecules to the windows. At high pressures and once the octahedral cages are full, Site I' becomes the preferential adsorption site.



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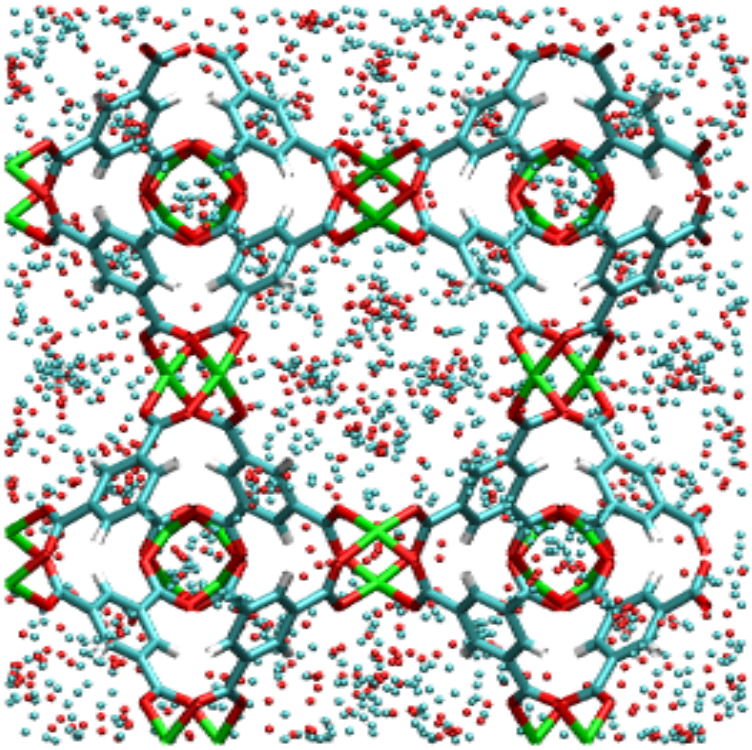

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Table 1s. No bonded van der Waals and charge parameters for the MOFs and adsorbed molecules used in this work.

IRMOF-1			
Atom type	ε/k_B [K]	σ [Å]	Charge [e^-]
Zn	27.7	4.04	1.275
Oa	48.19	3.03	-1.5
Ob	48.19	3.03	-0.6
Ca	47.86	3.47	0.475
Cb	47.86	3.47	0.125
Cc	47.86	3.47	-0.15
H	7.65	2.85	0.15
Cu-BTC			
Atom type	ε/k_B [K]	σ [Å]	Charge [e^-]
Cu	2.518	3.114	1.0
Ob	48.19	3.03	-0.6
Ca	47.86	3.47	0.7
Cb	47.86	3.47	0.0
Cc	47.86	3.47	-0.15
H	7.65	2.85	0.15
Adsorbed molecules			
Atom type	ε/k_B [K]	σ [Å]	Charge [e^-]
CH_4	158.5	3.72	-
CH_3	108.0	3.76	-
CH_2	56.0	3.96	-
C (CO_2)	27.0	2.80	0.7
O (CO_2)	79.0	3.05	-0.35
N (N_2)	36.4	3.32	-0.40484
Dummy (N_2)	-	-	0.80968

Cu-BTC and IRMOF-1 frameworks are considered rigid with Lennard-Jones parameters taken from DREIDING[4] forcefield, except the value for Cu, that was taken from the UFF[5] forcefield. Lorentz-Berthelot mixing rules were used to calculate mixed Lennard-Jones parameters and the atomic charges for the MOFs are taken from Frost *et al.* and Dubbeldam *et al.*[6]. One unit cell of the IRMOF-1 (a = b = c = 25.832 Å) and one unit cell of Cu-BTC (a = b = c = 26.343 Å) were used in our simulations. We obtained a helium void fraction of 0.82 for IRMOF-1 and of 0.76 for Cu-BTC.

Table 2s. Preferential adsorption sites for pure component methane, ethane, propane, CO_2, and N_2 in Cu-BTC at 298 K.

