Simulations of Slow Dynamic Processes in Nanoconfined Aqueous Solutions

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Nanoconfined water and aqueous solutions exhibit a number of properties, which are fundamental in geology and have a great practical importance for medical and industrial applications. Many of these processes are still not completely understood, such as the mechanism of SiO2 dissolution or the dynamic transition of confined aqueous solutions [1] at low temperatures, which share common features with the dynamic crossover of hydration water at biomolecules [2].

Here we present a study of the diffusion and dynamic transitions of water, and transport properties of ions confined in mesoporous silicates (MCM-41 and SBA-15). The complex dynamics of the system also involves surface reactions, such as water dissociation and SiO2 dissolution, and water diffusion in bulk silica. We evaluate the effects of pore size and shape, ion concentration, and temperature on the dynamics of different processes. The results obtained from simulations are compared with available quasi-elastic neutron scattering (QENS) experiments.

Since most of the studied processes are characterized by very long diffusion relaxation times or rare reactive events, typically in the order of nano- to microseconds, theypose a challenge for usual atomistic simulations. To overcome these complications, we use a combination of the reaction ensemble Monte Carlo technique (RxMC) [3] and long molecular dynamics simulations accelerated by the processing power of a GPU. The force fields used include common non-reactive models (e.g. SPC/E) for speed as well as reactive potential models (ReaxFF [4]) for the details of reactive steps.

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