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Connecting Spectroscopy and Computational Chemistry to Study Interfacial Phenomena

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Interpretation of spectra in systems of environmental interest is not generally straightforward due to the lack of close analogs and a clear structure of some components of the system. Computational chemistry can be used as an objective method to test interpretations of spectra. This talk will focus on applying ab initio methods to complement vibrational, NMR, and EXAFS spectroscopic information. Examples of systems studied include phosphate/Fe-hydroxides, arsenate/Al- and Fe-hydroxide, fractured silica surfaces. Phosphate interactions with Fe-hydroxides are important in controlling nutrient availability in soils and transport within streams. In addition, organo-phosphate bonding may be a key attachment mechanism for bacteria at Fe-oxide surfaces. Interpretation of IR spectra is enhanced by model predictions of vibrational frequencies for various surface complexes. Ab initio calculations were used to help explain As(V) and As(III) adsorption behavior onto amorphous Al- and Fe-hydroxides in conjunction with EXAFS measurements. Fractured silica surfaces have been implicated in silicosis. These calculations test structures that could give rise to radical formation on silica surfaces. Calculations to simulate the creation of Si and SiO radical species on sufaces and their subsequent production of OH radicals will be discussed.