Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Carbon dioxide adsorption to UiO-66: theoretical analysis of binding energy and NMR properties

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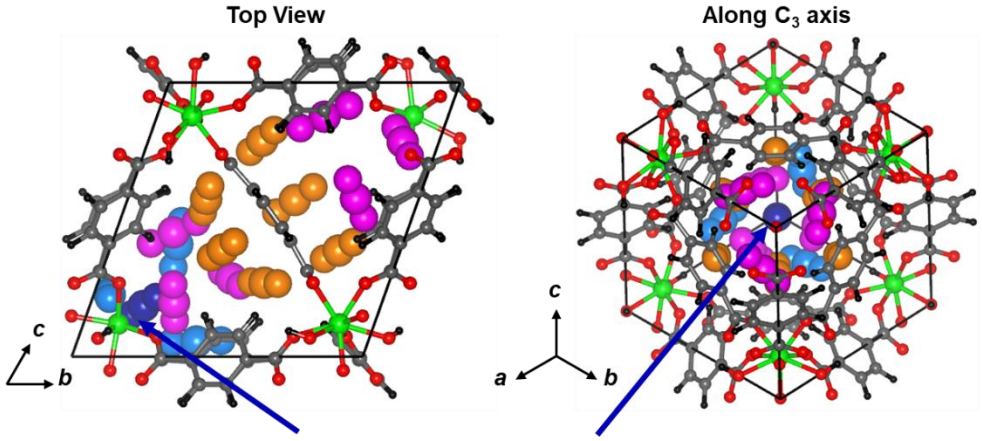
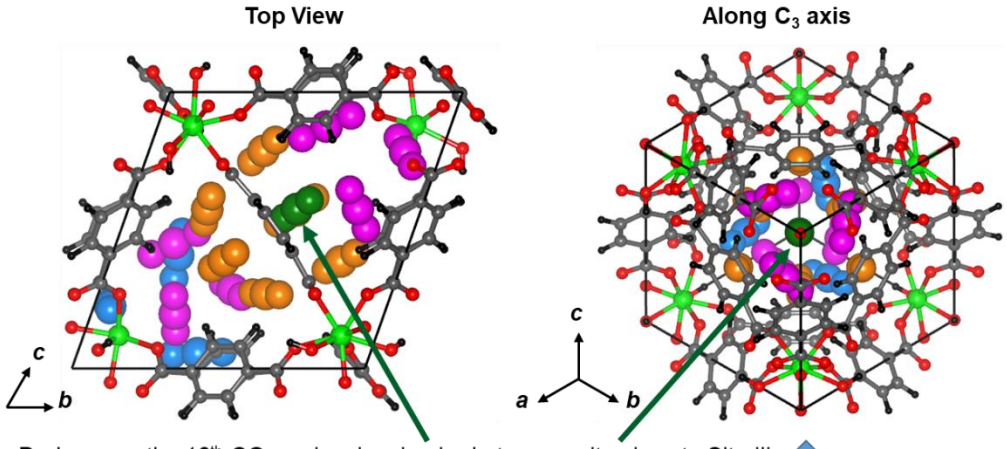
1. Adsorption of sixteen CO_2 molecules

(A) The 16th CO_2 at Site I



Dark blue; the 16th CO_2 molecule adsorbed at the fourth Site I

(B) The 16th CO_2 at a new site close to Site III



Dark green; the 16th CO_2 molecule adsorbed at a new site close to Site III

In the figure at the left-hand side, the sixteenth CO_2 molecule exists at a different position from Sites II and III, but it almost overlaps with the sixteenth CO_2 molecule at Site I in the figure at the right-hand side; in other words, the sixteenth CO_2 at the new site is above the sixteenth CO_2 at Site I (the fourth HO-Zr site; Figure S1(A)).

Figure S1. Adsorption structure of sixteen CO_2 molecules optimized by the DFT calculation with PBE-D3 under periodic boundary condition. The sixteenth CO_2 molecule is shown by different color (dark blue in (A) and green color in Figure (B)) in the presence of fifteen CO_2 molecules.

