Electronic supplementary information

In silico screening of 4764 computation-ready, experimental metal–organic frameworks for CO_2 separation

Zhiwei Qiao, Kang Zhang and Jianwen Jiang[*]

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

Table S1. Lennard-Jones parameters of CoRE-MOFs.

Atom	ε/k_B [K]	σ [Å]	Atom	ε/k_B [K]	σ [Å]	Atom	ε/k_B [K]	σ [Å]
Ac	16.60	3.10	Ge	190.69	3.81	Po	163.52	4.20
Ag	18.11	2.80	Gd	4.53	3.00	Pr	5.03	3.21
Al	254.09	4.01	H	22.14	2.57	Pt	40.25	2.45
Am	7.04	3.01	Hf	36.23	2.80	Pu	8.05	3.05
Ar	93.08	3.45	Hg	193.71	2.41	Ra	203.27	3.28
As	155.47	3.77	Ho	3.52	3.04	Rb	20.13	3.67
At	142.89	4.23	I	170.57	4.01	Re	33.21	2.63
Au	19.62	2.93	In	301.39	3.98	Rh	26.67	2.61
B	90.57	3.64	Ir	36.73	2.53	Rn	124.78	4.25
Ba	183.15	3.30	K	17.61	3.40	Ru	28.18	2.64
Be	42.77	2.45	Kr	110.69	3.69	S	137.86	3.59
Bi	260.63	3.89	La	8.55	3.14	Sb	225.91	3.94
Bk	6.54	2.97	Li	12.58	2.18	Sc	9.56	2.94
Br	126.29	3.73	Lu	20.63	3.24	Se	146.42	3.75
C	52.83	3.43	Lr	5.53	2.88	Si	202.27	3.83
Ca	119.75	3.03	Md	5.53	2.92	Sm	4.03	3.14
Ca	119.75	3.03	Mg	55.85	2.69	Sn	285.28	3.91
Cd	114.72	2.54	Mn	6.54	2.64	Sr	118.24	3.24
Ce	6.54	3.17	Mo	28.18	2.72	Ta	40.75	2.82
Cf	6.54	2.95	N	34.72	3.26	Tb	3.52	3.07
Cl	114.21	3.52	Na	15.09	2.66	Tc	24.15	2.67
Cm	6.54	2.96	Ne	21.13	2.66	Te	200.25	3.98
Co	7.04	2.56	Nb	29.69	2.82	Th	13.08	3.03
Cr	7.55	2.69	Nd	5.03	3.18	Ti	8.55	2.83
Cu	2.52	3.11	No	5.53	2.89	TI	342.14	3.87
Cs	22.64	4.02	Ni	7.55	2.52	Tm	3.02	3.01
Dy	3.52	3.05	Np	9.56	3.05	U	11.07	3.02
Eu	4.03	3.11	O	30.19	3.12	V	8.05	2.80
Er	3.52	3.02	Os	18.62	2.78	W	33.71	2.73
Es	6.04	2.94	P	153.46	3.69	Xe	167.04	3.92
F	25.16	3.00	Pa	11.07	3.05	Y	36.23	2.98
Fe	6.54	2.59	Pb	333.59	3.83	Yb	114.72	2.99
Fm	6.04	2.93	Pd	24.15	2.58	Zn	62.39	2.46
Fr	25.16	4.37	Pm	4.53	3.16	Zr	34.72	2.78
Ga	208.81	3.90						

Table S2. Lennard-Jones parameters and charges of CO_2, N_2 and CH_4.

Atom	ε/k_B [K]	σ [Å]	Charge	Atom	ε/k_B [K]	σ [Å]	Charge
C_CO_2	27.0	2.80	+0.70	N_N_2	36.0	3.31	−0.482
O_CO_2	79.0	3.05	−0.35	com_N_2	0.00	0.00	+0.964
CH_4	148.0	3.73	0.00				

