Supporting Information

Kinetic Effects in Predicting Adsorptions Using GCMC Method – Using CO_2 Adsorption on ZIFs as an Example

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Table S1. Chemical potential (K) of CO_2 calculated at different pressures and 298K

Pressure (kPa)	Chemical Potential (K)
0.01	-7592.297
0.05	-7112.890
0.1	-6906.055
0.5	-6426.704
1	-6220.019
5	-5740.344
10	-5533.726
20	-5327.698
30	-5206.790
40	-5121.303
50	-5055.190
60	-5000.872
70	-4954.931
80	-4915.098
90	-4880.221
100	-4849.459
120	-4794.889
150	-4728.988
200	-4644.168
500	-4374.358
1000	-4175.098
2000	-3981.250
2500	-3921.657
3000	-3875.054

Table S2. MSM force field parameters for CO_2.

	$R^0(\text{Å})$	ε (kJ/mol)	q(e)
C_CO_2	3.13	0.2467	0.576
O_CO_2	3.38	0.6903	0.288

Figure S1. The models using MD simulation to investigate desorption behaviors (a) and adsorption behaviors (b).
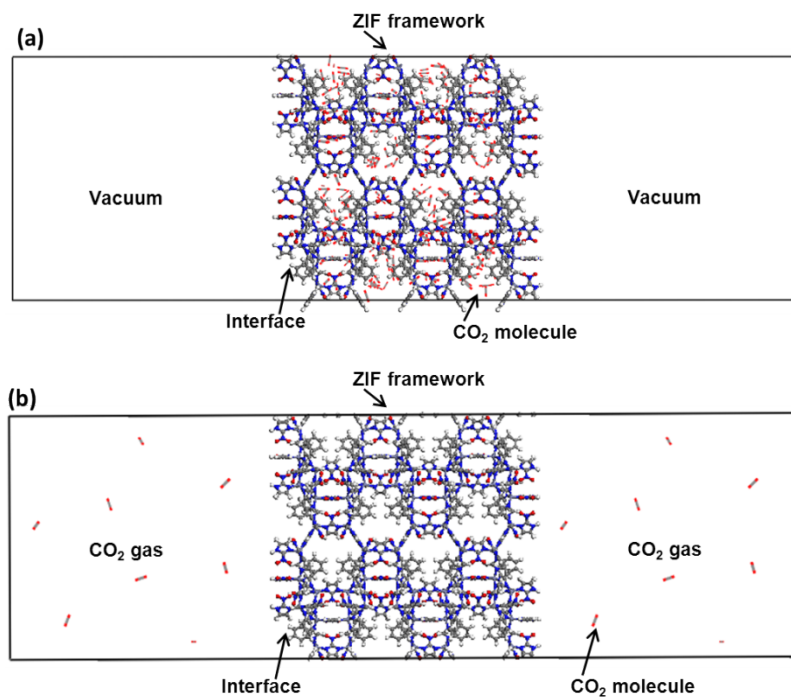
Figure S2. Comparison of energy differences between the FF and ab initio results of all data.