Electrolytes at the (0001) alpha-quartz/water interface investigated by DFT-MD simulations

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This talk is dedicated to probing the microscopic organization of silica-water interfaces including electrolytes by first principles DFT-based molecular dynamics simulations (DFT-MD).

Ions from electrolytic solutions play key roles on interfacial water/mineral interfaces: their adsorption typically drives pollutant transport in groundwater, mineral dissolution, clay swelling, and electrolytes can strongly affect the binding of organic molecules because of competitive interactions.

We will present our DFT-MD simulations of electrolytic quartz-water interfaces (KCl, NaCl, NaI) in order to unravel the structural properties of these electrolytes at the interface between the quartz surface and liquid water. We provide some understanding on how the chemical properties and reactivity of the interface can be modified by the presence of the electrolytes. Vibrational spectra at these interfaces (IR, Raman and SFG) are calculated from the trajectories in order to relate structural properties to vibrational signatures, and make a direct link to experiments. Vibrational signatures are interpreted in relation with the microscopic structure of interfacial water molecules and electrolytes. The acido-basic characters of the quartz surface sites are also investigated once the aqueous surface is in contact with the electrolytes.

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