(a) United-atom model of CH_4

(b) Three-site model of N_2

(c) Three-site model of CO_2
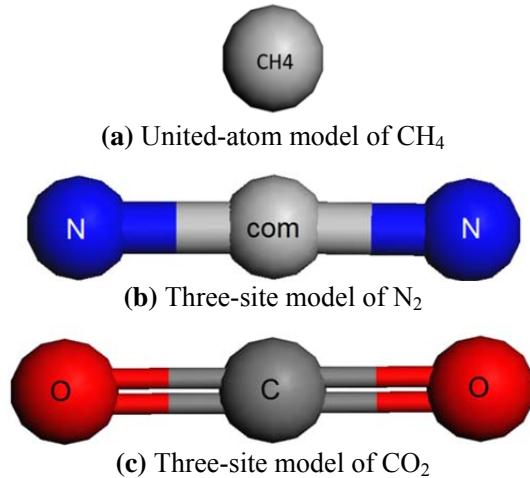
Figure S1. Models of CH_4, N_2 and CO_2.
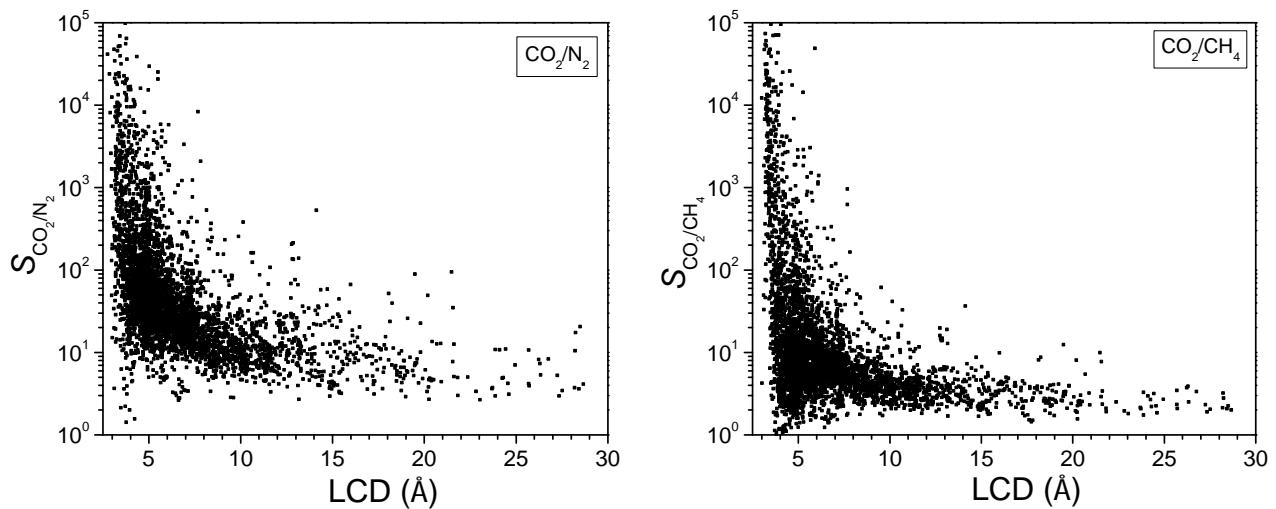

