Molecular dynamics simulation prediction of quartz wetting by water and supercritical CO_2 and the potential impact of organic residues

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Fundamental physical and chemical features governing multiphase flow in water-CO_2-quartz nanopore systems directly impact the mobility and trapping of supercritical CO_2 injected into the subsurface as part of Carbon Capture and Sequestration (CCS). CCS is a potentially important approach to mitigating anthropogenic emissions, and depends largely on the capillary trapping capacities of subsurface formations. However, published experimental data on relevant properties, such as water-CO_2 contact angles (CA), vary widely.

The fundamental basis of this variability remains poorly known, though surface contamination is hypothesized to be a significant source. Molecular Dynamics (MD) simulations have shown significant promise in elucidating CA at the nanoscale and we have been able to predict trends with respect to changes in pressure in ideal systems. An important remaining knowledge gap in CCS is the influence of organic residues naturally present in sedimentary rocks on water-CO_2-solid wetting and multiphase flow. We carry out a series of MD simulations to probe CAs in the presence of organic molecules. Using small organic molecules as proxies, we simulate a CO_2 bubble in a water-filled 6.6 nm quartz nanopore with varying fluid pressures. We find that high concentrations of organics may influence the water-CO_2 wetting behavior of quartz.