Electronic Supplementary Information

Carbon Flakes based Metal Organic Frameworks for H_2, CH_4 and CO_2 Gas Storage: A GCMC Simulation Study

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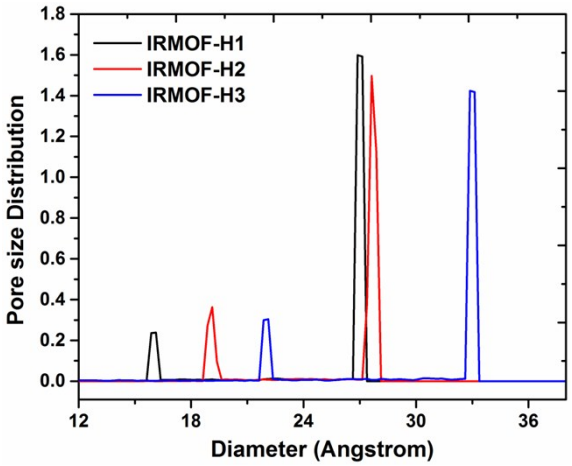

Fig. S1 Pore size distribution of IRMOF-H1, IRMOF-H2, and IRMOF-H3.

Table S1 Pore size analysis for IRMOF-H1, IRMOF-H2, and IRMOF-H3

	IRMOF-H1	**IRMOF-H2**	**IRMOF-H3**
Pore limiting diameter (Å)	10.72	12.98	14.98
Maximum pore diameter (Å)	27.20	27.82	33.11

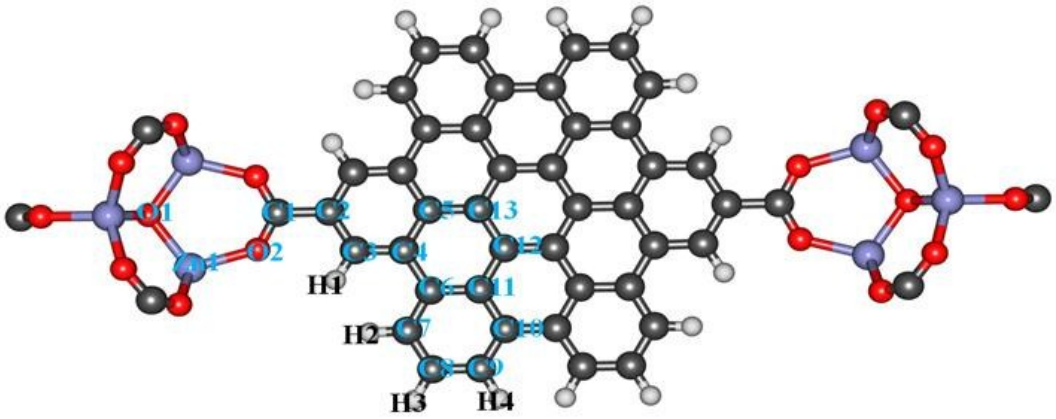

Fig. S2 Clusters were used to calculating partial charges on IRMOF-H1 atoms. The methyl groups are used for termination. Hydrogen (White), Carbon (Black), Oxygen (Red), Zinc (violet).

Table S2 Partial atomic charges for atoms in IRMOF-H1

Atom	O1	Zn1	O2	C1	C2
Charge (e)	-1.685	1.481	-0.714	0.647	0.133
Atom	C3	C4	C5	C6	C7
Charge (e)	-0.271	0.066	0.001	0.042	-0.186
Atom	C8	C9	C10	C11	C12
Charge (e)	-0.109	-0.171	0.031	0.045	-0.042
Atom	C13	H1	H2	H3	H4
Charge (e)	0.020	0.169	0.143	0.118	0.128