2. Adsorption structure of CO_2 at Site III

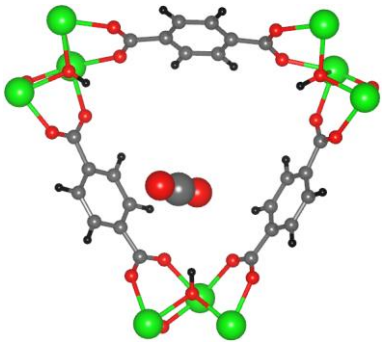


Figure S2. CO_2 adsorption structure at Site III shown from different direction. This structure resembles well the Wt site reported previously.[S1]

3. Adsorption Structures of Acetone

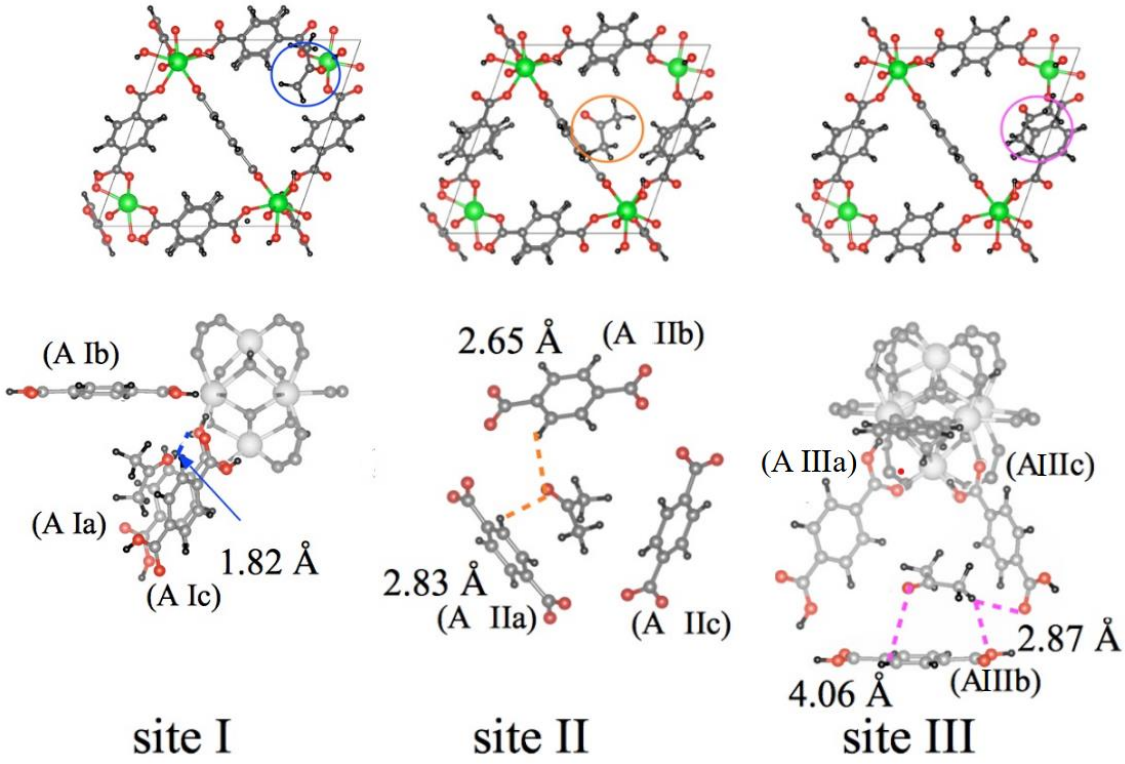


Figure S3. Acetone adsorption structures at Site I, II, and III.

Upper: Optimized geometry of one unit cell of UiO-66 with one adsorbed acetone molecule.

Lower: Three adsorption sites.

Small cluster models used for post-Hartree-Fock correction are represented by A Ia, A Ib, A Ic etc. where A means acetone.

