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ISEQ Work Summary as of December 2004

Chemical reactions that occur in the environment have the characteristic of being exceptionally complicated due to the heterogeneous nature of the environment and its multiple interfaces (air-water, solid-water, and solid-solid). Furthermore, environmental and geochemical reactions of interest often encompass toxic, mutagenic, and carcinogenic compounds that have entered our environment inadvertently or as a consequence of our ignorance.

Laboratory experiments in environmental chemistry and geochemistry are designed to achieve an understanding of a pollutant's behavior in the environment, ultimately leading to the desired outcome of remediating the anthropogenically altered system. However, as mentioned in the preceding paragraph, studying these chemical reactions is extremely difficult due to the complexity of the environment and the health risks posed to experimentalists working with pollutants. The experimental results are also highly complicated, a reflection of the nature of the environment.

During the last decade, computer technology has dramatically altered and affected the field of chemistry and our ability to understand and gain insight into chemical reactions not accessible through experiment. Theoretical and computational chemistry is complimentary to experimental chemistry and is often a tool whereby the theoretician is able to interpret highly complicated experimental results. Moreover, it is preferable to study chemical reactions that pose danger or health risk to a researcher with the aid of massively-parallel computer servers. Theoretical chemistry codes and the development of improved algorithms are allowing theoreticians the ability to solve difficult chemical problems much quicker than conventional experiments without having to ever step into a laboratory.

I am involved in research that deals with understanding the behavior of pollutants and their reactions at mineral surfaces through the use of theoretical and computational chemistry. Pollutant interactions with mineral surfaces are important with respect to their transport and bioavailability in the environment. I also study the interaction of biomolecules (molecules synthesized by plants and/or microbes biochemically) and toxic metal ions and the mechanisms whereby organisms are able to tolerate high concentrations of otherwise toxic metals. This research involves collaboration with experimentalists in order to verify the accuracy of the theoretical/computational results and leads to an improved understanding of contaminated environmental systems.

The theoretical and computational work that is being currently performed will lay a foundation for future work that relies heavily on these methods. Experimentalists are now able to integrate theoretical tools into their research enabling them to interpret and assist them in unprecedented ways.