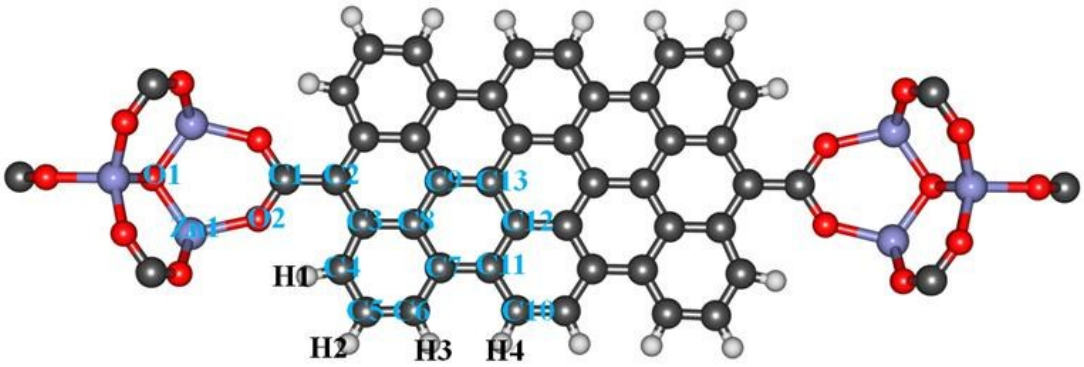

Fig. S3 Clusters were used to calculating partial charges on IRMOF-H2 atoms. The methyl groups are used for termination. Hydrogen (White), Carbon (Black), Oxygen (Red), Zinc (violet).

Table S3 Partial atomic charges for atoms in IRMOF-H2

Atom	O1	Zn1	O2	C1	C2
Charge (e)	-1.917	1.668	-0.837	0.804	-0.237
Atom	C3	C4	C5	C6	C7
Charge (e)	0.133	-0.176	-0.151	-0.147	0.034
Atom	C8	C9	C10	C11	C12
Charge (e)	0.002	-0.001	-0.183	0.047	0.024
Atom	C13	H1	H2	H3	H4
Charge (e)	-0.033	0.199	0.136	0.130	0.144

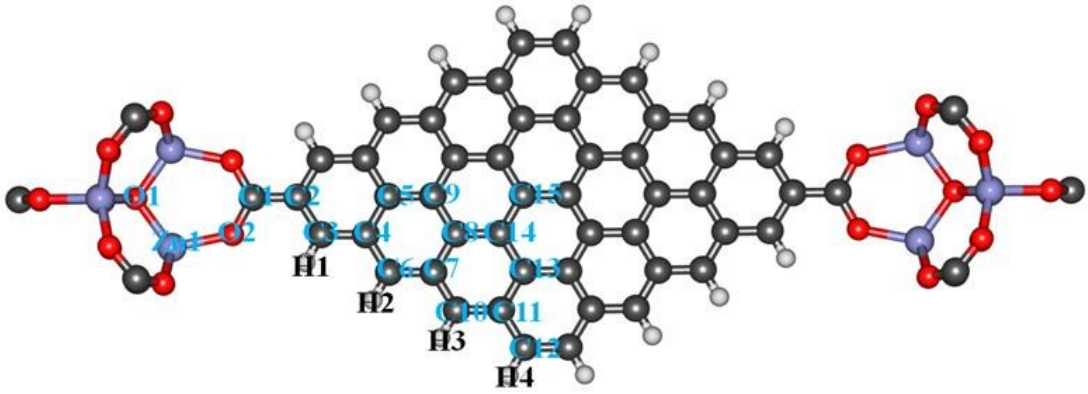

Fig. S4 Clusters were used to calculating partial charges on IRMOF-H3 atoms. The methyl groups are used for termination. Hydrogen (White), Carbon (Black), Oxygen (Red), Zinc (violet).

Table S4 Partial atomic charges for atoms in IRMOF-H3

Atom	O1	Zn1	O2	C1	C2
Charge (e)	-1.671	1.460	-0.679	0.500	0.222
Atom	C3	C4	C5	C6	C7
Charge (e)	-0.325	0.187	-0.039	-0.327	0.193
Atom	C8	C9	C10	C11	C12
Charge (e)	-0.002	-0.005	-0.366	0.193	-0.230
Atom	C13	C14	C15	H1	H2
Charge (e)	-0.003	-0.025	0.019	0.193	0.174
Atom	H3	H4			
Charge (e)	0.181	0.152			

