The Journal of Physical Chemistry B

Methane Aqueous Fluids in Montmorillonite Clay Interlayer under Near-Surface Geological Conditions: A Grand Canonical Monte Carlo and Molecular Dynamics Simulation Study

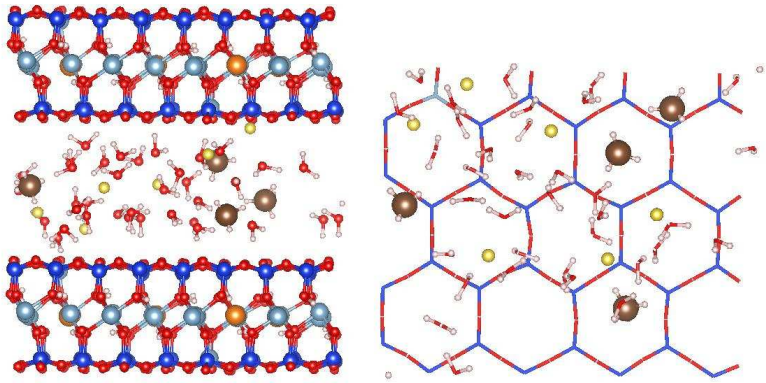
Qi Rao and Yongsheng Leng*

Department of Mechanical and Aerospace Engineering

The George Washington University

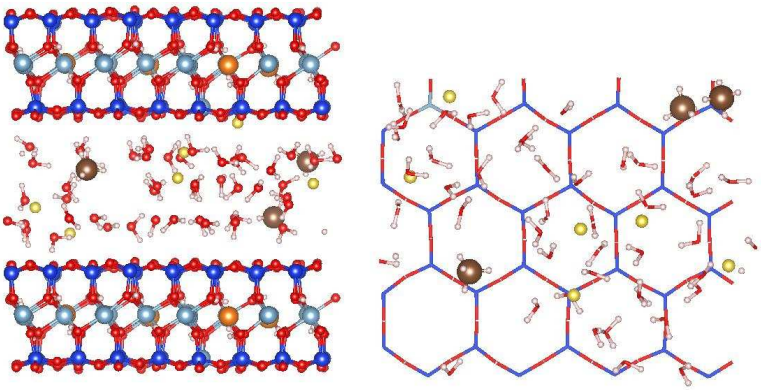
Washington, DC 20052, USA

Supplemental information for Figure S1 and S2:

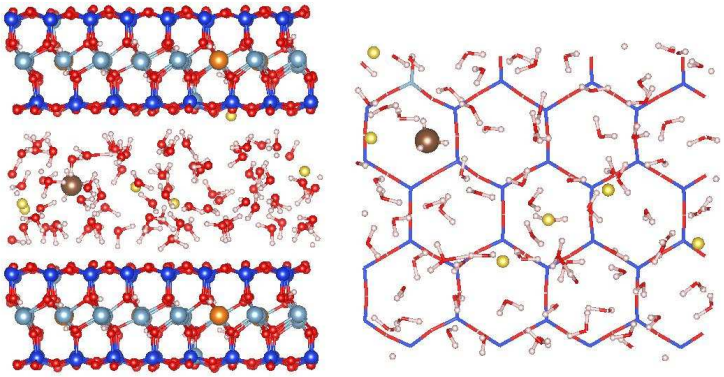


(a)

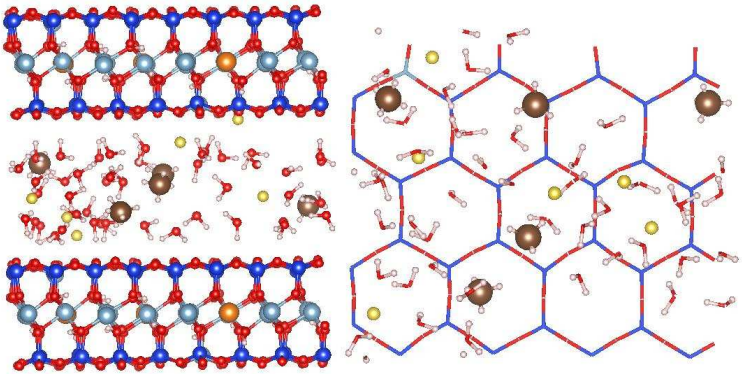
* Corresponding author, Tel.: 202-994-5964; e-mail: leng@gwu.edu.