Figure S2. Relationships between selectivity S and LCD.
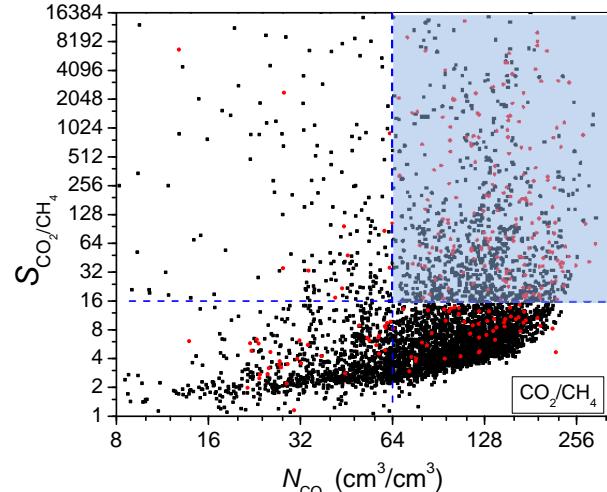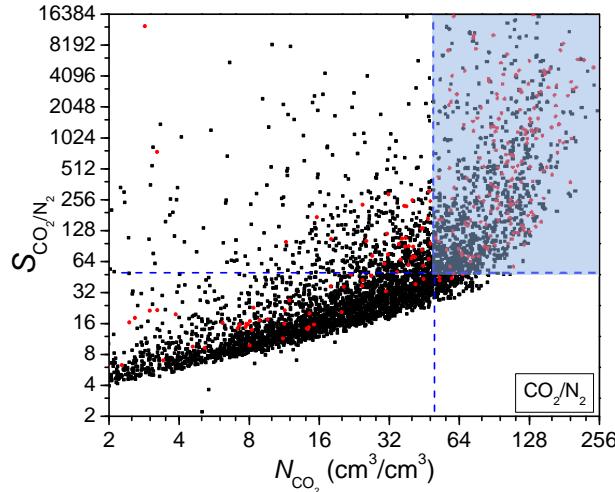
Figure S3. Relationships between selectivity S and CO_2 adsorption capacity N_{CO_2}. The red points indicate alkali- and alkaline-MOFs.
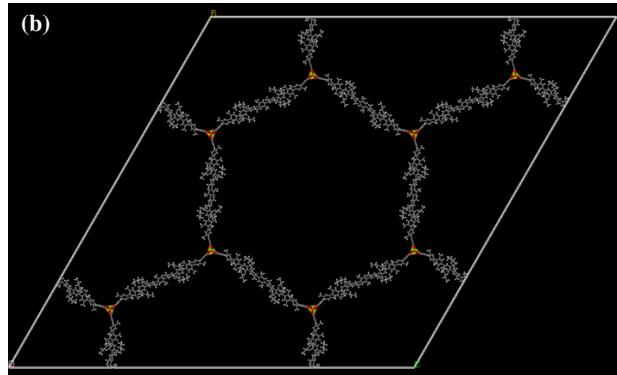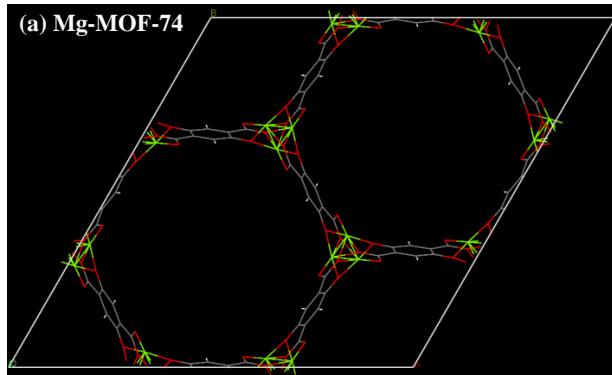