4. Adsorption Structures of Methanol

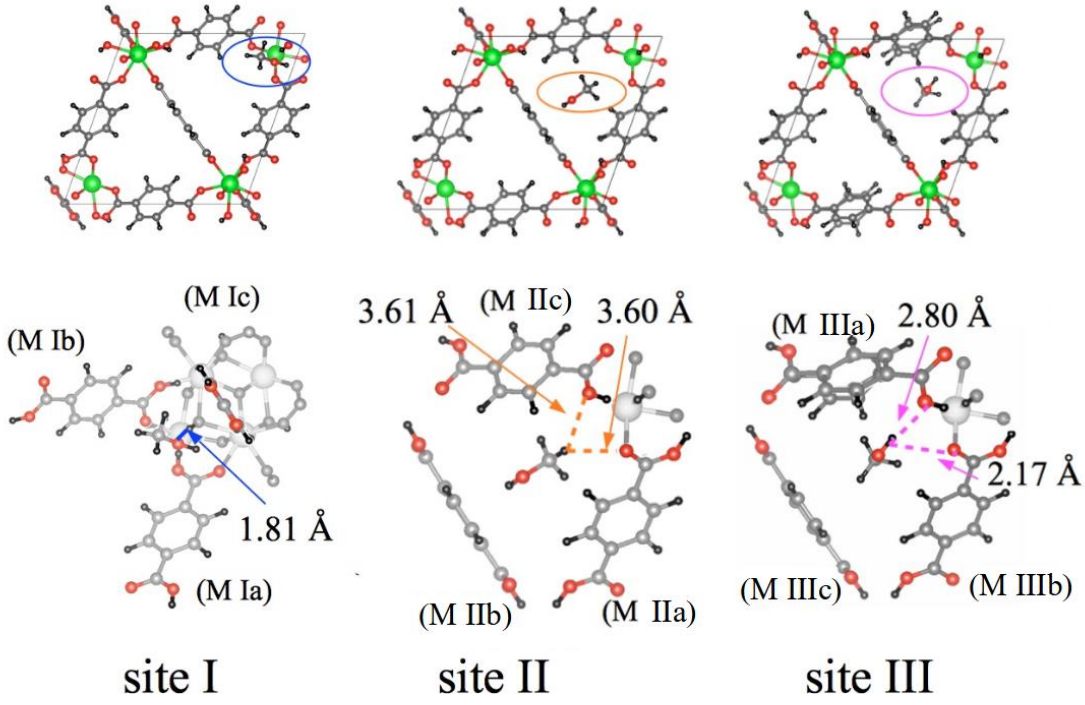


Figure S4. Methanol adsorption structures at Sites I, II, and III.

Upper: Optimized geometry of one unit cell in UiO-66 with one adsorbed methanol molecule.

Lower: Three adsorption sites.

Small cluster models used for post-Hartree-Fock correction are represented by M Ia, M Ib, M Ic etc. where M means methanol.

5. Comparison of interaction energy (in kcal/mol) of gas molecule with ligand moiety among several computational methods

Table S1. Comparison of interaction energy (in kcal/mol) between gas molecule and ligand moiety among CCSD(T), SCS-MP2, and MP2.5.[a]

	CCSD(T)	SCS-MP2	MP2.5
CO_2 Adsorption			
Site I_M [a]	-4.68	-3.88	-4.40
Site II	-2.61	-1.89	-2.37
Site III	-2.72	-1.95	-2.46
Acetone Adsorption			
Site I_M [a]	-9.36	-7.63	-9.08
Site II	-7.26	-6.09	-7.18
Site III	-7.48	-5.89	-7.32
Methanol Adsorption			
Site I_M [a]	-5.93	-4.3	-5.54
Site II	-6.62	-5.11	-6.45
Site III	-5.47	-4.51	-5.42

[a] Sites II and III are shown in Figure 2. Site I_M represents that the Zr-OH moiety is removed from Site I (Figure 2). We employed Site I_M here because CCSD(T) calculations could not be carried out due to the large size of Site I.

6. Comparison of interaction energy (in kcal/mol) of gas molecule with ligand moiety among several computational methods

Table S2. Interaction energies (in kcal/mol) between gas molecule (CO_2, acetone, and methanol) and ligand moieties.[a]

