

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

The Role of Water and Carbon Dioxide Intercalation on Na-Montmorillonite Swelling Behavior at Geological Carbon Sequestration Conditions¹ MEYSAM MAKAREMI, KENNETH JORDAN, GEORGE GUTHRIE, EVGENIY MYSHAKIN, National Energy Technology Laboratory, and University of Pittsburgh, Pittsburgh, PA — Swelling of Na-montmorillonite in the environment relevant to geological CO₂ sequestration in deep underground formations is investigated by conducting classical Monte Carlo and molecular dynamics simulations. Both the binary (clay-water or clay- CO₂) and the ternary (clay-water-CO₂) systems containing the clay, water and carbon dioxide phases are simulated, and the free energy for clay swelling is calculated as a function of the interlayer distance. The calculations indicate that while water intercalates into the clay layer and forms stable monolayer and bilayer hydration states, in the absence of interlayer water adsorption of dry carbon dioxide is thermodynamically unfavorable. In the ternary system, two hydration states are observed with interlayer spacings corresponding closely to those of the pure water binary system. In addition, the simulations of the ternary system show that the incomplete first hydration state is more effective at adsorbing CO₂ molecules than is the incomplete second hydration state.

¹Work was performed in support of the NETL's ongoing research in Subtask 4000.4.641.061.002.254 under the RES contract DE-FE0004000.

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Date submitted: 10 Nov 2014

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