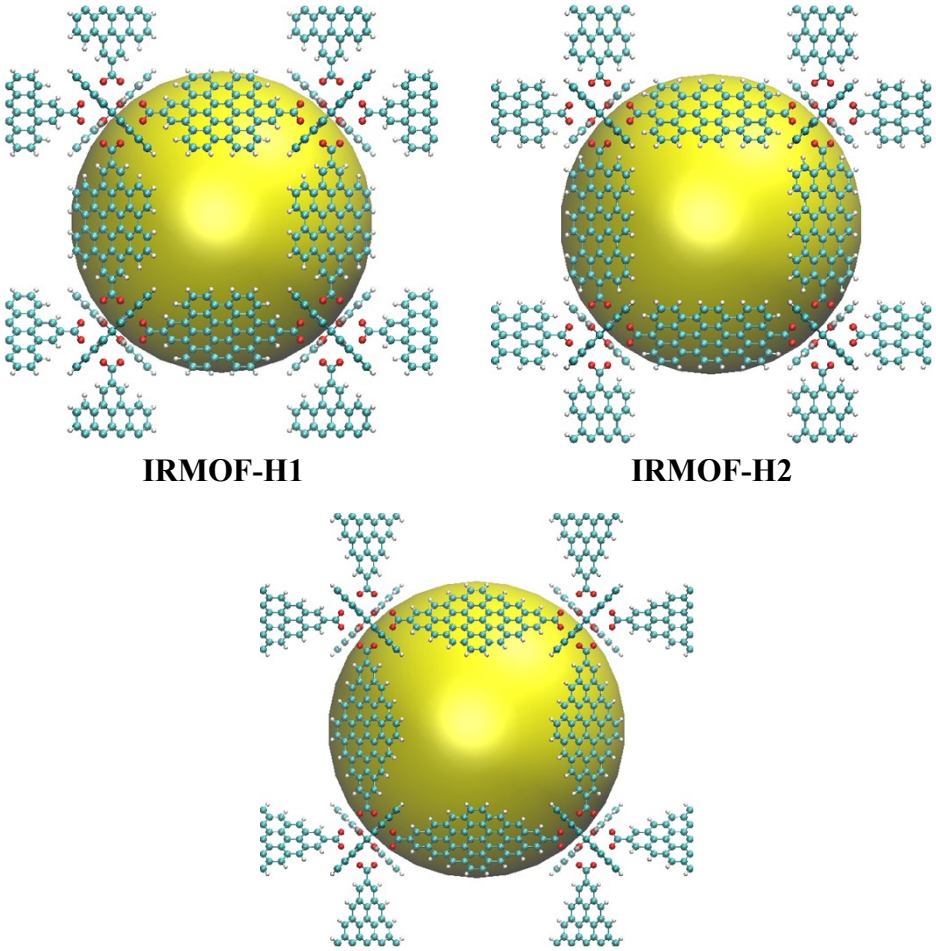

Fig. S5 Unit cell of IRMOF-H1, IRMOF-H2, and IRMOF-H3. The yellow color sphere represents the available free volume in the MOFs.

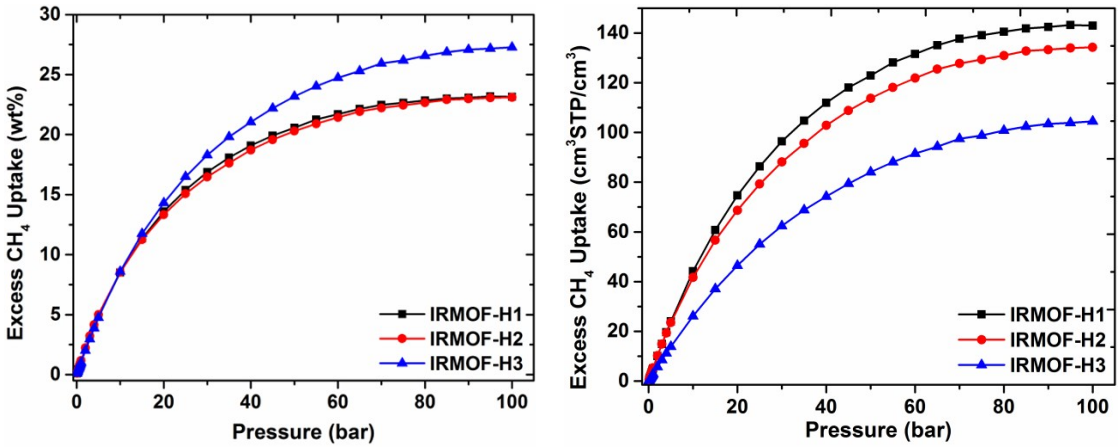

Fig. S6 Simulated excess adsorption isotherm for CH_4 in IRMOF-H1, IRMOF-H2, and IRMOF-H3: gravimetric (left) and volumetric (right) at 298 K.