	MP2	SCS-MP2	MP3	MP2.5
	CO_2 Adsorption			
Ia	-1.02	-0.74	-0.59	-0.80
Ib	-1.82	-1.09	-0.73	-1.28
Ic	-2.78	-2.05	-1.86	-2.32
IIa	-1.19	-0.79	-0.77	-0.98
IIb	-0.88	-0.60	-0.55	-0.72
IIc	-0.88	-0.50	-0.46	-0.67
IIIa	-1.00	-0.70	-0.74	-0.87
IIIb	-0.68	-0.37	-0.34	-0.51
IIIc	-1.23	-0.88	-0.94	-1.08
	Acetone Adsorption			
Ia	-2.90	-1.81	-1.60	-2.25
Ib	-5.00	-3.58	-3.35	-4.17
Ic	-3.21	-2.24	-2.10	-2.66
IIa	-4.02	-2.69	-2.30	-3.16
IIb	-1.15	-0.88	-0.90	-1.03
IIc	-3.51	-2.52	-2.47	-2.99
IIIa	-1.83	-1.18	-1.31	-1.57
IIIb	-2.16	-1.24	-1.24	-1.70
IIIc	-4.49	-3.47	-3.61	-4.05
	Methanol Adsorption			
Ia	-1.48	-0.77	-0.68	-1.08
Ib	-2.09	-1.11	-1.12	-1.60
Ic	-3.10	-2.42	-2.61	-2.86
IIa	-3.41	-2.57	-2.91	-3.16
IIb	-3.28	-2.14	-2.33	-2.81
IIc	-0.53	-0.40	-0.44	-0.48
IIIa	-1.93	-1.40	-1.45	-1.69
IIIb	-2.14	-1.57	-1.62	-1.88
IIIc	-2.12	-1.54	-1.58	-1.8

[a] Ia, Ib, etc. are small cluster models presented in Figure 2.

7. Computational results of NMR shielding constants and skews.

Table S3. Hydrogen, carbon, and oxygen NMR shielding constants at each atom.

		UiO66+15CO_2	UiO-66 + CO_2			UiO66
atom			site I	site II	site III	
H	1	-16.9459	-18.8761	-18.8903	-18.9278	-19.0308
H	2	-16.946	-18.9297	-18.8404	-18.9539	-19.0308
H	3	-16.9459	-18.8453	-18.858	-19.0252	-19.0308
H	4	-17.0815	-18.8583	-18.8815	-18.912	-19.0308
H	5	-17.0815	-18.8619	-18.9437	-18.9045	-19.0308
H	6	-17.0815	-18.8609	-18.8599	-18.9162	-19.0308
H	7	-17.1234	-18.8427	-18.8706	-18.9104	-19.0307
H	8	-17.1234	-18.8476	-18.9484	-18.8883	-19.0307
H	9	-17.1234	-18.8616	-18.8484	-18.9355	-19.0307
H	10	-16.7647	-18.8663	-18.8609	-18.8857	-19.0308
H	11	-16.7646	-18.9273	-18.8295	-18.9254	-19.0307
H	12	-16.7646	-18.8491	-18.7075	-18.9758	-19.0308
H	13	-16.8522	-18.9154	-18.8131	-18.9004	-19.0307
H	14	-16.8521	-18.8431	-18.8313	-18.9614	-19.0308
H	15	-16.8522	-18.8425	-18.8527	-18.8967	-19.0307
H	16	-17.1244	-18.8616	-18.9536	-18.9074	-19.0308
H	17	-17.1245	-18.8786	-18.8887	-18.9543	-19.0308
H	18	-17.1244	-18.8373	-18.8744	-18.9322	-19.0308
H	19	-17.0707	-18.8759	-18.9658	-18.8925	-19.0308
H	20	-17.0707	-18.8755	-18.8851	-18.9299	-19.0308
H	21	-17.0707	-18.8607	-18.8602	-18.9428	-19.0308
H	22	-16.9669	-18.9157	-18.8288	-18.9191	-19.0308
H	23	-16.9669	-18.8748	-18.8369	-19.0062	-19.0307
H	24	-16.9669	-18.8588	-18.7178	-18.9258	-19.0307
H	25	-24.1366	-25.994	-25.9781	-26.0488	-26.1834
H	26	-24.1365	-24.7531	-25.969	-26.0325	-26.1839
H	27	-24.1366	-25.9947	-25.9741	-26.0249	-26.1839
H	28	-24.0899	-25.9925	-25.9868	-26.0345	-26.1833
C	1	166.0027	165.9329	165.5089	164.6864	164.5496
C	2	166.0022	165.8018	165.8641	164.6538	164.5497
C	3	166.002	166.1919	166.2359	164.8347	164.5492

