Adsorption in the electrical double layer at clay-brine interfaces

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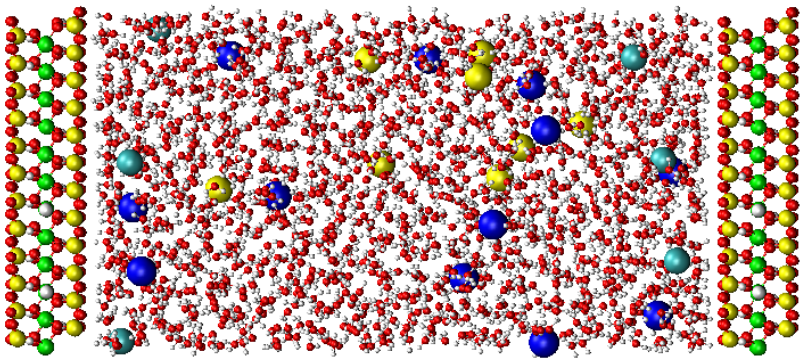
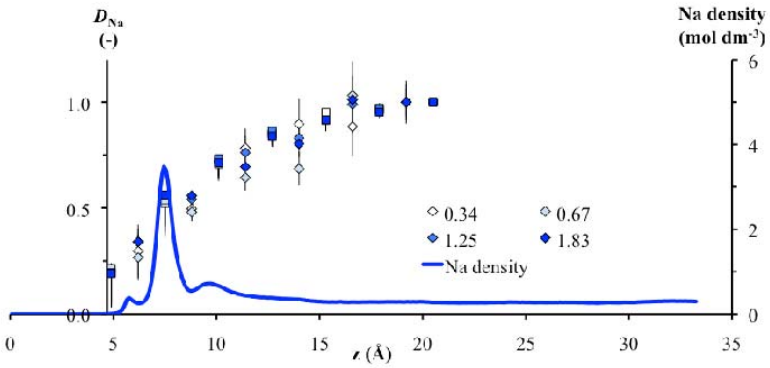
EFRC: Nano-scale controls on Geologic CO_2



MD simulation snapshot of a 0.3 M NaCl-$CaCl_2$ brine confined in a 6 nm-wide nanopore between smectite clay surfaces (with Na, Ca, and Cl ions in dark blue, light blue, and yellow).



Plot of Na^+ density (curve) and diffusion coefficients (symbols) as a function of distance from the clay surface.

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- Caprocks such as clay shales play a key role in the performance of CO_2 repositories: they must prevent the buoyant rise of the CO_2 plume until trapping is ensured by mechanisms such as carbonate mineral precipitation. Potential CO_2 leakage mechanisms through clay caprocks depend on the behavior of water and ions near clay mineral surfaces (adsorption, diffusion, interfacial energy).
- The electrical double layer (EDL) is a key feature of ion adsorption at clay-water interfaces. However, molecular-scale structure and dynamics in the EDL are not fully understood especially at the high electrolyte concentrations of brine aquifers considered for CO_2 sequestration.
- Molecular dynamics (MD) simulations of 6 nm-wide nanopores between smectite clay surfaces were carried out for a range of brine concentrations (0.3 to 1.8 M NaCl-$CaCl_2$; upper figure) to determine the properties of the EDL as a function of salinity.
- This study yielded an unprecedentedly-detailed view of water and ion distribution and dynamics near charged clay surfaces (lower figure) that will help to constrain reactive transport models of clay caprocks.
- Interestingly, anion exclusion balances a significant fraction of the clay structural charge at high ionic strengths. This may shed light into the ionic-strength-dependence of the clay-water interfacial energy and of clay-water-CO_2 wetting angles.