Supporting Information

for

Effects of Force Field Selection on the Computational Ranking of MOFs for CO_2 Separations

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Table S1. Potential parameters of the MOF atoms in UFF and Dreiding

Atom	σ_{UFF} (Å)	ε_{UFF} (K)	$\sigma_{Dreiding}$ (Å)	$\varepsilon_{Dreiding}$ (K)
Ag	2.80	18.13	2.80	18.13
Al	4.01	254.30	3.91	151.07
Be	2.45	42.80	2.45	42.80
C	3.43	52.87	3.47	47.89
Cd	2.54	114.81	2.54	114.81
Co	2.56	7.05	2.56	7.05
Cu	3.11	2.52	3.11	2.52
Fe	2.59	6.55	2.59	6.55
H	2.57	22.16	2.85	7.65
In	3.98	301.63	4.09	276.96
Mn	2.64	6.55	2.64	6.55
N	3.26	34.75	3.26	38.98
Ni	2.52	7.55	2.52	7.55
O	3.12	30.21	3.03	48.19
V	2.80	8.06	2.80	8.06
Zn	2.46	62.44	4.04	27.70
Zr	2.78	34.75	2.78	34.75

Table S2. The number of common MOFs in top 10 material rankings based on molecular simulations performed using Dreiding and UFF.

Performance evaluation metrics	CO_2/H_2	CO_2/N_2	CO_2/CH_4
S	8	8	9
ΔN (mol/kg)	6	6	8
S_{sp}	8	7	7
R (%)	7	8	8

Table S3. The Spearman's ranking correlation coefficient (SRCC) between Dreiding-based and UFF-based rankings of 100 MOFs.

All MOFs	CO_2/H_2	CO_2/N_2	CO_2/CH_4
S	0.9795	0.9826	0.9774
ΔN (mol/kg)	0.9567	0.9568	0.9521
S_{sp}	0.9774	0.9796	0.9726
R (%)	0.9635	0.9693	0.9699

Table S4. The five MOFs with the highest and lowest FFFs.

MOF	C	H	O	N	Metals	Others	FFF
EMIHAK	144	144	0	32	80 (In)	128 (S)	0.003
OWITIY	148	52	96	0	20 (Mn)	0	0.011
OWITAQ	144	48	96	0	16 (Zn)	0	0.014
OWIVAS	144	48	96	0	16 (Zn)	0	0.014
AVEROJ	12	12	0	18	6 (Cd)	6 (Cl)	0.014
FAYPUS	680	640	128	144	40 (Zn)	0	0.294
NUJCIE	56	80	0	48	8/8 (Cd/Ni)	0	0.333
OFERUN	96	120	0	48	12 (Zn)	0	0.387
LUXDEO	152	184	8	40	8 (Ag)	0	0.418
GUPCOK	480	672	0	192	48 (Cd)	0	0.466