C	4	167.6376	166.3393	165.872	164.5406	164.5497
C	5	167.6378	165.8853	166.7109	164.6485	164.5491
C	6	167.637	165.8335	165.7848	164.44	164.5492
C	7	169.1585	165.9389	165.9968	164.5894	164.5503
C	8	169.1584	165.7783	165.5752	165.236	164.5501
C	9	169.1591	165.8225	166.0614	164.534	164.5498
C	10	166.4998	165.9033	166.0749	164.6707	164.5496
C	11	166.5006	165.9832	165.9006	164.5912	164.5495
C	12	166.5003	165.9445	165.2003	164.4406	164.5501
C	13	167.0291	165.9294	165.8711	164.5374	164.5495
C	14	167.0294	165.8881	165.6022	164.4111	164.5501
C	15	167.0288	165.8235	166.1947	165.2196	164.5498
C	16	168.3677	165.7978	166.7716	164.7091	164.5496
C	17	168.3666	165.9118	165.886	164.606	164.5497
C	18	168.3668	166.0099	165.7996	164.5964	164.5492
C	19	166.3168	165.8871	165.5788	164.4226	164.5497
C	20	166.3179	165.9213	166.0241	164.4647	164.5496
C	21	166.3176	165.9825	166.0648	164.652	164.5492
C	22	167.2221	165.8006	165.9486	164.5817	164.5491
C	23	167.2218	166.3072	166.0868	164.7855	164.5501
C	24	167.2218	165.8558	165.2842	164.6387	164.5503
C	25	207.0273	206.3722	206.5504	205.1243	205.0333
C	26	207.0275	206.4852	206.7229	205.033	205.0331
C	27	207.0275	206.4963	206.5649	205.2711	205.0332
C	28	206.7781	206.5299	206.5809	205.1436	205.0333
C	29	206.7783	206.5755	206.5408	205.1898	205.0329
C	30	206.7787	206.5232	206.4048	205.3557	205.0329
C	31	206.7912	206.4822	206.5808	205.1379	205.0330
C	32	206.7915	206.5604	206.5308	205.1995	205.0332
C	33	206.7919	206.4832	206.4309	205.3611	205.0329
C	34	207.1763	206.4084	206.573	205.1537	205.0332
C	35	207.1764	206.5611	206.7275	205.0522	205.0329
C	36	207.1763	206.4696	206.5589	205.2329	205.0330
C	37	174.9014	172.4469	172.6455	171.4424	171.0610
C	38	174.9014	172.3619	172.4888	171.1795	171.0610
C	39	174.9013	172.15	172.4931	171.0756	171.0610
C	40	172.6362	172.7831	172.3721	171.1332	171.0612

C	41	172.636	172.7742	172.1193	171.154	171.0609
C	42	172.6364	172.4029	172.3709	170.8648	171.0610
C	43	173.7921	172.0878	172.3665	171.0745	171.0612
C	44	173.7919	172.2447	172.0637	171.2737	171.0611
C	45	173.7927	172.4084	172.3485	171.6976	171.0612
C	46	174.0853	172.436	172.8128	171.0812	171.0609
C	47	174.0856	172.3907	172.4901	171.1299	171.0611
C	48	174.0858	172.8741	172.6721	171.0627	171.0610
C	49	158.3677	158.0275	161.0757	156.6128	
C	50	158.3685				
C	51	158.3682				
C	52	162.5638				
C	53	162.5639				
C	54	162.5637				
C	55	162.6277				
C	56	162.6272				
C	57	162.6267				
C	58	159.1279				
C	59	159.1287				
C	60	159.1294				
C	61	158.9415				
C	62	158.9411				
C	63	158.9414				
O	1	330.0151	327.4032	327.8758	326.4889	325.7059
O	2	330.014	328.0384	327.3926	326.3536	325.7060
O	3	330.0124	325.8849	327.2065	326.5583	325.7055
O	4	330.2722	327.5082	327.3298	325.9145	325.7053
O	5	330.2773	326.6794	327.7815	326.8263	325.7054
O	6	330.2743	327.2787	327.076	325.5806	325.7078
O	7	329.3369	327.1927	327.5559	325.9483	325.7044
O	8	329.3378	327.4176	327.7519	326.3006	325.7041
O	9	329.3375	327.363	328.1322	325.7596	325.7059
O	10	329.0065	327.4417	327.557	325.1181	325.7055
O	11	329.0059	327.4692	327.2887	326.303	325.7059
O	12	329.0061	327.3757	327.9765	326.1704	325.7051
O	13	329.0019	327.3583	327.3932	326.0752	325.7059
O	14	329.0073	327.1642	327.3445	326.0191	325.7051

