Molecular Simulation of Carbon Dioxide, Water and Kaolinite Interactions

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Safe long-term storage of carbon dioxide (CO_2) will reduce CO_2-emissions to the atmosphere. This can be achieved by injecting captured CO_2 in geological formations. CO_2 injection in reservoirs is also a well-known method used in enhanced oil-recovery (EOR). Lastly, injection of carbon dioxide in methane hydrate is a promising method, both due to energy aspects as well as climate aspects. The above mentioned reasons have several challenging common problems, there among, how the microscopic interactions between reservoirs species governs the behavior of injected CO_2. To study the behavior of super-critical CO_2 at the nanoscale, we have performed Molecular Dynamics (MD) simulations of a water, CO_2 and clay system. The mineral used in our simulations is kaolinite, a common clay found in the earth's crust. We have initially focused on a slab of kaolinite with the hydrophilic gibbsite layer exposed to a water phase that is in contact with a super-critical CO_2 phase. The interactions of the CO_2 phase with the water phase have been analyzed. As well as the impact of varying temperature on CO_2 dissolution from the super-critical phase into the kaolinite adsorbed water. Results shows that water adsorbs strongly on the gibbsite surface of kaolinite, but this strongly adsorbed water also creates following exclusion zones where adsorption of CO_2 can be facilitated.