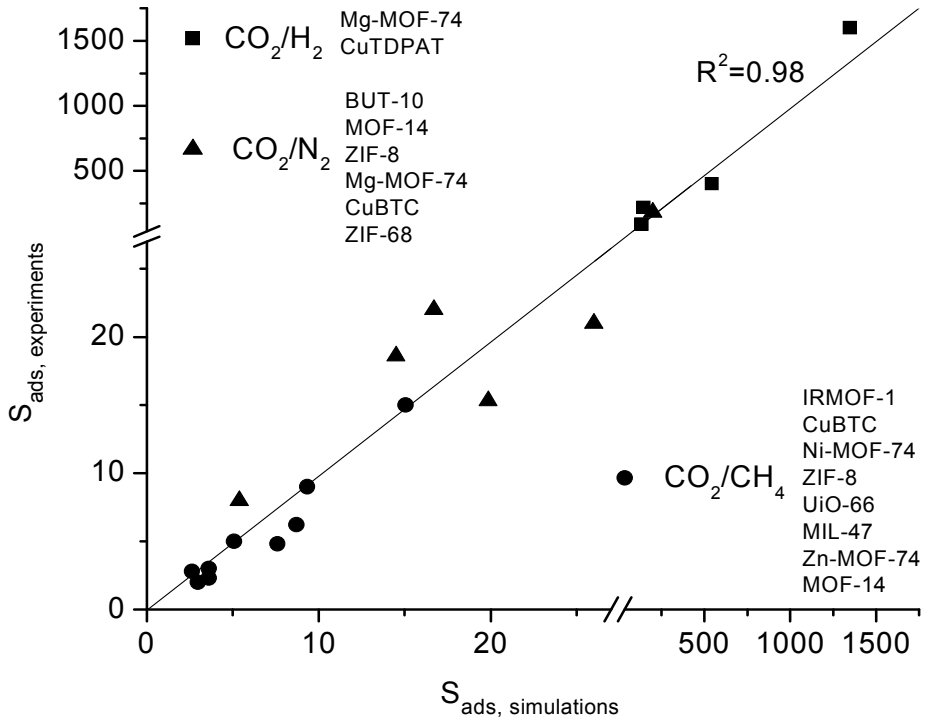

Figure S1. Comparison of simulation results with the experiments for CO_2/H_2, CO_2/N_2 and CO_2/CH_4 selectivities of various MOFs. The details of selectivity measurements can be seen in our previous publication.[1]

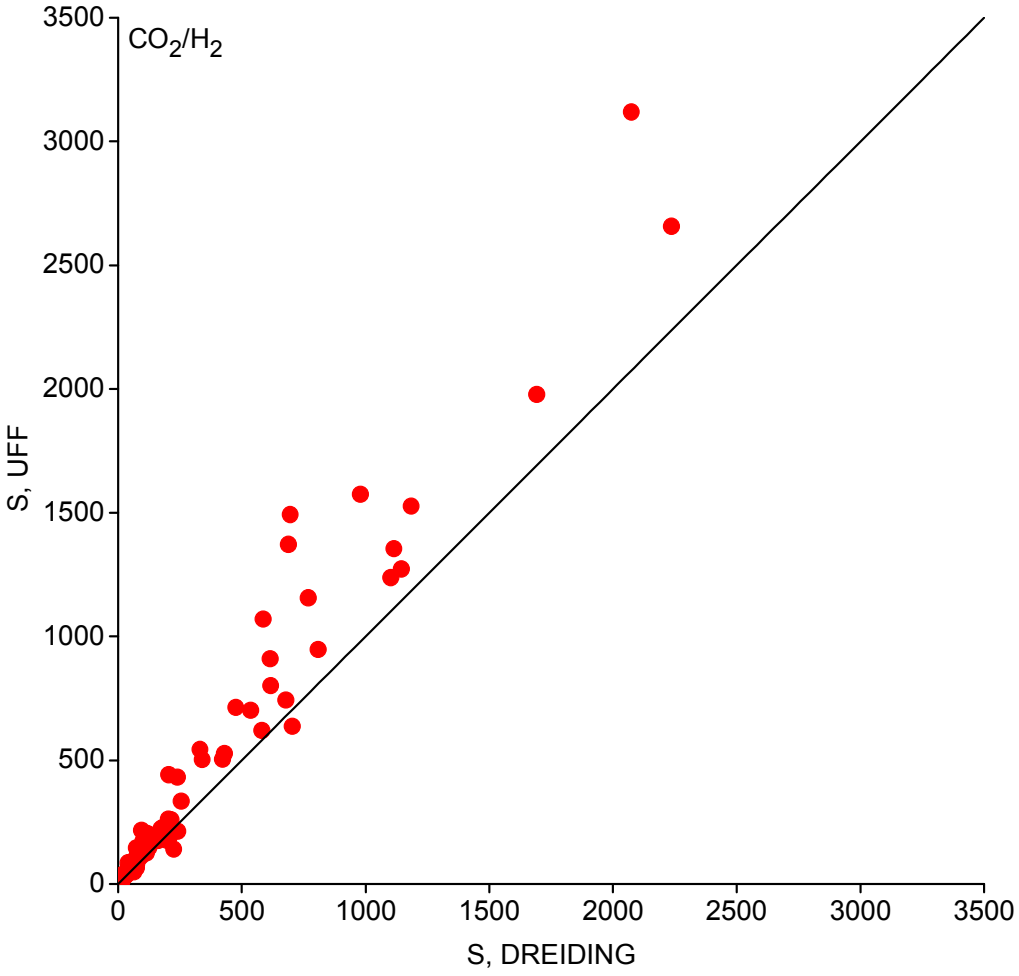

Figure S2. Comparison of CO_2/H_2 selectivities of MOFs calculated with Dreiding and UFF at 1 bar.