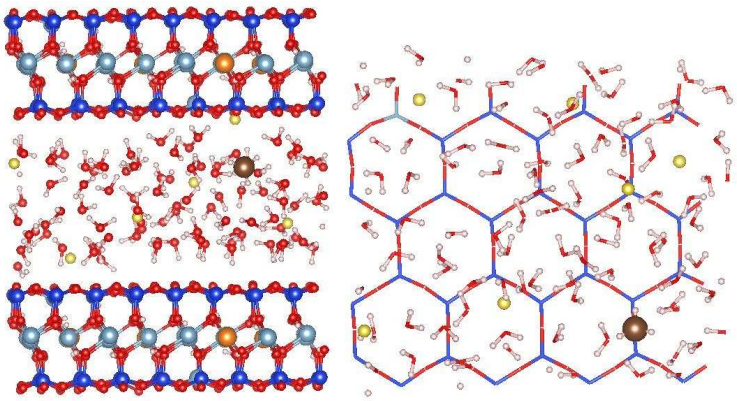
(b)



(c)

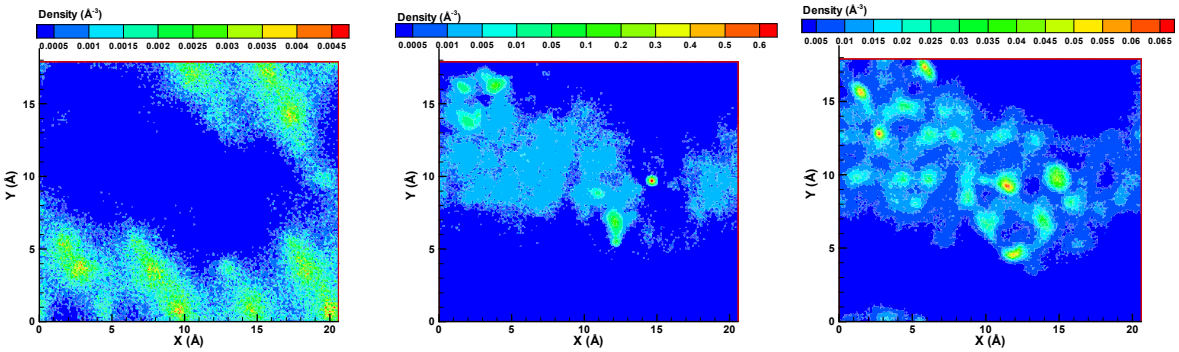


(d)

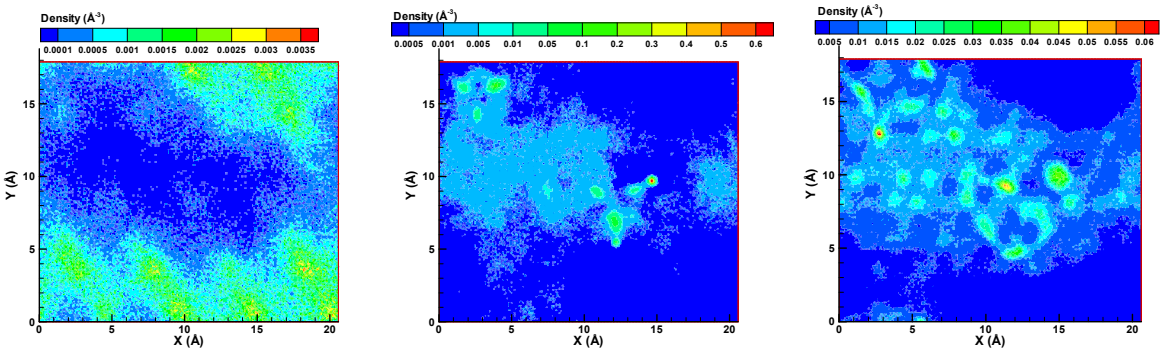


(e)

Figure S1. Snapshots of methane aqueous hydration structure in Na-montmorillonite interlayer in the other five *T/P/RH* simulation cases. The left and right panels show the side and top views of the molecular configurations. (a) *T/P/RH* = 300 K/20 bar/5% at an equilibrium basal spacing of 15.5 Å; (b) *T/P/RH* = 300 K/20 bar/10% at an equilibrium basal spacing of 16 Å; (c) *T/P/RH* = 300 K/20 bar/20% at an equilibrium basal spacing of 17 Å; (d) *T/P/RH* = 300 K/30 bar/10% at an equilibrium basal spacing of 16.1 Å; and (e) *T/P/RH* = 300 K/50 bar/30% at an equilibrium basal spacing of 17.9 Å. Color scheme: oxygen – red, hydrogen – white, carbon – brown, silicon – blue, aluminum – cyan, magnesium – orange, and sodium – yellow.