Table S5 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H1 at 77 K

IRMOF-H1					
	gravimetric density (wt%)		volumetric density (g/L)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.44	0.43	1.50	1.47	6.9
0.2	0.83	0.82	2.86	2.81	6.9
0.3	1.19	1.16	4.10	4.03	6.9
0.4	1.50	1.47	5.21	5.11	6.9
0.5	1.79	1.76	6.25	6.12	6.8
0.6	2.05	2.01	7.15	7.00	6.7
0.7	2.29	2.25	8.03	7.86	6.8
0.8	2.51	2.46	8.81	8.62	6.7
0.9	2.71	2.65	9.53	9.31	6.8
1	2.89	2.82	10.18	9.94	6.7
2	4.22	4.09	15.05	14.56	6.4
3	5.05	4.86	18.20	17.46	6.1
4	5.68	5.42	20.58	19.60	5.8
5	6.20	5.88	22.58	21.35	5.6
10	7.95	7.32	29.51	27.00	5.6
15	9.12	8.19	34.32	30.49	5.1
20	10.01	8.76	38.01	32.82	5.5
25	10.76	9.21	41.23	34.67	4.7
30	11.36	9.49	43.82	35.86	4.8
35	11.88	9.69	46.07	36.69	4.7
40	12.35	9.85	48.16	37.35	5.0
45	12.71	9.90	49.79	37.56	4.8
50	13.06	9.94	51.36	37.72	4.7
55	13.38	9.95	52.81	37.78	4.6
60	13.65	9.91	54.02	37.62	5.1
65	13.90	9.87	55.19	37.43	5.0
70	14.11	9.79	56.17	37.10	5.0
75	14.30	9.69	57.02	36.67	4.8
80	14.51	9.63	58.01	36.41	5.3
85	14.70	9.55	58.91	36.10	5.1
90	14.85	9.44	59.61	35.63	4.9
95	14.99	9.33	60.29	35.18	4.6
100	15.14	9.24	61.00	34.80	5.3

Table S6 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H2 at 77 K

IRMOF-H2					
	gravimetric density (wt%)		volumetric density (g/L)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.49	0.48	1.68	1.65	7.2
0.2	0.88	0.86	3.03	2.98	7.2
0.3	1.21	1.19	4.19	4.11	7.1
0.4	1.49	1.46	5.17	5.06	6.9
0.5	1.73	1.70	6.04	5.90	6.9
0.6	1.96	1.92	6.84	6.69	6.8
0.7	2.16	2.11	7.56	7.37	6.7
0.8	2.34	2.28	8.20	7.99	6.8
0.9	2.51	2.45	8.82	8.58	6.6
1	2.67	2.59	9.36	9.10	6.6
2	3.79	3.65	13.47	12.94	6.3
3	4.54	4.33	16.27	15.47	6.2
4	5.12	4.84	18.46	17.39	5.5
5	5.60	5.25	20.30	18.95	5.7
10	7.31	6.62	26.98	24.25	5.2
15	8.51	7.48	31.81	27.65	4.8
20	9.48	8.11	35.78	30.15	4.7
25	10.27	8.56	39.12	31.99	4.6
30	10.97	8.92	42.11	33.46	4.9
35	11.53	9.13	44.55	34.36	4.7
40	12.05	9.31	46.82	35.08	4.7
45	12.52	9.44	48.91	35.64	4.9
50	12.90	9.49	50.64	35.83	4.5
55	13.26	9.51	52.25	35.92	4.6
60	13.62	9.55	53.90	36.08	5.0
65	13.89	9.49	55.14	35.86	5.0
70	14.15	9.44	56.36	35.65	4.7
75	14.38	9.37	57.43	35.33	5.0
80	14.61	9.29	58.48	35.02	4.5
85	14.84	9.24	59.59	34.82	4.7
90	15.01	9.12	60.36	34.32	4.9
95	15.15	8.99	61.03	33.76	4.8
100	15.35	8.94	62.01	33.54	4.6

Table S7 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H3 at 77 K

IRMOF-H3					
	gravimetric density (wt%)		volumetric density (g/L)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.36	0.34	1.23	1.18	6.6
0.2	0.68	0.66	2.35	2.26	6.6
0.3	0.98	0.94	3.38	3.24	6.5
0.4	1.25	1.20	4.33	4.15	6.5
0.5	1.50	1.44	5.22	4.99	6.4
0.6	1.74	1.66	6.05	5.78	6.5
0.7	1.96	1.87	6.84	6.53	6.3
0.8	2.17	2.07	7.59	7.23	6.2
0.9	2.36	2.25	8.26	7.85	6.3
1	2.55	2.42	8.94	8.49	6.3
2	3.99	3.74	14.21	13.29	6.1
3	5.00	4.64	18.01	16.63	5.8
4	5.81	5.33	21.09	19.25	5.6
5	6.50	5.91	23.77	21.46	5.4
10	8.90	7.74	33.39	28.70	4.8
15	10.62	8.92	40.63	33.47	4.6
20	12.02	9.77	46.68	37.00	4.7
25	13.21	10.43	52.05	39.79	4.2
30	14.25	10.93	56.82	41.95	4.3
35	15.15	11.29	61.02	43.50	4.3
40	15.95	11.56	64.85	44.68	3.9
45	16.70	11.79	68.53	45.70	4.2
50	17.36	11.94	71.81	46.35	4.2
55	17.96	12.04	74.84	46.77	4.2
60	18.54	12.12	77.80	47.16	4.2
65	19.04	12.14	80.38	47.23	4.4
70	19.52	12.16	82.92	47.31	4.4
75	19.96	12.14	85.23	47.22	4.2
80	20.33	12.07	87.24	46.90	4.6
85	20.71	12.02	89.28	46.68	4.4
90	21.06	11.96	91.22	46.44	4.8
95	21.36	11.85	92.83	45.93	4.9
100	21.69	11.80	94.67	45.72	4.6

