

Supporting information

Adsorption properties of CH₄ and CO₂ in quartz nanopores studied by molecular simulation

Haoyang Sun,^a Wenchao Sun,^b Hui Zhao,^a Yange Sun,^a Dianrui Zhang,^a Xiaoqing Qi,^a
and Ying Li*,^a

^aKey Laboratory of Colloid and Interface Chemistry of State Education Ministry, Shandong University, Jinan, Shandong 250100, P. R. China

^bSchool of Petroleum Engineering, China University of petroleum (East China), Qingdao, Shandong 266580, P. R. China

Corresponding author:

Ying Li

Tel:(86) 0531-88362078

Fax: (86) 0531-88364464

Email: yingli@sdu.edu.cn

Table S1. Parameters of the Langmuir isotherms model of pure CH₄ in nanopore

Temperature (K)	Langmuir constants		correlation coefficient (R ²)
	V _L (N/nanopore)	b (1/kPa)	
313	75.12	9.39×10 ⁻⁵	0.9997
323	74.03	8.44×10 ⁻⁵	0.9998
333	73.88	1.10×10 ⁻⁴	0.9995
353	71.95	7.05×10 ⁻⁵	0.9994
373	69.16	6.19×10 ⁻⁵	0.9996

Table S2. Parameters of the Langmuir isotherms model of pure CO₂ in nanopore

Temperature (K)	Langmuir constants		correlation coefficient (R ²)
	V _L (N/nanopore)	b (1/kPa)	
303	95.48	8.25×10 ⁻⁴	0.9989
313	94.87	6.18×10 ⁻⁴	0.9993
323	93.81	4.86×10 ⁻⁴	0.9988
333	91.61	4.25×10 ⁻⁴	0.9981
353	90.23	2.87×10 ⁻⁴	0.9994
373	89.55	1.97×10 ⁻⁴	0.9980