SAND2017-7577C

Molecular simulations of adsorption and transport in subsurface porous media

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Understanding nano-structural properties of subsurface porous media including kerogen and clays, and the adsorption and transport in subsurface porous media are important to numerous applications such as shale gas, carbon sequestration, and nuclear waste disposal. Kerogen is the host for CH_4 and CO_2 in petroleum-rich systems. Despite its importance in organic-rich shale, the interaction of kerogen with methane, carbon dioxide, and water remains poorly understood. On the other hand, clay is the backbone of any geological system. Understanding the properties of clay including nano-structural properties is important to determine the permeability, ion exchange capacity, gas loading, and fluid migration in mudstones and shales. In this poster, I report molecular dynamics simulation methods to build complex and realistic kerogen and clay aggregates. These models are then used to investigate the effects of porous media structure, porosity, and connectivity on gas adsorption and transport. The results provide a mechanistic understanding at the atomistic level of the effect of the porous media properties on the behaviors of fluid.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research was funded, partly, by DOE National Energy Technology Laboratory and Basic Energy Sciences projects.