O	15	329.002	327.3352	327.491	326.4042	325.7059
O	16	330.33	327.383	327.8829	326.0288	325.7055
O	17	330.3291	327.5191	327.4406	325.9208	325.7053
O	18	330.3323	325.3275	327.3758	326.2577	325.7055
O	19	328.5539	326.873	327.6034	324.7851	325.7060
O	20	328.5557	327.3962	327.6656	325.7403	325.7059
O	21	328.5573	327.1504	327.8988	326.1512	325.7078
O	22	330.5802	328.0267	327.5914	326.0688	325.7054
O	23	330.5799	327.832	327.2794	326.4734	325.7041
O	24	330.5807	327.3739	328.7638	327.2736	325.7044
O	25	63.7493	68.539	67.9152	66.7867	66.6637
O	26	63.7489	64.2276	68.2994	67.2213	66.6665
O	27	63.7489	68.1203	68.2173	66.8249	66.6663
O	28	462.7973	462.4736	462.1935	460.419	66.6637
O	29	462.7945	462.2118	462.3387	460.4511	458.8087
O	30	462.798	462.4086	462.3794	461.1064	458.8079
O	31	87.3862	84.3407	88.7191	85.2981	458.8052
O	32	87.388	92.5063	86.5382	88.4151	458.8087
O	33	87.3876				
O	34	96.4756				
O	35	96.4775				
O	36	96.477				
O	37	97.1338				
O	38	97.1332				
O	39	97.1341				
O	40	91.5988				
O	41	91.5983				
O	42	91.5986				
O	43	88.1321				
O	44	88.1308				
O	45	88.1314				
O	46	97.7963				
O	47	97.7955				
O	48	97.7943				
O	49	96.6988				
O	50	96.6985				
O	51	96.7007				

O	52	93.5792				
O	53	93.5813				
O	54	93.5829				
O	55	105.5691				
O	56	105.5679				
O	57	105.5692				
O	58	92.8741				
O	59	92.8729				
O	60	92.8734				
O	61	67.9223	68.3149	67.8232	67.0971	
O	62	461.4949	462.3966	461.9827	460.4866	
Zr	1	1828.04	1823.766	1824.7781	1823.7208	1822.8816
Zr	2	1828.0276	1822.0395	1824.5496	1823.1292	1822.8855
Zr	3	1828.0603	1823.4958	1823.822	1823.1603	1822.8855
Zr	4	1825.8328	1822.2325	1824.5466	1823.8851	1822.8816
Zr	5	1825.8271	1823.9865	1824.5359	1823.1862	1822.8741
Zr	6	1825.7891	1824.6699	1823.7439	1823.1419	1822.8998

Table S4. Skews of hydrogen, carbon, and oxygen NMR peaks at each atom.

atom		UiO66+15CO_2	UiO66+1CO_2 site I	UiO66+1CO_2 site II	UiO66+1CO_2 site III	UiO66
H	1	0.1167	0.5267	0.5996	0.5176	0.5271
H	2	0.1167	0.4884	0.435	0.5363	0.5271
H	3	0.1167	0.5779	0.4532	0.5945	0.5271
H	4	0.5724	0.5827	0.4328	0.5713	0.5271
H	5	0.5724	0.5843	0.4484	0.5477	0.5271
H	6	0.5723	0.5231	0.5199	0.5465	0.5271
H	7	0.6206	0.505	0.5154	0.5418	0.5271
H	8	0.6205	0.5301	0.4573	0.6214	0.5271
H	9	0.6206	0.5553	0.3437	0.6187	0.5271
H	10	0.1047	0.5353	0.448	0.6001	0.5271
H	11	0.1048	0.591	0.5208	0.546	0.5271
H	12	0.1048	0.5153	0.1023	0.5009	0.5271
H	13	0.4152	0.5997	0.471	0.576	0.5271