Table S8 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H1 at 298 K

IRMOF-H1					
	gravimetric density (wt%)		**volumetric density (g/L)**		**Q_{st} (kJ/mol)**
pressure (bar)	**absolute**	**excess**	**absolute**	**excess**	
0.1	0.00	0.00	0.01	0.00	4.2
0.2	0.01	0.00	0.02	0.01	4.4
0.3	0.01	0.00	0.03	0.01	4.4
0.4	0.01	0.00	0.04	0.02	4.5
0.5	0.01	0.01	0.05	0.02	4.5
0.6	0.02	0.01	0.06	0.02	4.3
0.7	0.02	0.01	0.07	0.03	4.4
0.8	0.02	0.01	0.08	0.03	4.5
0.9	0.03	0.01	0.09	0.03	4.4
1	0.03	0.01	0.10	0.04	4.5
2	0.06	0.02	0.20	0.08	4.5
3	0.09	0.03	0.30	0.11	4.5
4	0.12	0.04	0.40	0.15	4.6
5	0.15	0.06	0.50	0.19	4.7
10	0.29	0.11	1.00	0.37	4.9
15	0.43	0.16	1.48	0.54	4.9
20	0.57	0.20	1.96	0.70	4.8
25	0.70	0.25	2.42	0.85	4.9
30	0.83	0.29	2.88	0.99	4.9
35	0.96	0.33	3.33	1.13	4.9
40	1.09	0.37	3.78	1.27	4.9
45	1.22	0.40	4.21	1.38	4.9
50	1.34	0.44	4.64	1.50	4.7
55	1.46	0.47	5.06	1.61	4.9
60	1.57	0.50	5.47	1.71	4.8
65	1.69	0.53	5.89	1.81	4.7
70	1.81	0.55	6.29	1.89	4.8
75	1.92	0.58	6.69	1.98	4.9
80	2.03	0.60	7.07	2.05	4.8
85	2.14	0.62	7.46	2.13	4.7
90	2.24	0.64	7.84	2.19	4.7
95	2.35	0.66	8.21	2.25	4.8
100	2.45	0.67	8.59	2.31	4.7

Table S9 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H2 at 298 K

IRMOF-H2					
	gravimetric density (wt%)		volumetric density (g/L)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.00	0.00	0.01	0.00	4.2
0.2	0.01	0.00	0.02	0.01	4.3
0.3	0.01	0.00	0.03	0.01	4.2
0.4	0.01	0.00	0.04	0.02	4.3
0.5	0.02	0.01	0.05	0.02	4.3
0.6	0.02	0.01	0.06	0.02	4.3
0.7	0.02	0.01	0.07	0.03	4.3
0.8	0.02	0.01	0.09	0.03	4.3
0.9	0.03	0.01	0.10	0.03	4.3
1	0.03	0.01	0.11	0.04	4.2
2	0.06	0.02	0.21	0.08	4.5
3	0.09	0.03	0.32	0.11	4.4
4	0.12	0.04	0.42	0.15	4.7
5	0.15	0.05	0.53	0.19	4.6
10	0.30	0.11	1.05	0.36	4.8
15	0.45	0.16	1.55	0.53	4.1
20	0.60	0.20	2.05	0.69	4.9
25	0.74	0.24	2.54	0.84	4.9
30	0.88	0.28	3.02	0.98	4.9
35	1.01	0.33	3.50	1.11	4.9
40	1.15	0.36	3.96	1.24	4.8
45	1.27	0.39	4.41	1.35	4.8
50	1.41	0.43	4.87	1.47	4.9
55	1.53	0.46	5.31	1.56	4.7
60	1.65	0.48	5.75	1.66	4.5
65	1.78	0.51	6.19	1.76	4.7
70	1.90	0.53	6.61	1.84	4.6
75	2.01	0.55	7.02	1.90	4.7
80	2.13	0.57	7.42	1.97	4.7
85	2.24	0.59	7.84	2.04	4.6
90	2.35	0.61	8.23	2.10	4.7
95	2.46	0.62	8.62	2.15	4.6
100	2.57	0.64	9.03	2.22	4.6