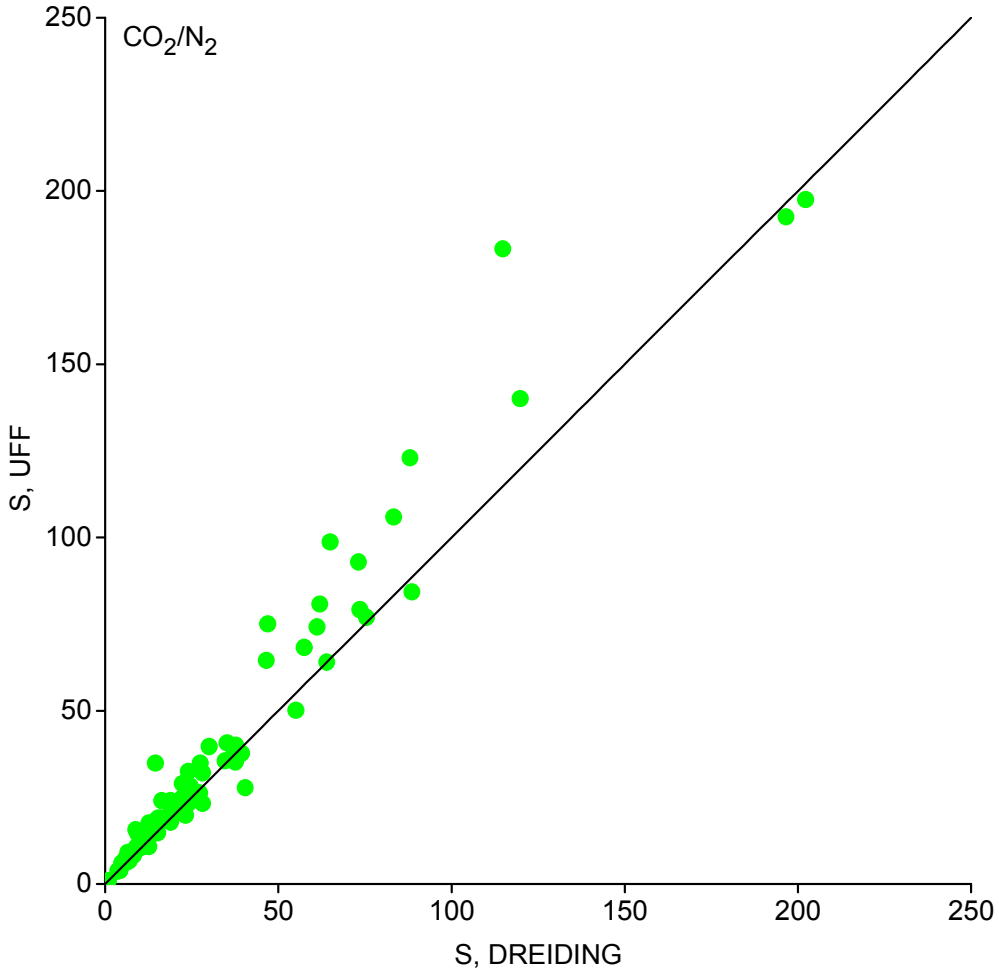

Figure S3. Comparison of CO_2/N_2 selectivities of MOFs calculated with Dreiding and UFF at 1 bar.

