Using Molecular Simulation to Study the Interfacial Properties of CO_2/Water/Silica Systems

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Carbon dioxide capture and storage via injection into saline aquifers is a promising option for the reduction of greenhouse gas emissions and the potential mitigation of global climate change. However, the estimation of reservoir capacity has been hampered by uncertainty in key interfacial properties of the CO_2/water/rock system, especially at high pressures where supercritical CO_2 is present. In order to prevent the leakage of sequestered gas through pores in caprock, the aquifer pressure must remain below the breakthrough pressure, which depends on (1) the interfacial tension between the CO_2-rich and water-rich phases and (2) the contact angle that a water-rich droplet forms on a mineral surface in a mother CO_2-rich background. We discuss here the use of Monte Carlo (MC) molecular simulation to measure these key properties for CO_2/water mixtures in the presence of an atomistically detailed silica surface. Specifically, we present an interface potential-based free energy method to measure interfacial properties over a range of CO_2/water compositions. Results are presented for the evolution of the contact angle and CO_2/water interfacial tension over a range of pressures at select temperatures. We also discuss connections between our results and those from experimental studies.