Table S10 Simulated H_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H3 at 298 K

IRMOF-H3					
	gravimetric density (wt%)		volumetric density (g/L)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.00	0.00	0.02	0.00	3.8
0.2	0.01	0.00	0.03	0.01	3.7
0.3	0.01	0.00	0.05	0.01	3.7
0.4	0.02	0.01	0.06	0.02	3.9
0.5	0.02	0.01	0.08	0.02	3.8
0.6	0.03	0.01	0.10	0.03	3.9
0.7	0.03	0.01	0.11	0.03	3.8
0.8	0.04	0.01	0.13	0.04	3.8
0.9	0.04	0.01	0.15	0.04	3.9
1	0.05	0.01	0.16	0.04	3.7
2	0.09	0.03	0.32	0.09	3.9
3	0.14	0.04	0.48	0.13	4.0
4	0.19	0.05	0.64	0.17	4.1
5	0.23	0.06	0.80	0.22	4.2
10	0.46	0.12	1.59	0.42	4.3
15	0.69	0.18	2.36	0.61	4.2
20	0.91	0.23	3.13	0.79	4.3
25	1.12	0.28	3.89	0.96	4.2
30	1.34	0.32	4.63	1.11	4.2
35	1.54	0.37	5.36	1.26	4.0
40	1.75	0.41	6.08	1.40	4.2
45	1.95	0.44	6.79	1.52	4.2
50	2.14	0.48	7.49	1.63	4.1
55	2.34	0.51	8.20	1.76	4.1
60	2.53	0.54	8.88	1.85	4.1
65	2.72	0.56	9.55	1.94	4.0
70	2.90	0.59	10.23	2.02	4.2
75	3.09	0.61	10.88	2.10	4.1
80	3.26	0.62	11.51	2.14	4.1
85	3.44	0.64	12.17	2.21	4.0
90	3.61	0.66	12.82	2.27	3.9
95	3.78	0.67	13.44	2.31	3.9
100	3.94	0.67	14.04	2.32	4.1

Table S11 Simulated CH_4 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H1 at 298 K

IRMOF-H1					
	gravimetric density (wt%)		volumetric density (cm^3 STP/ cm^3)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.12	0.11	0.59	0.52	10.8
0.2	0.25	0.22	1.17	1.03	11.2
0.3	0.37	0.32	1.76	1.55	11.7
0.4	0.49	0.43	2.34	2.06	11.8
0.5	0.61	0.54	2.92	2.58	12.1
0.6	0.73	0.65	3.50	3.09	12.1
0.7	0.85	0.75	4.09	3.60	12.2
0.8	0.97	0.86	4.67	4.11	12.2
0.9	1.09	0.96	5.25	4.62	12.4
1	1.21	1.07	5.83	5.13	12.5
2	2.37	2.09	11.51	10.12	12.5
3	3.46	3.05	17.03	14.94	12.3
4	4.51	3.97	22.44	19.64	12.5
5	5.49	4.82	27.57	24.06	12.7
10	9.74	8.51	51.24	44.15	12.4
15	13.09	11.34	71.48	60.73	12.1
20	15.82	13.60	89.22	74.73	12.1
25	18.07	15.39	104.69	86.38	12.1
30	19.99	16.88	118.62	96.41	12.1
35	21.62	18.08	130.93	104.75	11.3
40	23.05	19.08	142.18	111.95	11.4
45	24.30	19.91	152.40	118.04	11.4
50	25.38	20.57	161.47	122.91	11.3
55	26.48	21.26	170.98	128.16	11.2
60	27.35	21.70	178.74	131.58	11.2
65	28.22	22.15	186.59	135.04	11.1
70	28.98	22.49	193.71	137.71	11.8
75	29.60	22.66	199.58	139.07	11.0
80	30.22	22.84	205.61	140.54	10.7
85	30.82	23.01	211.52	141.86	11.2
90	31.35	23.08	216.75	142.46	11.3
95	31.88	23.18	222.20	143.24	12.7
100	32.31	23.15	226.64	142.99	12.1

Table S12 Simulated CH_4 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H2 at 298 K

