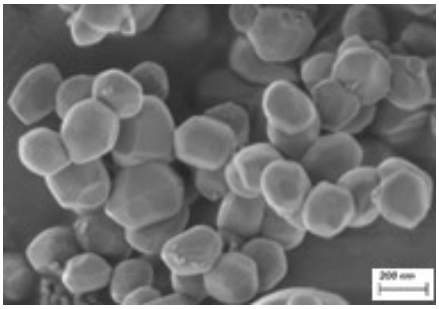
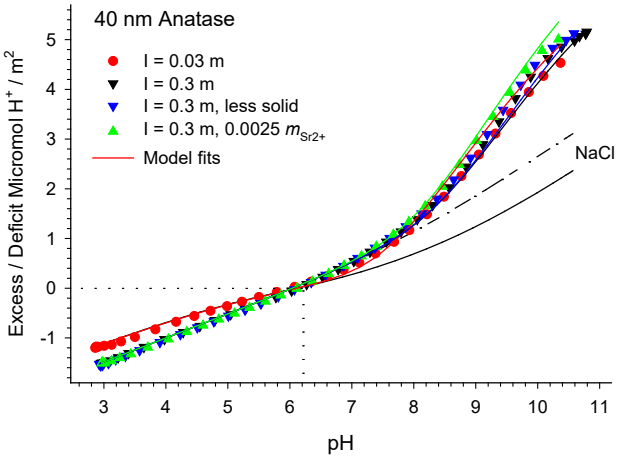
Taking Mineral-Water Interface Studies to the Molecular-Scale

Metal contamination of water and soils, dissolution and precipitation of minerals, redox reactions, environmental toxicity of natural and engineered nanoparticles, water filtration processes, and remediation of radioactive elements by clays are just a few examples of the myriad mineral-water interface reactions. Aqueous geochemistry research at TTU, aims to understand the inherently complex interactions at the interface of minerals, water, and the ions and compounds present in natural waters.

Adsorption at Mineral Surfaces: Experimental Studies and Empirical Modeling



SEM Characterization of Corundum

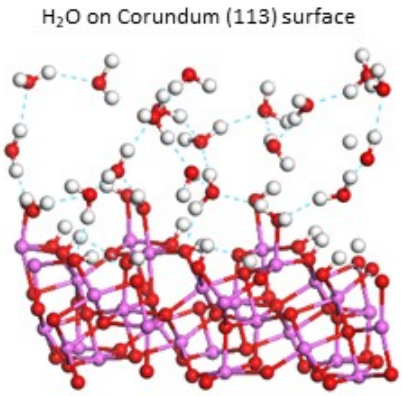


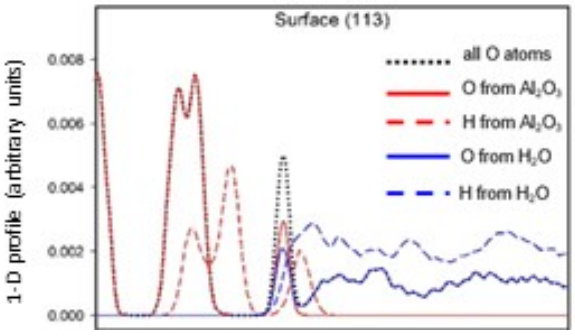
Experimental data with empirical model fits for Sr^{2+} adsorption on nanometer sized anatase (TiO_2)

Our approach to studying the solid-water domain combines high-resolution characterization of mineral surfaces with detailed laboratory studies. We then integrate molecular-scale information with the observable experimental results into constrained Surface Complexation Models. Our aim is to improve the understanding of chemical reactions and processes taking place at mineral-water interfaces that affect the environment.

Examples of research projects include, the adsorption behavior of rutile – important for remediation of metals and radionuclides; the behavior of nanoparticle anatase – found in household items such as suntan lotion and paint; surface charging of barite – used in hydraulic fracturing fluids and a cause of scaling in wells; and studies of the environmentally relevant manganese-oxides – found in soils and used in water treatment plants.

Mineral Surfaces at the Molecular-Scale





Atomic density 1-D profile of atoms at the interface of H_2O and Corundum

Many minerals of environmental importance are highly soluble, making them difficult to study experimentally. Consequently, we conduct computational studies to evaluate surface reactivity towards water and ions present in water. These studies aim to investigate the underlying molecular mechanisms occurring at mineral-water interfaces. Project examples include, evaluating the interaction of water with specific corundum surfaces; and the interaction of ions with rutile and anatase.