Figure S4. Mg-MOFs with different organic linkers.
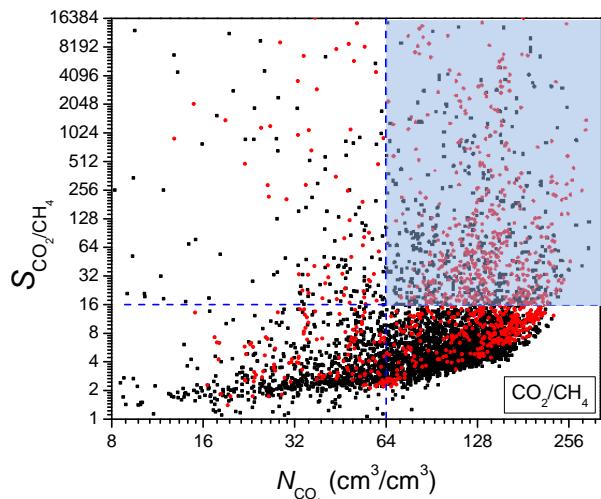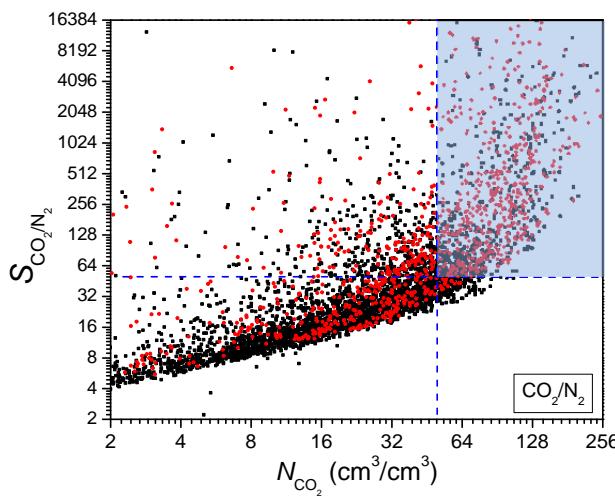
Figure S5. Relationships between selectivity S and CO_2 adsorption capacity N_{CO_2}. The red points indicate lanthanide-MOFs.
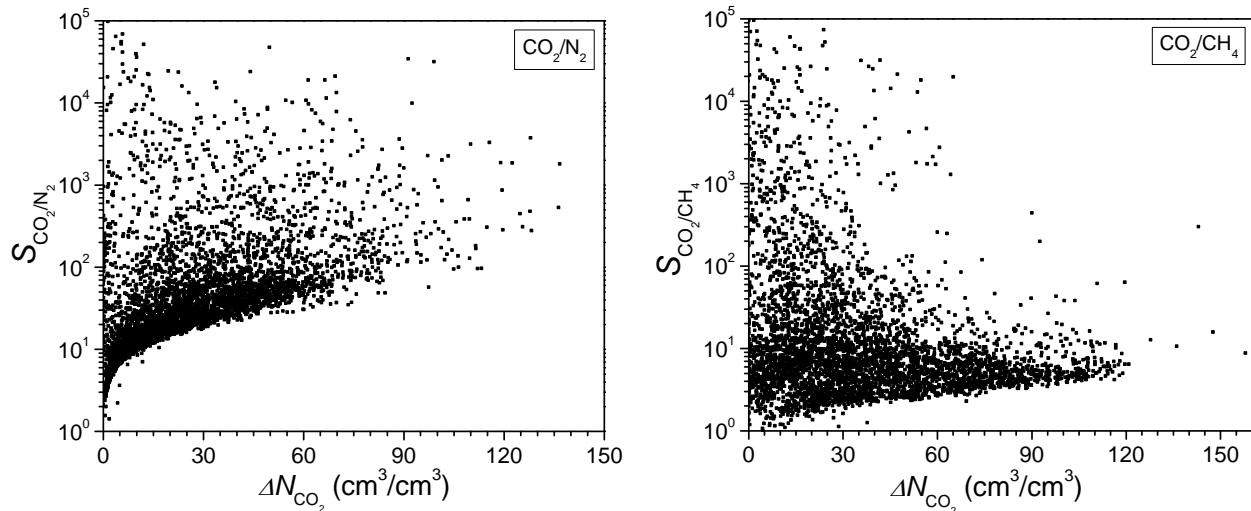
Figure S6. Relationships between selectivity S and working capacity ΔN_{CO_2}.
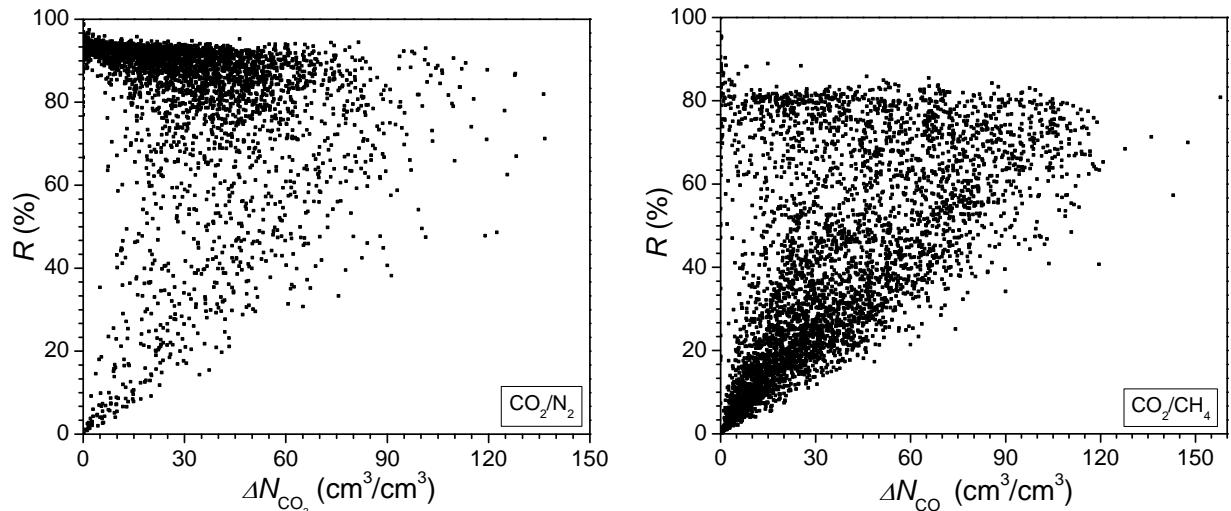
Figure S7. Relationships between regenerability R and working capacity ΔN_{CO_2}.

Table S3. Fixed-bed parameters.

Notation	Meaning	Value
L_b	bed length (m)	0.2
ε_b	bed voidage	0.4
v	interstitial feed velocity (m/s)	0.07
R_p	particle radius (cm)	0.15
τ_p	tortuosity	3