(a)



(b)

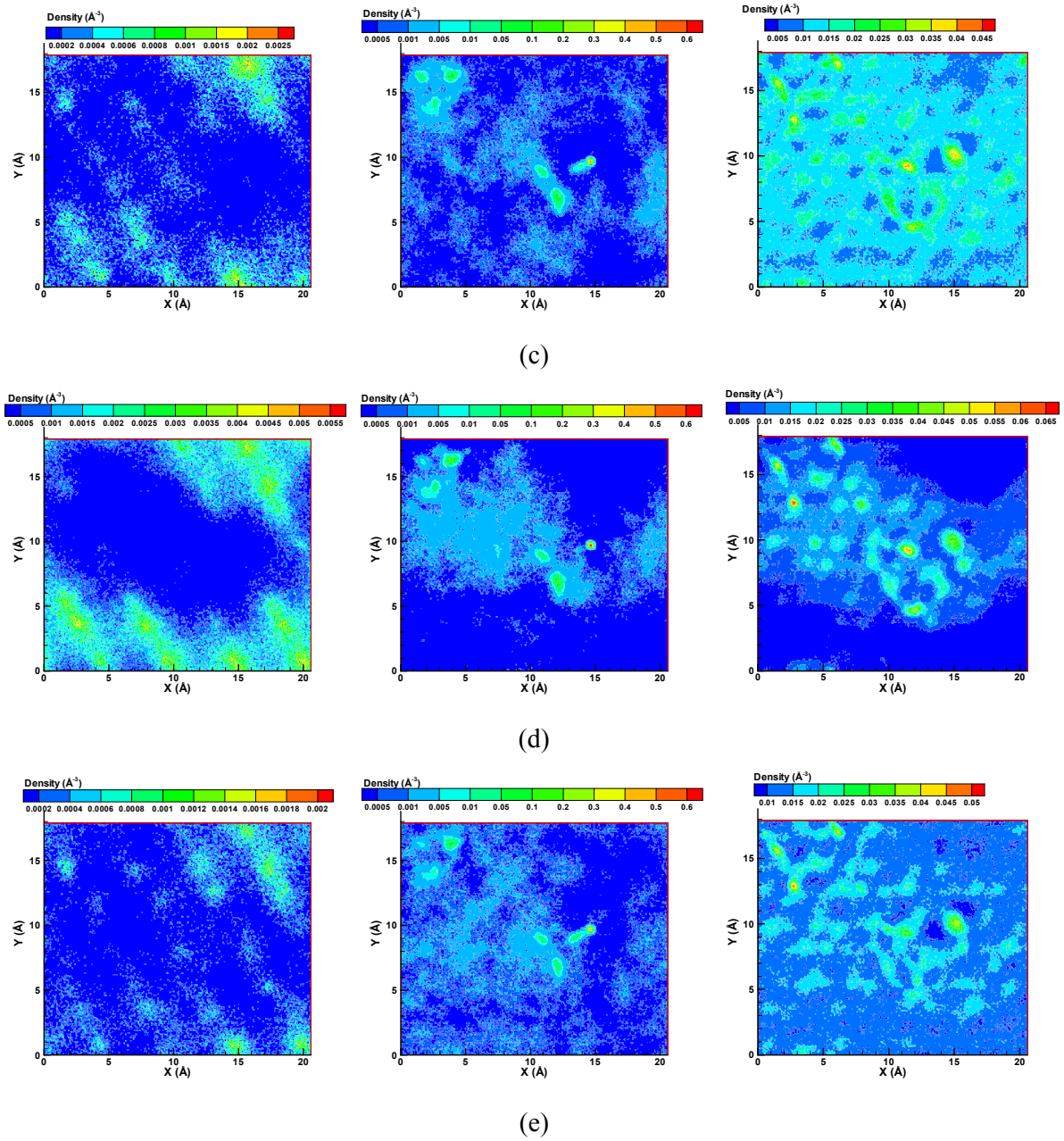


Figure S2. In-plane two-dimensional (2D) density distributions of methane (left), sodium ions (middle), and water molecules (right) in clay interlayer under other five *T/P/RH* conditions: (a) *T/P/RH* = 300 K/20 bar/5% at an equilibrium basal spacing of 15.5 Å; (b) *T/P/RH* = 300 K/20 bar/10% at an equilibrium basal spacing of 16 Å; (c) *T/P/RH* = 300 K/20 bar/20% at an equilibrium basal spacing of 17 Å; (d) *T/P/RH* = 300 K/30 bar/10% at an equilibrium basal spacing of 16.1 Å; and (e) *T/P/RH* = 300 K/50 bar/30% at an equilibrium basal spacing of 17.9 Å.