

Effect of molecular interactions on macroscopic phenomena in geological CO₂ storage

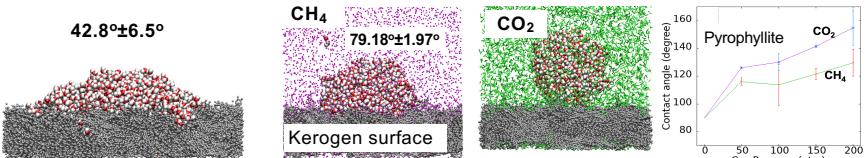
Tuan A. Ho and Yifeng Wang



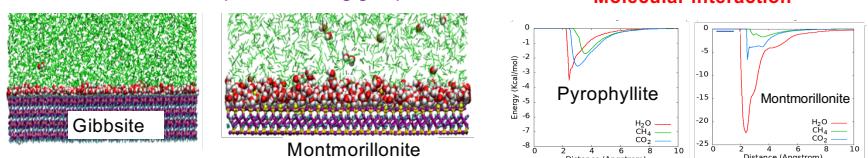
Wettability Alteration upon CO₂ Sequestration

ACS Applied Materials & Interfaces 13, 41330

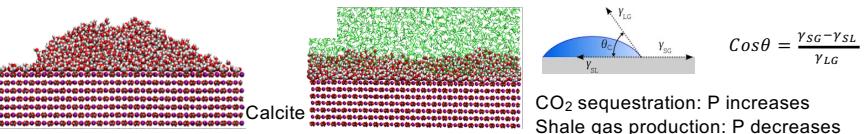
1. Contact angle increases upon increasing pressure



2. Surface remains wet upon increasing gas pressure



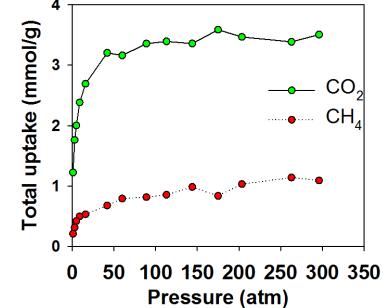
3. Contact angle decreases upon increasing pressure



CO₂ and CH₄ competitive adsorption onto kerogen structure

Scientific Reports 6, 28053 and Fuel 220, 1-7, 2018

1:1 binary gas adsorption

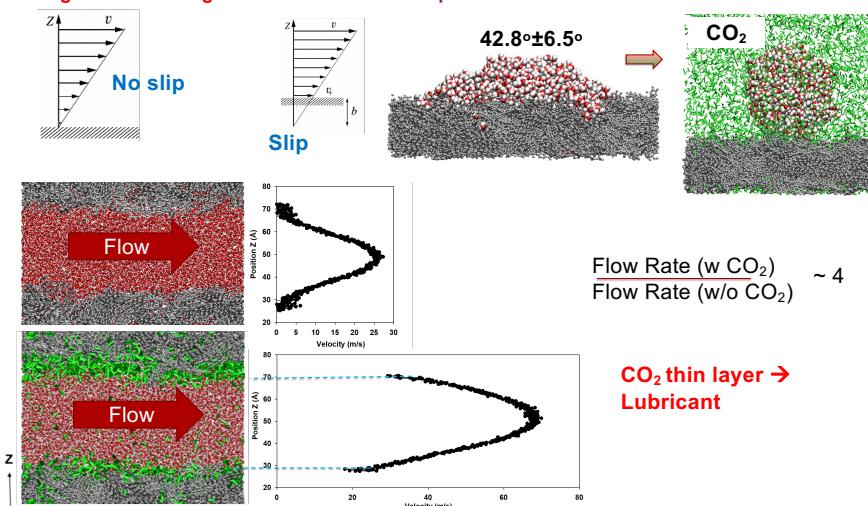


Kerogen preferentially retains CO₂ over CH₄

Effect of scCO₂ on water transport

Nanoscale 10, 19957

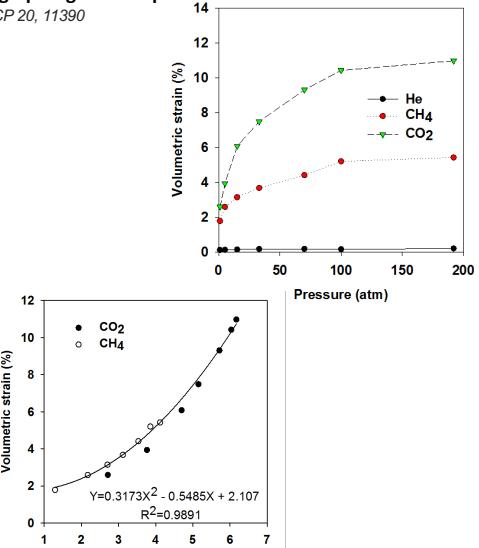
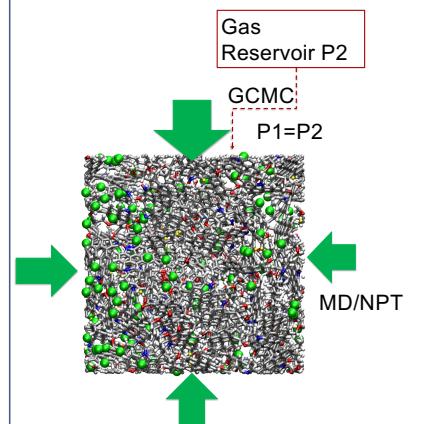
Wetting to non-wetting transition → Stick to slip flow transition



Kerogen swelling upon gas adsorption

PCCP 20, 11390

Simulation: Hybrid MD/MC



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