Supplementary Information

Molecular Modeling of CO_2 and *n*-octane in Solubility Process and α-quartz Nanoslit

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Table S1. Lennard-Jones parameters and charges for the CO_2 and *n*-octane.

	σ (nm)	ε (kJ/mol)	q (e)
C (CO_2)	0.2800	0.2340	+0.6516
O (CO_2)	0.3028	0.6682	-0.3258
CH_3 (*n*-octane)	0.3910	0.8647	0.0000
CH_2 (*n*-octane)	0.3930	0.3808	0.0000

Table S2. Lennard-Jones parameters and charges for α-quartz.

	σ (nm)	ε (kJ/mol)	q (e)
Si	0.3303	7.7×10^{-6}	+2.1000
O_B[1]	0.3166	0.6506	-1.0500
O_H[2]	0.3166	0.6506	-0.9500
H	0.0000	0.0000	+0.4250

[1] OB refers to the bridging oxygen.[2] OH refers to the hydroxyl oxygen.

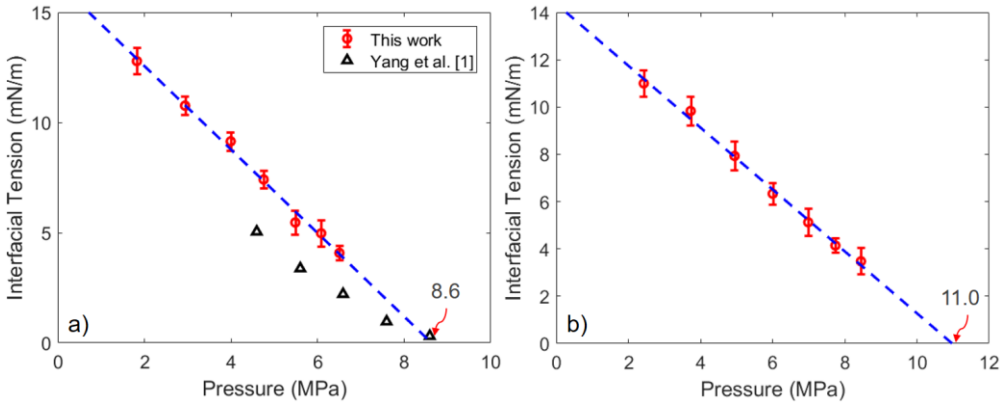

Figure S1. Interfacial tensions of CO_2 + *n*-octane binary system as a function of the pressure at (**a**) 323.15K and (**b**) 348.25 K. Red circles are the simulation results. Black triangles are the experimental results of Yang et al [1]. Blue dash line comes from the linear fitting: IFT = −1.894P + 16.3526 (323.15K) and IFT = −1.3089P + 14.3639 (348.25K).

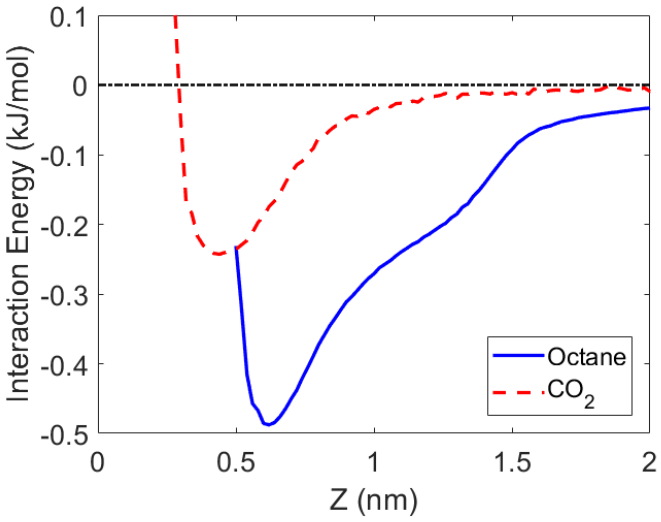

Figure S2. The interaction energy of *n*-octane and CO_2 on *α*-quartz surface.

To understand the stronger adsorption of CO_2, the interaction energies of *n*-octane and CO_2 on *α*-quartz surface are calculated. The interaction energy consists of two parts: van der Waals interaction (Lennard-Jones potential in this work) and Coulomb interaction. Although the potential well of *n*-octane is lower, the following three reasons still make CO_2 easier to adsorb on the surface of *α*-quartz: (1) the position of CO_2 potential well is closer to the surface, which will mainly determine the position of adsorbed layer. This position is affected by the parameter σ in Lennard-Jones potential. Other impact parameters include orientation of molecules, rigidity of molecules and so on. (2) The volume of CO_2 is small that CO_2 is easily absorbed in the gap between oil and *α*-quartz surface, which is determined by the size of molecules. Mehana et al. also found that the molecular size of the gas plays an important role in the adsorption process [2]. (3) This interaction energy is the interaction of whole molecule with *α*-quartz surface. The lower potential well is mainly because there are more atoms in oil molecule. If the interaction energy per atom or the interaction energy per unit weight are calculated, the CO_2 potential well will be lower, which is determined by the parameter both σ and ε in Lennard-Jones potential.

Reference

1. Yang, Z.; Li, M.; Peng, B.; Lin, M.; Dong, Z.; Ling, Y. Interfacial tension of CO_2 and organic liquid under high pressure and temperature. *Chin. J. Chem. Eng.* **2014**, *22*, 1302–1306, doi:10.1016/j.cjche.2014.09.042.
2. Mehana, M.; Fahes, M.; Huang, L. The Density of Oil/Gas Mixtures: Insights From Molecular Simulations. *SPE Journal* **2018**, 10.2118/187297-PA, doi:10.2118/187297-PA.