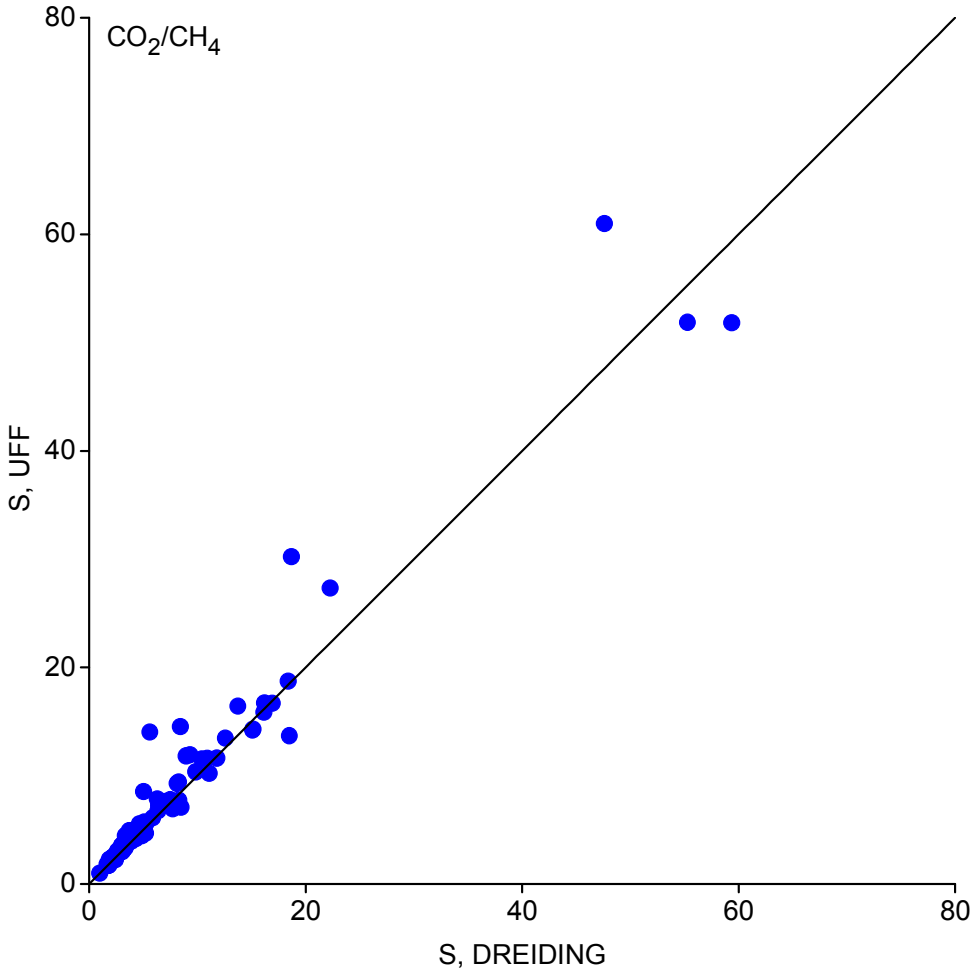

Figure S4. Comparison of CO_2/CH_4 selectivities of MOFs calculated with Dreiding and UFF at 1 bar.

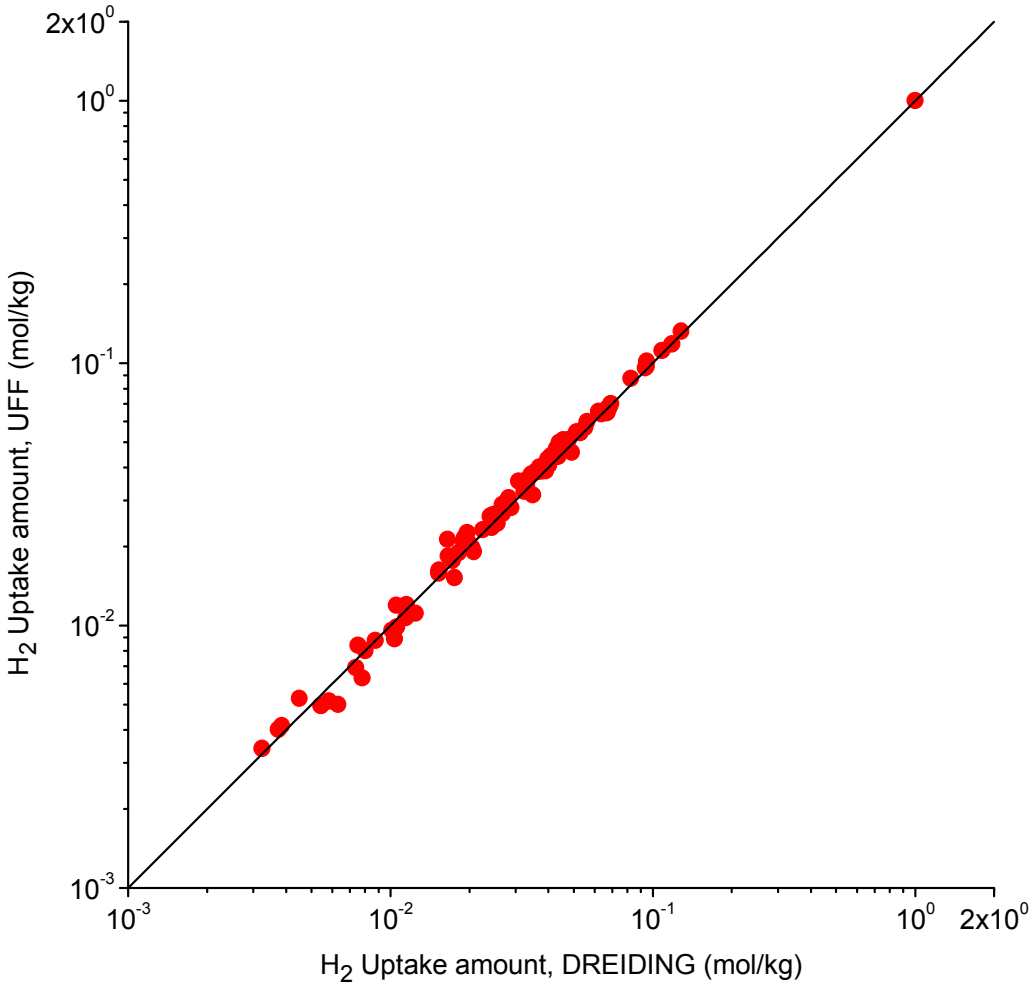

Figure S5. Comparison of H_2 uptakes of MOFs for CO_2/H_2 mixture calculated with Dreiding and UFF at 1 bar.