H	14	0.4152	0.5286	0.5693	0.5118	0.5271
H	15	0.4152	0.5357	0.4576	0.5871	0.5271
H	16	0.7125	0.5241	0.4195	0.5193	0.5271
H	17	0.7124	0.5267	0.4285	0.6007	0.5271
H	18	0.7124	0.6529	0.5101	0.5449	0.5271
H	19	0.5523	0.5686	0.4499	0.6703	0.5271
H	20	0.5523	0.5318	0.5055	0.5381	0.5271
H	21	0.5523	0.5001	0.3439	0.5365	0.5271
H	22	0.5104	0.4969	0.509	0.5418	0.5271
H	23	0.5104	0.5441	0.4609	0.6015	0.5271
H	24	0.5104	0.5524	0.1787	0.5644	0.5271
H	25	0.8937	0.9603	0.9453	0.91	1
H	26	0.8937	0.9868	0.929	0.8915	1
H	27	0.8937	0.9571	0.9331	0.9601	1
H	28	1	0.9513	0.902	0.8807	1
C	1	0.3384	0.2922	0.2834	0.2989	0.2902
C	2	0.3384	0.292	0.291	0.2937	0.2902
C	3	0.3384	0.2992	0.2966	0.2983	0.2902
C	4	0.3366	0.3015	0.2911	0.2905	0.2902
C	5	0.3366	0.2895	0.3076	0.2978	0.2902
C	6	0.3366	0.2909	0.2879	0.2888	0.2902
C	7	0.3747	0.2949	0.2905	0.2909	0.2902
C	8	0.3747	0.2883	0.2908	0.3022	0.2902
C	9	0.3747	0.2902	0.297	0.2908	0.2902
C	10	0.3231	0.2909	0.2924	0.2972	0.2902
C	11	0.3231	0.2937	0.2896	0.2913	0.2902
C	12	0.3231	0.296	0.2924	0.2892	0.2902
C	13	0.3212	0.2923	0.2887	0.2891	0.2902
C	14	0.3212	0.2942	0.2826	0.2877	0.2902
C	15	0.3212	0.2896	0.2938	0.3011	0.2902
C	16	0.345	0.2894	0.31	0.298	0.2902
C	17	0.345	0.292	0.2915	0.2926	0.2902
C	18	0.345	0.2984	0.2892	0.2924	0.2902
C	19	0.3577	0.2909	0.2923	0.2988	0.2902
C	20	0.3577	0.2918	0.2917	0.2903	0.2902
C	21	0.3577	0.2979	0.2977	0.2932	0.2902
C	22	0.3284	0.2906	0.2904	0.2915	0.2902

C	23	0.3284	0.3018	0.2927	0.2961	0.2902
C	24	0.3284	0.2905	0.2967	0.2995	0.2902
C	25	0.0133	-0.0039	0.0032	0.0073	0.0132
C	26	0.0133	0.0207	0.0251	0.0066	0.0132
C	27	0.0133	0.0062	0.0103	0.0162	0.0132
C	28	-0.0164	0.0053	0.0048	0.0085	0.0132
C	29	-0.0165	0.0138	0.0019	0.0102	0.0132
C	30	-0.0164	0.015	-0.0052	0.0248	0.0132
C	31	-0.0231	0.0068	-0.0007	0.0151	0.0132
C	32	-0.0231	0.0134	0.0081	0.0098	0.0132
C	33	-0.0231	0.0029	-0.011	0.025	0.0132
C	34	0.0308	0.0085	0.0103	0.0074	0.0132
C	35	0.0308	0.0139	0.0261	0.0002	0.0132
C	36	0.0308	0.0062	0.004	0.0294	0.0132
C	37	0.3009	0.2785	0.2808	0.2861	0.2801
C	38	0.3009	0.2791	0.2771	0.2799	0.2801
C	39	0.3009	0.2903	0.2767	0.281	0.2801
C	40	0.293	0.2828	0.2747	0.2787	0.2801
C	41	0.293	0.2853	0.2753	0.288	0.2801
C	42	0.293	0.2781	0.2772	0.2812	0.2801
C	43	0.298	0.2866	0.277	0.2778	0.2801
C	44	0.298	0.2807	0.2752	0.2828	0.2801
C	45	0.298	0.2784	0.2747	0.2894	0.2801
C	46	0.2935	0.2793	0.2771	0.292	0.2801
C	47	0.2935	0.2789	0.2789	0.2795	0.2801
C	48	0.2935	0.2859	0.2722	0.2807	0.2801
C	49	0.99	0.9799	0.9851	0.9792	
C	50	0.99				
C	51	0.99				
C	52	0.9897				
C	53	0.9897				
C	54	0.9897				
C	55	0.98				
C	56	0.98				
C	57	0.98				
C	58	0.972				
C	59	0.972				