Methane					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.34	21.6	0.1	68.8	9.5
20	2.92	25.9	0.1	63.9	10.1
200	15.38	44.9	0.0	38.0	17.1
500	28.92	59.6	0.0	21.4	19.0
Ethane					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	5.98	9.2	0.0	89.1	1.7
20	14.95	44.6	0.0	49.6	5.8
200	71.10	77.1	0.0	10.8	12.1
1000	90.96	78.2	0.0	8.5	13.3
Propane					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	13.29	40.7	0.0	58.4	0.9
20	69.23	83.4	0.0	11.5	5.1
200	84.56	85.9	0.0	9.4	4.7
500	85.59	85.3	0.0	9.1	5.6
CO_2					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	1.02	24.2	0.1	38.9	36.8
20	8.68	32.4	0.1	30.5	37.0
200	58.07	63.0	0.2	9.6	27.2
1000	132.83	77.6	0.2	4.2	18.0
5000	132.83	77.6	0.2	4.1	18.1
N_2					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.06	44.9	0.1	42.6	12.4
20	0.59	45.9	0.3	40.6	13.2
200	4.99	40.4	0.0	40.3	19.3
1000	17.31	60.9	0.2	23.4	15.5
6000	46.65	74.5	0.7	9.0	15.8

Table 3s. Preferential adsorption sites for pure component methane, ethane, propane, CO_2, and N_2 in IRMOF-1 at 298 K.

Methane									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.13	32.7	0.8	37.1	13.4	5.4	0.6	4.8	5.2
100	2.78	32.8	0.7	36.3	13.8	5.2	0.9	4.8	5.5
500	13.36	30.0	0.8	36.9	14.1	6.0	1.1	5.0	6.1
2000	47.02	21.7	0.5	40.5	15.6	7.4	1.8	5.5	7.0
6000	81.35	16.3	1.2	41.3	12.8	7.1	3.6	6.1	11.6
Ethane									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.82	46.2	0.1	31.1	11.7	3.1	0.2	4.2	3.4
100	20.52	40.9	0.1	33.2	11.2	3.7	1.0	4.9	5.0
500	93.90	18.8	0.3	40.5	8.9	6.5	4.3	5.2	15.5
1000	104.84	16.1	0.4	41.5	9.0	5.8	4.8	5.0	17.4
Propane									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	4.51	53.8	0.0	26.8	11.1	2.0	0.3	4.0	2.0
100	85.48	24.0	0.7	35.1	6.4	7.8	4.5	5.1	16.4
500	93.25	20.6	0.8	38.4	6.0	7.7	4.3	3.2	19.0
CO_2									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.28	36.1	0.8	41.9	11.7	3.0	0.4	2.9	3.2
100	5.56	34.0	0.9	41.5	12.9	3.5	0.5	3.4	3.3
500	32.60	27.2	1.3	43.0	14.4	4.3	1.4	4.1	4.3
2000	128.00	15.2	1.9	40.3	15.2	8.9	4.3	6.1	8.1
5000	135.32	12.9	2.1	40.6	16.5	7.9	4.7	6.1	9.2
N_2									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.05	28.0	0.4	37.3	13.3	7.4	1.2	6.2	6.2
100	1.05	26.4	0.8	37.0	15.9	6.6	1.8	5.9	5.6
500	4.99	26.7	0.8	36.7	15.6	6.9	1.6	5.8	5.9
2000	4.99	24.6	0.9	40.5	12.5	9.4	1.3	3.4	7.4
6000	34.65	19.6	1.2	37.1	18.5	8.0	2.9	4.4	8.3

Table 4s. Preferential adsorption sites for CO_2 and methane from a CH_4/CO_2 equimolar mixture in Cu-BTC at 298 K.

CO_2 50 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
1	0.22	25.1	0.2	43.4	31.3
13	2.85	26.9	0.1	34.8	38.2
100	15.71	42.9	0.1	21.0	36.0
1000	90.53	74.2	0.2	5.0	20.6
4000	120.17	78.0	0.3	4.0	17.7
Methane 50 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
1	0.08	22.5	0.0	66.8	10.7
13	0.87	26.2	0.0	62.5	11.3
100	3.71	47.8	0.1	38.1	14.0
1000	14.70	76.3	0.6	9.4	13.7
4000	12.33	76.3	0.6	9.4	13.7

Table 5s. Preferential adsorption sites for CO_2 and methane from a CH_4/CO_2 equimolar mixture in IRMOF-1 at 298 K.

CO_2 50 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.29	37.4	0.8	41.6	11.7	2.7	0.2	2.8	2.8
100	2.80	34.5	0.8	41.8	13.1	3.1	0.7	3.0	3.0
500	14.53	30.5	1.1	43.2	13.3	3.8	0.9	3.6	3.6
1000	31.81	26.7	1.1	39.7	15.6	6.0	2.0	4.8	4.1
4000	91.63	16.5	1.6	42.8	15.0	7.3	3.1	6.1	7.6
Methane 50 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.14	31.8	0.9	35.9	15.0	4.8	0.9	5.6	5.1
100	1.37	32.2	0.7	36.4	14.0	5.6	1.0	4.7	5.4
500	6.65	27.1	0.8	38.0	14.5	6.2	1.5	5.4	6.5
1000	13.36	20.7	1.0	39.5	14.0	9.2	1.0	6.7	7.9
4000	24.28	11.8	1.1	36.6	15.9	10.0	5.4	6.5	12.7

Table 6s. Preferential adsorption sites for CO_2 and methane from a CO_2/CH_4 10:90 mixture in Cu-BTC at 298 K.