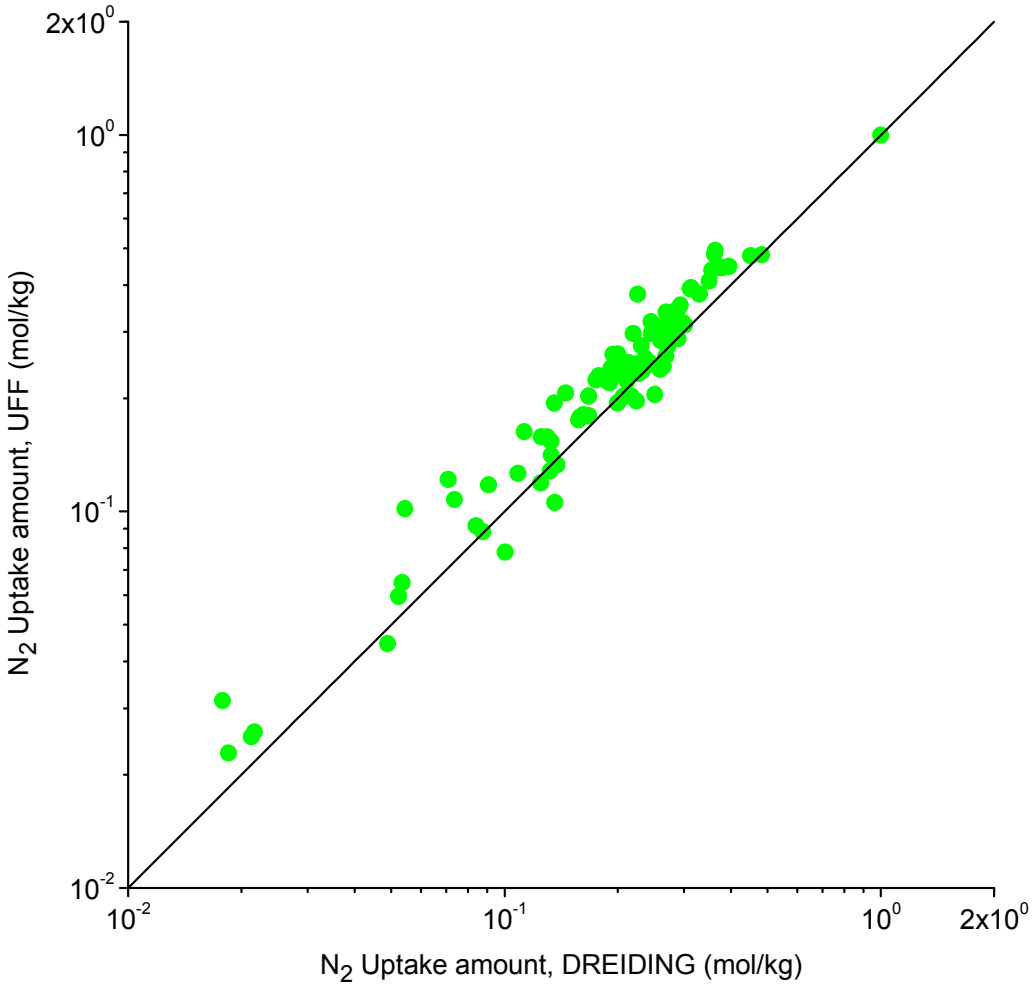

Figure S6. Comparison of N_2 uptakes of MOFs for CO_2/N_2 mixture calculated with Dreiding and UFF at 1 bar.