C	60	0.972				
C	61	0.9853				
C	62	0.9853				
C	63	0.9853				
O	1	0.5011	0.4663	0.472	0.4681	0.4621
O	2	0.5011	0.4698	0.4687	0.4688	0.4621
O	3	0.5011	0.473	0.4673	0.4646	0.4621
O	4	0.5084	0.4676	0.4641	0.4599	0.4621
O	5	0.5084	0.4634	0.4558	0.4726	0.4621
O	6	0.5084	0.4632	0.462	0.4625	0.4621
O	7	0.4967	0.4808	0.4625	0.4609	0.4621
O	8	0.4967	0.4589	0.4551	0.4646	0.4621
O	9	0.4967	0.4607	0.4613	0.4621	0.4621
O	10	0.4646	0.4662	0.4593	0.4524	0.4621
O	11	0.4646	0.4522	0.4614	0.4624	0.4621
O	12	0.4646	0.4606	0.4686	0.4559	0.4621
O	13	0.4794	0.4509	0.4609	0.4556	0.4621
O	14	0.4794	0.4774	0.4674	0.4555	0.4621
O	15	0.4794	0.4615	0.4554	0.4584	0.4621
O	16	0.4996	0.4589	0.4575	0.4673	0.4621
O	17	0.4996	0.4661	0.465	0.4628	0.4621
O	18	0.4996	0.4733	0.464	0.4648	0.4621
O	19	0.5044	0.4623	0.4603	0.4612	0.4621
O	20	0.5043	0.4637	0.4653	0.4622	0.4621
O	21	0.5044	0.4667	0.4654	0.4677	0.4621
O	22	0.4824	0.4692	0.4649	0.4625	0.4621
O	23	0.4824	0.4695	0.4685	0.4642	0.4621
O	24	0.4824	0.4612	0.4697	0.4732	0.4621
O	25	0.928	0.992	0.9923	0.9968	1
O	26	0.928	0.9396	0.9851	0.9843	1
O	27	0.928	0.9988	0.9838	0.9822	1
O	28	0.9734	0.9492	0.972	0.9863	1
O	29	0.9733	0.9989	0.9778	0.9614	0.9999
O	30	0.9734	0.9506	0.9844	0.9647	0.9999
O	31	0.9499	0.9594	0.9616	0.9328	0.9999
O	32	0.9499	0.9499	0.988	0.957	0.9999
O	33	0.9499				

O	34	0.9532				
O	35	0.9532				
O	36	0.9532				
O	37	0.9858				
O	38	0.9858				
O	39	0.9858				
O	40	0.9916				
O	41	0.9916				
O	42	0.9916				
O	43	0.9435				
O	44	0.9435				
O	45	0.9435				
O	46	0.971				
O	47	0.971				
O	48	0.971				
O	49	0.9615				
O	50	0.9615				
O	51	0.9616				
O	52	0.9399				
O	53	0.9399				
O	54	0.9399				
O	55	0.9435				
O	56	0.9435				
O	57	0.9435				
O	58	0.9149				
O	59	0.9149				
O	60	0.9149				
O	61	0.9999	0.9855	0.9914	0.9829	
O	62	0.9999	0.9425	0.996	0.9641	
Zr	1	-0.7916	-0.8231	-0.8239	-0.8233	-0.8287
Zr	2	-0.7915	-0.8214	-0.8237	-0.8176	-0.8287
Zr	3	-0.7913	-0.8212	-0.818	-0.8201	-0.8287
Zr	4	-0.7965	-0.8218	-0.8235	-0.8197	-0.8287
Zr	5	-0.7966	-0.8234	-0.8211	-0.8178	-0.8287
Zr	6	-0.7968	-0.8224	-0.8242	-0.8178	-0.8287

8. Reference

(S1) Chevreau, H.; Liang, W.; Kearley, G. J.; Duyker, S. G.; D'Alessandro, D. M.; Peterson, V. K. Concentration-dependent binding of CO_2 and CD_4 in UiO-66 (Zr). *J. Phys. Chem. C* **2015**, *119*, 6980–6987.