Nanoscale CO$_2$-brine-mineral interactions

Scientific Achievement
Developed accurate molecular models of CO$_2$–H$_2$O–solute structure and dynamics...
1) within clay slit pores to study solute partitioning and wetting behavior.
2) within Na-montmorillonite interlayer to investigate CO$_2$ intercalation by clay.

Significance and Impact
1) Distribution of CO$_2$, H$_2$O, and ion species controls dissolution and precipitation of minerals, influencing transport and long-term mineralization of injected carbon. Models show nanoscale distribution of species can vary significantly in spite of similar macroscopic wetting behavior.
2) CO$_2$ intercalation by smectite clays influences permeability, mechanical strength, and integrity of shale-mudstone caprock. Models show swelling caused by intercalation of CO$_2$ strongly depends on interlayer H$_2$O content and alters interlayer Na$^+$ adsorption.
CO$_2$ and brine wetting in muscovite nanopores
INTERCALATION OF CO$_2$-H$_2$O BY CLAY MINERALS

Molecular Dynamics Simulations of Carbon Dioxide Intercalation in Hydrated Na-Montmorillonite
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