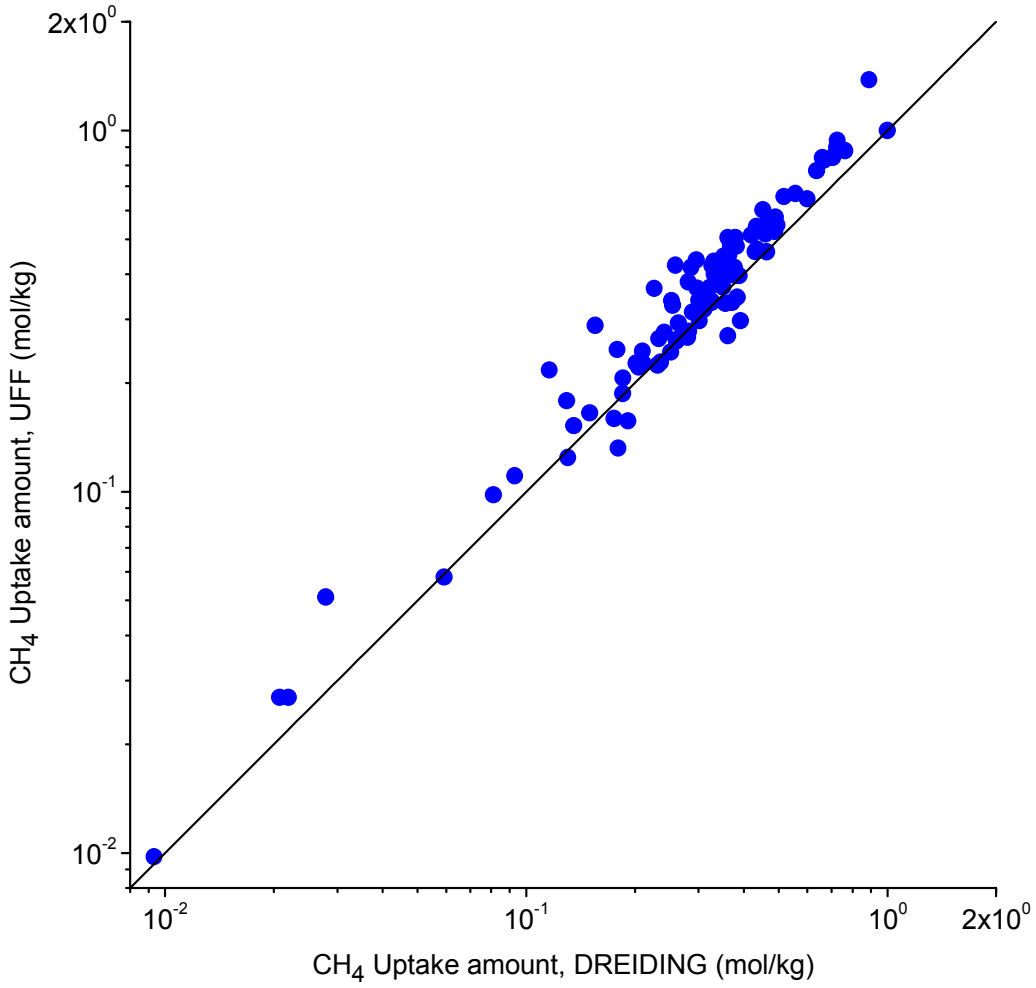

Figure S7. Comparison of CH_4 uptakes of MOFs for CO_2/CH_4 mixture calculated with Dreiding and UFF at 1 bar.

