Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supplementary Material

**Modeling Carbon Dioxide and Methane Adsorption on Illite and Calcite: Enhancing the Simplified Local Density Model through Crystal Structure Modifications**

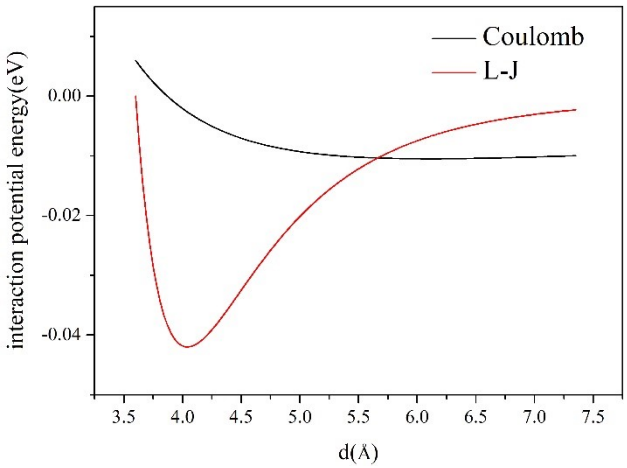


**Fig S1. Comparison of L-J potential and Coulomb potential**

The L-J potential between the Ca atom on the calcite surface and methane molecule is compared with coulomb potential at different distance. When the distance between Ca and methane is less than 5.6 Å, the L-J interaction potential plays a dominant role. In addition, the well depth of the Coulomb potential is about 24% of L-J potential. Therefore, the interaction between the fluid and the pore is simplified to the LJ potential to improve the simulation speed of the model.