Molecular Dynamics Simulation of Super-Critical CO_2 and Water Adsorbed on Calcite

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To slow down global warming there is an increasing focus on reducing carbon dioxide (CO_2) emissions to the atmosphere. Geologic storage of CO_2 is one method that can contribute to nations reaching the desired limits on emissions of greenhouse gases. Long-term storage of CO_2 in geological formations requires knowledge on several different trapping processes that run on different time-scales. In order to understand these complex systems on a field-scale, it is important to understand the nanoscale behavior. Among other, how the solubility trapping of CO_2 occurs. Dissolved CO_2 can react with reservoir rocks and form carbonate minerals. This process is known as mineral trapping and is the most stable form of storage. But insight into the microscopic effects that governs the macroscopic thermodynamic observables can often be hard to obtain, especially when it comes to interfacial systems. We have used molecular dynamics (MD) and focused on carbon dioxide and water adsorbed on calcite. The system consisted of a calcite slab with the (1014) surface exposed to a water phase interacting with a super-critical CO_2 phase. The effect of varying temperature was also investigated through several large-scale simulations at different temperatures. Results show that the density of water increases towards the mineral surface. This creates voids that can facilitate increasing dissolution of CO_2 into the water phase.