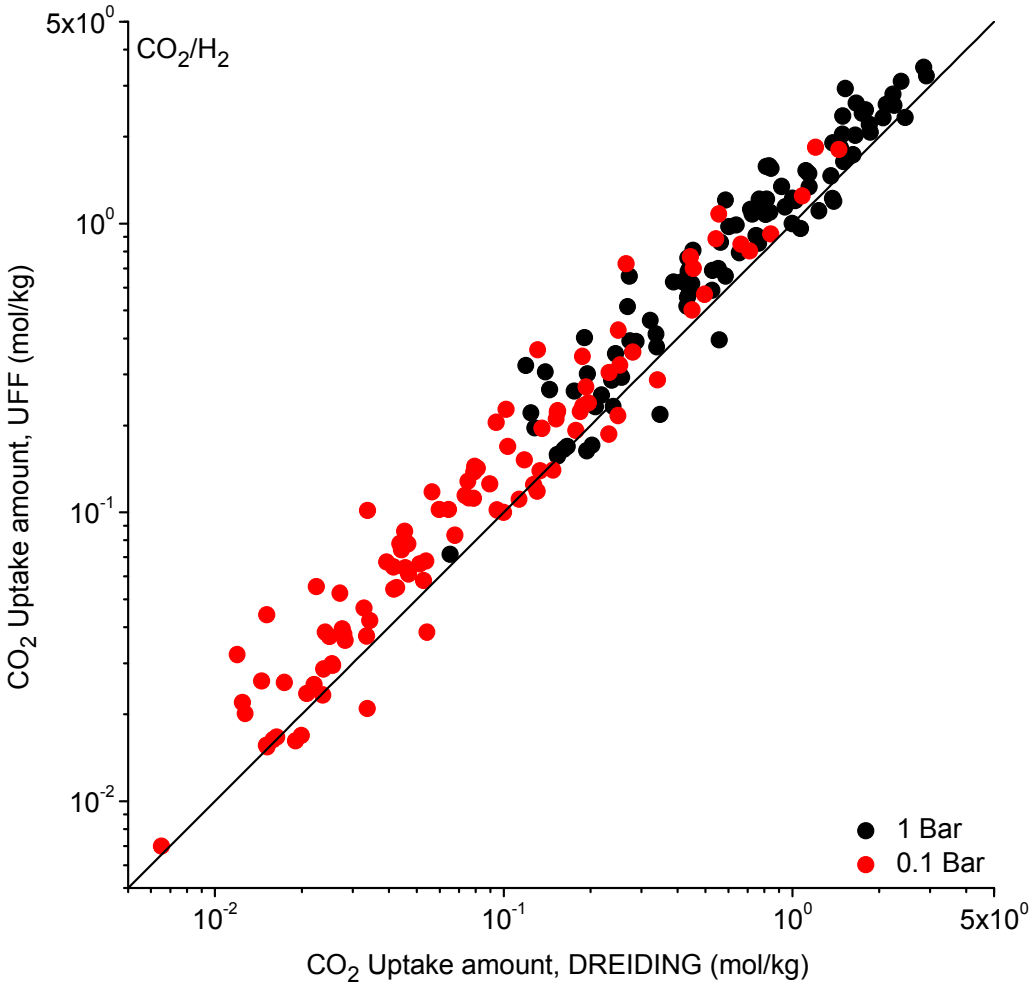

Figure S8. Comparison of CO_2 uptakes of MOFs for CO_2/H_2 mixture calculated with Dreiding and UFF at 0.1 and 1 bar.