IRMOF-H2					
	gravimetric density (wt%)		**volumetric density (cm^3 STP/ cm^3)**		**Q_{st} (kJ/mol)**
pressure (bar)	**absolute**	**excess**	**absolute**	**excess**	
0.1	0.14	0.12	0.61	0.54	11.3
0.2	0.27	0.24	1.23	1.08	11.8
0.3	0.41	0.36	1.84	1.62	12.3
0.4	0.54	0.48	2.44	2.15	12.7
0.5	0.68	0.60	3.04	2.68	12.7
0.6	0.81	0.71	3.63	3.20	12.6
0.7	0.94	0.83	4.23	3.73	12.9
0.8	1.07	0.94	4.81	4.25	13.0
0.9	1.20	1.06	5.41	4.77	13.0
1	1.32	1.17	5.98	5.27	13.1
2	2.54	2.23	11.63	10.21	12.8
3	3.67	3.23	17.03	14.89	13.1
4	4.74	4.15	22.21	19.35	13.0
5	5.72	5.00	27.12	23.53	12.7
10	9.87	8.53	48.93	41.69	12.0
15	13.15	11.25	67.64	56.65	11.8
20	15.75	13.33	83.54	68.72	11.3
25	17.99	15.07	98.00	79.28	11.4
30	19.88	16.48	110.84	88.14	11.6
35	21.49	17.62	122.31	95.55	10.6
40	23.04	18.71	133.77	102.86	11.2
45	24.36	19.58	143.91	108.79	10.7
50	25.53	20.29	153.17	113.75	10.5
55	26.59	20.91	161.87	118.10	10.4
60	27.57	21.43	170.09	121.88	11.1
65	28.51	21.92	178.16	125.46	11.2
70	29.28	22.23	184.98	127.73	10.4
75	29.97	22.45	191.22	129.36	10.8
80	30.65	22.67	197.46	130.95	11.3
85	31.35	22.91	204.00	132.79	10.7
90	31.90	22.98	209.27	133.32	11.1
95	32.45	23.07	214.68	133.96	10.9
100	32.97	23.11	219.76	134.26	10.9

Table S13 Simulated CH_4 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H3 at 298 K

IRMOF-H3					
	gravimetric density (wt%)		volumetric density (cm^3 STP/ cm^3)		Q_{st} (kJ/mol)
pressure (bar)	absolute	excess	absolute	excess	
0.1	0.13	0.11	0.37	0.29	9.5
0.2	0.26	0.21	0.73	0.58	9.8
0.3	0.39	0.31	1.10	0.87	10.3
0.4	0.53	0.42	1.47	1.17	10.5
0.5	0.65	0.52	1.83	1.45	10.7
0.6	0.79	0.62	2.21	1.75	11.1
0.7	0.91	0.72	2.55	2.02	11.0
0.8	1.04	0.82	2.93	2.32	11.2
0.9	1.17	0.93	3.29	2.60	11.1
1	1.30	1.03	3.66	2.90	11.3
2	2.54	2.01	7.25	5.72	11.2
3	3.72	2.96	10.78	8.48	10.9
4	4.88	3.87	14.28	11.22	11.1
5	5.98	4.75	17.72	13.88	11.1
10	10.86	8.59	33.94	26.17	10.5
15	14.92	11.75	48.86	37.08	10.8
20	18.30	14.31	62.38	46.50	9.9
25	21.24	16.50	75.13	55.06	10.1
30	23.74	18.30	86.72	62.39	10.1
35	25.94	19.82	97.55	68.86	9.9
40	27.83	21.05	107.39	74.26	9.7
45	29.60	22.19	117.10	79.45	9.2
50	31.20	23.18	126.31	84.06	9.9
55	32.65	24.03	135.05	88.13	8.9
60	33.95	24.73	143.18	91.51	9.5
65	35.13	25.30	150.83	94.35	9.8
70	36.32	25.93	158.88	97.51	9.4
75	37.21	26.18	165.10	98.79	8.5
80	38.19	26.57	172.10	100.81	9.3
85	39.09	26.88	178.73	102.40	9.8
90	39.89	27.08	184.83	103.42	9.4
95	40.60	27.17	190.42	103.90	9.0
100	41.32	27.28	196.16	104.50	9.3

Table S14 Simulated CO_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H1 at 298 K

