OPEN ACCESS
computation
ISSN 2079-3197
www.mdpi.com/journal/computation

Supplementary Information

Molecular Simulation of Shale Gas Adsorption and Diffusion in Clay Nanopores. *Computation* 2015, *3*, 687-700

Hongguang Sui, Jun Yao * and Lei Zhang

School of Petroleum Engineering, China University of Petroleum, Qingdao, Shandong 266580, China; E-Mail: suihg@upc.edu.cn (H.S.); zhlei84@163.com (L.Z.)

* Author to whom correspondence should be addressed; E-Mail: RCOGFR_UPC@126.com; Tel.: +86-532-86981829.

Table S1. Atomic positions and effective charges in the unit cell.

Atom	*x* (nm)	*y* (nm)	*z* (nm)	*q* (e)
O	0.264	0.0	0.328	−0.8
O	0.132	0.228	0.328	−0.8
O	0.396	0.228	0.328	−0.8
O (OH)	0.0	0.0	0.106	−1.7175
H (OH)	0.08815	0.0	0.1434	0.7175
Si	0.264	0.152	0.273	1.2
Si	0.0	0.305	0.273	1.2
O	0.264	0.152	0.106	−1.0
O	0.0	0.305	0.106	−1.0
Al	0.44	0.152	0.0	3.0
Al	0.44	−0.152	0.0	3.0
O	0.0	0.457	0.328	−0.8
O	0.396	0.685	0.328	−0.8
O	0.132	0.685	0.328	−0.8
O (OH)	0.264	0.457	0.106	−1.7175
H (OH)	0.35215	0.457	0.1434	0.7175
Si	0.0	0.609	0.0.273	1.2
Si	0.264	0.762	0.273	1.2
O	0.0	0.609	0.106	−1.0
O	0.264	0.762	0.106	−1.0
Al	0.704	0.609	0.0	3.0
Al	0.704	0.305	0.0	3.0
O	0.088	0.914	−0.328	−0.8
O	0.22	0.686	−0.328	−0.8
O	−0.044	0.686	−0.328	−0.8
O (OH)	0.352	0.914	−0.106	−1.7175

Table S1. *Cont.*

Atom	*x* (nm)	*y* (nm)	*z* (nm)	*q* (e)
H (OH)	0.26385	0.914	−0.1434	0.7175
Si	0.088	0.762	−0.273	1.2
Si	0.352	0.609	−0.273	1.2
O	0.088	0.762	−0.106	−1.0
O	0.352	0.609	−0.106	−1.0
O	0.352	0.457	−0.328	−0.8
O	−0.044	0.229	−0.328	−0.8
O	0.22	0.229	−0.328	−0.8
O (OH)	0.088	0.457	−0.106	−1.7175
H (OH)	−0.00015	0.457	−0.1434	0.7175
Si	0.352	0.305	−0.273	1.2
Si	0.088	0.152	−0.273	1.2
O	0.352	0.305	−0.106	−1.0
O	0.088	0.152	−0.106	−1.0
Mg	0.704	0.609	0.0	2
Na^+				1

The total potential of COMPASS force field is described by the equation

$$\begin{aligned} E_{poential} &= \sum_b \left[k_2 (b-b_0)^2 + k_3 (b-b_0)^3 + k_4 (b-b_0)^4 \right] \\ &+ \sum_\theta \left[k_2 (\theta-\theta_0)^2 + k_3 (\theta-\theta_0)^3 + k_4 (\theta-\theta_0)^4 \right] \\ &+ \sum_\phi \left[k_1 (1-\cos\phi) + k_2 (1-\cos 2\phi) + k_3 (1-\cos 3\phi) \right] \\ &+ \sum_\chi k_2 \chi + \sum_{b,b'} k (b-b_0)(b'-b_0') + \sum_{b,\theta} k (b-b_0)(\theta-\theta_0) \\ &+ \sum_{b,\theta} k (b-b_0)\left[k_1 \cos\phi + k_2 \cos 2\phi + k_3 \cos 3\phi \right] \\ &+ \sum_{\theta,\phi} k (\theta-\theta_0)\left[k_1 \cos\phi + k_2 \cos 2\phi + k_3 \cos 3\phi \right] \\ &+ \sum_{b,\theta} k (\theta'-\theta_0')(\theta-\theta_0) + \sum_{\theta,\theta,\phi} k (\theta'-\theta_0')(\theta-\theta_0)\cos\phi \\ &+ E_{el} + E_{vdW} \end{aligned} \tag{A1}$$

where the equation consists of two parts, which were bond terms include bond stretching term (b), angle bending term (θ), torsion angle term (φ) and out-of-plane bending term (χ) and nonbond terms, namely a LJ-9-6 function for the van der Waals (vdW) term and a Coulombic function for an electrostatic interaction, described by the following equations

$$E_{vdW} = \sum_{i,j} \varepsilon_{ij} \left[2 \left(\frac{r_{ij}^0}{r_{ij}} \right)^9 - 3 \left(\frac{r_{ij}^0}{r_{ij}} \right)^6 \right] \tag{A2}$$

$$E_{el} = \sum_{i,j} \frac{q_i q_j}{r_{ij}} \tag{A3}$$

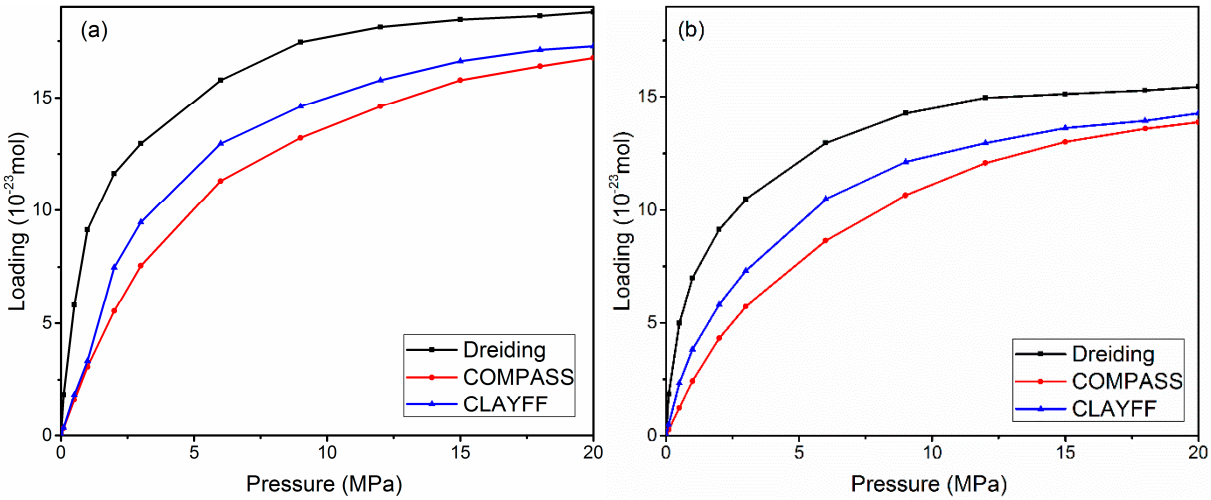

Figure S1. The adsorption isotherm of methane in 1.0 nm MMT pores with different forcefields. (**a**) Without cation exchange structure and (**b**) with cation exchange structure.