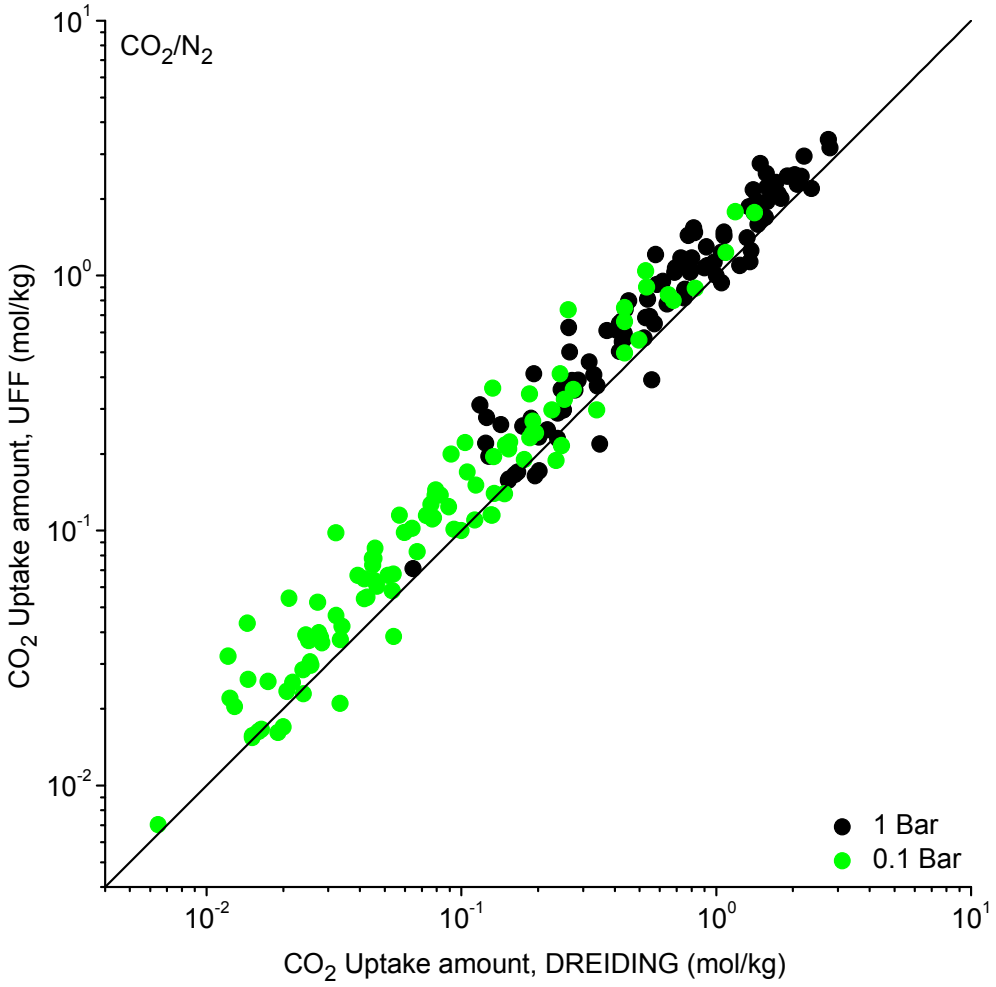

Figure S9. Comparison of CO_2 uptakes of MOFs for CO_2/N_2 mixture calculated with Dreiding and UFF at 0.1 and 1 bar.

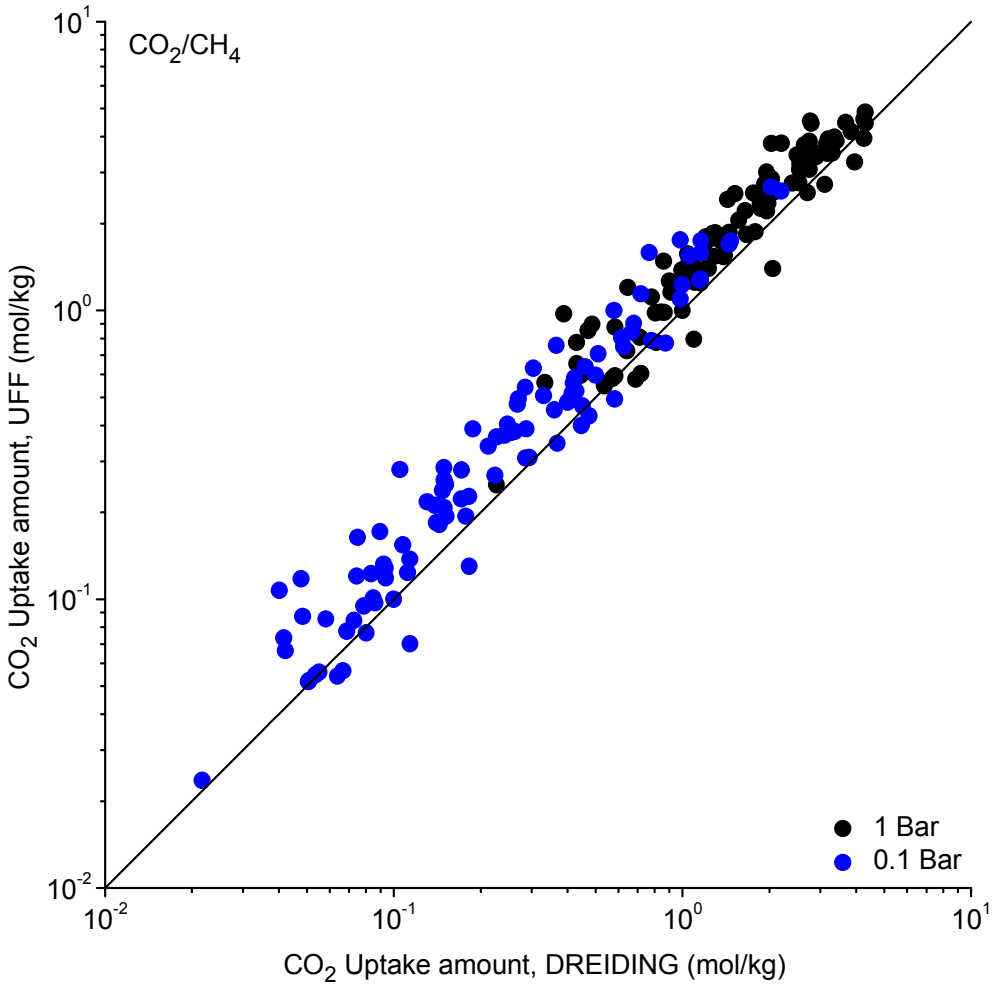

Figure S10. Comparison of CO_2 uptakes of MOFs for CO_2/CH_4 mixture calculated with Dreiding and UFF at 0.1 and 1 bar.

References:

1.Sumer, Z.; Keskin, S., Ranking of MOF Adsorbents for CO_2 Separations: A Molecular Simulation Study. *Ind Eng Chem Res* 2016, *55* (39), 10404-10419.