IRMOF-H1					
	gravimetric density (mg/g)		**volumetric density (cm^3 STP/ cm^3)**		**Q_{st} (kJ/mol)**
pressure (bar)	**absolute**	**excess**	**absolute**	**excess**	
0.1	9.87	9.46	1.71	1.64	22.1
0.2	19.66	18.88	3.40	3.26	21.3
0.3	29.29	28.08	5.07	4.86	21.5
0.4	39.20	37.58	6.78	6.51	20.8
0.5	48.91	46.91	8.46	8.12	21.8
0.6	58.04	55.63	10.04	9.63	20.1
0.7	67.91	65.09	11.75	11.26	20.1
0.8	76.96	73.76	13.32	12.76	19.1
0.9	87.05	83.44	15.06	14.44	20.3
1	96.48	92.46	16.70	16.00	20.2
2	186.58	178.46	32.29	30.89	18.5
3	265.93	253.71	46.02	43.91	18.6
4	339.33	322.94	58.72	55.89	18.7
5	407.76	387.15	70.56	67.00	18.8
10	662.15	619.69	114.59	107.24	15.0
15	847.47	781.73	146.66	135.28	14.5
20	999.16	908.48	172.91	157.21	14.4
25	1134.68	1017.05	196.36	176.01	14.7
30	1244.00	1097.10	215.28	189.86	15.6
35	1346.86	1167.73	233.08	202.08	16.4
40	1428.27	1213.20	247.17	209.95	13.0
45	1501.09	1245.15	259.77	215.48	16.5
50	1570.67	1266.84	271.81	219.23	17.9
55	1614.04	1251.44	279.32	216.57	19.8

Table S15 Simulated CO_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H2 at 298 K

IRMOF-H2					
	gravimetric density (mg/g)		**volumetric density (cm^3 STP/ cm^3)**		**Q_{st} (kJ/mol)**
pressure (bar)	**absolute**	**excess**	**absolute**	**excess**	
0.1	10.52	10.08	1.71	1.64	21.6
0.2	20.73	19.85	3.38	3.24	20.9
0.3	30.96	29.66	5.04	4.83	21.1
0.4	40.66	38.90	6.62	6.34	20.4
0.5	50.02	47.84	8.15	7.79	20.0
0.6	59.79	57.17	9.74	9.31	19.7
0.7	68.94	65.88	11.23	10.73	19.7
0.8	78.34	74.86	12.76	12.19	19.5
0.9	87.18	83.22	14.20	13.56	19.3
1	96.10	91.71	15.65	14.94	19.6
2	175.95	167.15	28.66	27.22	18.2
3	245.56	232.28	40.00	37.83	17.9
4	309.15	291.34	50.35	47.45	17.9
5	364.38	341.99	59.35	55.70	16.3
10	587.39	541.27	95.67	88.16	16.6
15	755.72	684.30	123.09	111.46	13.8
20	910.37	811.88	148.28	132.23	13.1
25	1034.74	906.98	168.53	147.72	14.0
30	1159.92	1000.32	188.92	162.93	13.5
35	1273.92	1079.32	207.49	175.80	12.7
40	1371.00	1137.37	223.30	185.25	15.0
45	1464.13	1186.09	238.47	193.19	12.5
50	1540.11	1210.07	250.85	197.10	15.4
55	1613.33	1219.49	262.77	198.63	16.2

Table S16 Simulated CO_2 absolute and excess adsorption amount and isosteric heat of adsorption (Q_{st}) for IRMOF-H3 at 298 K

IRMOF-H3					
	gravimetric density (mg/g)		**volumetric density (cm^3 STP/ cm^3)**		**Q_{st} (kJ/mol)**
pressure (bar)	**absolute**	**excess**	**absolute**	**excess**	
0.1	7.99	6.56	0.81	0.74	18.6
0.2	15.93	13.07	1.62	1.47	18.3
0.3	23.98	19.72	2.43	2.21	18.6
0.4	31.58	25.92	3.21	2.90	17.9
0.5	39.89	32.79	4.05	3.67	18.0
0.6	47.06	38.60	4.78	4.32	17.5
0.7	54.78	44.89	5.56	5.03	16.9
0.8	62.51	51.23	6.35	5.74	17.8
0.9	70.00	57.34	7.11	6.42	17.5
1	77.43	63.37	7.86	7.10	17.2
2	152.86	124.90	15.52	13.99	17.1
3	222.24	180.83	22.57	20.25	15.6
4	285.99	231.58	29.04	25.93	15.9
5	350.99	283.37	35.64	31.73	15.1
10	615.90	486.61	62.54	54.49	15.4
15	839.08	649.53	85.20	72.73	12.1
20	1025.06	775.92	104.09	86.89	13.9
25	1193.98	883.48	121.24	98.93	11.6
30	1352.06	977.22	137.29	109.43	11.6
35	1498.13	1055.12	152.12	118.15	11.7
40	1634.18	1117.61	165.93	125.15	10.6
45	1756.34	1159.15	178.34	129.80	14.5
50	1874.05	1184.81	190.29	132.67	11.4
55	1968.34	1170.82	199.87	131.10	14.2