# Density Functional Theory Calculations on Mineral Surfaces Compared to Experimental Observations

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The mineral-water interface is a complex region because the nature of the mineral surface influences water behavior and vice versa. Most geochemistry occurs at this type of interface, so it would be useful to understand the general principles that govern chemistry in this nanoscale regime. This talk will compare behavior of water at quartz, rutile and goethite interfaces. Density functional theory (DFT) molecular dynamics simulations of each interface will be compared in terms of the H-bonding structure & energetics, proton transfer and effect on adsorbed ions. Discussion particularly focuses on the ability of water to interact with bridging oxygen groups on each type of surface to investigate the hypothesis that it is hydrolysis of these oxygen atoms that leads to dissolution of the mineral.

Modeling of quartz and amorphous silica has focused on hydrolysis of Si-O-Si linkages leading to dissolution. Current work is using periodic DFT calculations to generate structures relevant to this reaction and MP2 calculations to attempt to reproduce experimental activation energies of dissolution. The rutile (110) surface has been studied extensively both through experimental and compuational methods. This talk will discuss comparisons of DFT simulations to X-ray reflectivity work and neutron scattering. Examination of model predictions on proton-exchange rates at the rutile and cassiterite (110) surfaces will also be explored. For goethite, modeling of organic surface complexation reactions will be presented that searches for a combined ligand- and reduction-promoted dissolution mechanism to solubilize relatively insoluble Fe(III).