CO_2 10%					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
1	0.05	29.6	0.0	35.9	34.5
10	0.45	26.6	0.0	36.9	36.5
100	3.24	39.0	0.1	23.8	37.1
1000	21.43	62.5	0.0	7.0	30.5
6000	45.84	75.8	0.6	4.0	19.6
Methane 90 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
1	0.14	21.7	0.0	68.2	10.1
10	1.26	25.0	0.0	64.3	10.7
100	7.97	41.3	0.1	45.0	13.6
1000	38.25	70.7	0.1	13.1	16.1
6000	57.89	74.5	0.3	6.6	18.6

Table 7s. Preferential adsorption sites for CO_2 and methane from a CO_2/CH_4 10:90 mixture in IRMOF-1 at 298 K.

CO_2 10 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.06	35.8	1.2	42.8	10.9	2.6	0.0	3.5	3.2
100	0.56	36.7	0.9	40.4	12.1	3.4	0.3	2.9	3.3
500	2.84	32.2	0.9	43.6	12.1	3.7	0.7	3.3	3.5
2000	10.84	26.5	0.4	42.7	13.3	6.0	3.0	4.7	3.4
6000	20.03	18.2	2.2	46.9	11.9	6.3	2.0	4.7	7.8
Methane 90 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.25	33.2	0.7	34.8	15.7	4.9	0.7	4.7	5.3
100	2.45	33.0	0.7	35.4	13.8	5.5	1.0	4.9	5.7
500	12.23	29.2	0.7	37.0	14.1	6.1	1.3	5.3	6.3
2000	43.12	18.3	1.1	37.9	16.4	8.2	2.9	5.5	9.7
6000	69.04	18.3	1.1	37.9	16.3	8.2	2.9	5.5	9.8

Table 8s. Preferential adsorption sites for CO_2 and N_2 from a CO_2/N_2 10:90 mixture in Cu-BTC at 298 K.

CO_2 10 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
10	0.47	26.2	0.1	39.6	34.1
100	4.03	29.0	0.1	33.4	37.5
1000	25.61	51.0	0.0	16.3	32.7
4000	61.83	67.9	0.3	7.2	24.6
8000	78.59	71.4	0.4	5.4	22.8
N_2 90 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
10	0.25	44.6	0.9	39.6	14.9
100	2.16	51.7	0.7	33.8	13.8
1000	12.54	79.9	2.1	9.0	9.0
4000	19.87	83.5	1.2	4.2	11.1
8000	19.87	83.5	1.2	4.2	11.1

Table 9s. Preferential adsorption sites for CO_2 and N_2 from a CO_2/N_2 10:90 mixture in IRMOF-1 at 298 K.

CO_2 10 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.06	37.4	1.4	39.4	10.3	3.6	0.6	3.6	3.7
100	0.56	36.5	0.6	42.4	10.9	3.1	0.5	2.8	3.3
300	1.65	35.9	0.9	41.0	12.1	3.2	0.5	3.3	3.1
2000	9.89	31.9	0.9	43.1	13.4	3.7	1.4	2.3	3.3
8000	28.88	23.9	1.4	44.4	13.8	4.4	2.7	3.8	5.6
10000	30.99	24.0	1.9	38.9	15.0	5.5	2.5	4.6	7.6
N_2 90 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
10	0.10	25.8	1.2	38.7	15.1	5.9	2.5	6.1	4.7
100	0.91	28.0	0.9	36.5	15.0	7.0	1.6	5.6	5.4
300	2.71	26.2	0.9	35.7	16.4	7.3	1.6	6.2	5.7
2000	14.50	22.3	0.4	36.2	14.6	8.7	2.4	10.1	5.3
8000	27.99	15.1	2.2	35.6	16.0	10.2	3.3	6.7	10.9
10000	27.99	15.1	2.2	35.6	16.0	10.2	3.3	6.7	10.9

Table 10s. Preferential adsorption sites for CO_2, ethane, methane, N_2, and propane from a five-component natural gas mixture (95:2.0:1.5:1.0:0.5) $CH_4/C_2H_6/N_2/CO_2/C_3H_8$ in Cu-BTC at 298 K.

CO_2 1%					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.01	32.2	0.0	34.9	32.9
20	0.06	46.5	0.1	21.0	32.4
200	0.42	65.5	0.0	1.2	33.3
1000	1.91	72.7	0.7	0.4	26.2
6000	4.47	81.1	0.4	1.0	17.5
Ethane 2 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.27	3.8	0.0	94.9	1.3
20	1.10	10.5	0.0	87.6	1.9
200	2.79	45.1	0.0	49.5	5.5
1000	7.77	72.6	0.0	17.7	9.8
6000	10.57	74.7	0.0	15.2	10.1
Methane 95 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.26	25.7	0.1	64.0	10.2
20	1.54	45.7	0.1	40.8	13.4
200	9.27	72.6	0.1	9.4	17.9
1000	31.92	78.3	0.3	2.5	18.9
N_2 1.5 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	0.00	40.7	0.0	40.7	18.6
20	0.01	69.5	0.3	18.4	11.8
200	0.04	88.9	0.0	11.1	0.0
1000	0.12	83.9	0.0	3.2	12.9
Propane 0.5 %					
Pressure (kPa)	Loading (molec uc^{-1})	Site I' (%)	Site I (%)	Site II (%)	Site III (%)
2	1.05	1.8	0.0	98.2	0.1
20	4.09	5.1	0.0	94.8	0.2
200	7.93	33.8	0.0	65.4	0.7
1000	17.70	65.7	0.1	32.1	2.1
6000	16.29	69.8	0.0	27.8	2.4

Table 11s. Preferential adsorption sites for CO_2, ethane, methane, N_2, and propane from a five-component natural gas mixture (95:2.0:1.5:1.0:0.5) $CH_4/C_2H_6/N_2/CO_2/C_3H_8$ in IRMOF-1 at 298 K.

CO_2 1 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.01	30.1	0.7	48.0	10.8	2.2	0.7	4.3	3.2
100	0.06	35.2	0.8	41.7	12.6	3.2	0.7	2.8	3.0
500	0.28	32.4	1.0	43.3	12.0	3.5	0.9	3.4	3.5
2000	1.09	22.5	2.5	45.8	9.8	4.7	3.4	5.5	5.8
6000	1.76	17.7	1.8	49.1	10.4	4.8	5.1	3.5	7.6
Ethane 2 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.02	46.0	0.1	31.8	11.3	3.1	0.4	3.7	3.6
100	0.33	46.8	0.1	31.1	11.5	2.9	0.4	3.8	3.4
500	1.77	42.9	0.1	32.8	11.2	3.5	0.6	4.6	4.3
2000	7.47	28.9	0.1	36.6	11.2	5.8	2.9	6.3	8.2
6000	10.39	21.8	0.4	41.3	9.6	6.0	3.2	4.3	13.4
Methane 95 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.13	33.8	0.7	35.6	14.4	4.9	0.9	4.6	5.1
100	2.62	32.4	0.7	36.3	13.9	5.5	0.9	4.9	5.4
500	12.95	28.7	0.8	37.6	13.6	6.2	1.4	5.3	6.4
2000	44.08	18.7	1.5	40.0	12.5	8.4	3.6	5.9	9.4
6000	62.61	13.5	1.8	42.1	12.0	8.4	4.7	5.5	12.0
N_2 1.5 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.01	23.6	0.9	37.7	21.7	8.5	0.0	3.8	3.8
100	0.02	25.6	0.9	37.6	15.3	6.9	2.0	5.5	6.2
500	0.07	23.4	0.9	37.3	15.5	7.9	2.4	5.9	6.7
2000	0.17	10.7	1.8	42.9	16.1	7.1	1.8	12.5	7.1
2000	0.09	10.7	1.8	42.9	16.1	7.1	1.8	12.5	7.1
Propane 0.5 %									
Pressure (kPa)	Loading (molec uc^{-1})	Site I (%)	Site II (%)	Site III (%)	Site IV (%)	Site V (%)	Site VI (%)	Site VII (%)	Site VIII (%)
5	0.02	55.4	0.1	26.1	11.0	2.3	0.1	3.5	1.5
100	0.37	53.8	0.0	26.8	11.6	2.0	0.2	3.9	1.7

500	2.23	51.8	0.0	27.3	11.2	2.5	0.3	4.4	2.5
2000	10.81	38.4	0.1	32.3	10.8	4.6	1.5	6.2	6.1
6000	12.35	32.9	0.3	33.4	9.9	5.6	2.7	5.9	9.3

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