



Events

[Current Events](#)[Lectures ▾](#)[Events Archive ▾](#)

CCT Colloquium Series

Molecular Simulations and Applications in Environmental Chemistry**Randall T. Cygan, Geochemistry Department, Sandia National Laboratories**

Johnston Hall 338

February 29, 2008 - 11:30 am

Abstract:

The fate of chemical and radioactive wastes in the environment is linked to the ability of natural phases to attenuate and immobilize contaminants through chemical adsorption and precipitation processes. Our ability to understand the molecular control of these processes is provided by a few experimental and analytical methods such as X-ray absorption, vibrational, and NMR spectroscopies. However, due to complexities in the structure and composition of clay and other hydrated minerals, and the inherent uncertainties of the experimental methods, it is important to apply theoretical molecular models for a fundamental understanding and interpretation of these phenomena. In this effort, we have developed a general force field suitable for the simulation of hydrated and multicomponent mineral systems. Interatomic potentials were derived from parameterizations incorporating structural and spectroscopic data from a variety of simple hydrated compounds. A flexible water model is used to describe the water and hydroxyl behavior. Bulk structures, interfacial behavior, and intercalation processes are evaluated and compared to experimental and spectroscopic findings. Classical molecular dynamics methods and ab initio molecular dynamics using quantum approaches provide additional insights into the structure, dynamics, and reactivity of these complex materials.

Speaker's Bio:

Randall Cygan received his Ph.D. degree in geochemistry and mineralogy in 1983 from the Pennsylvania State University. In late 1983, he joined the Geochemistry Department of Sandia National Laboratories in Albuquerque, New Mexico where he is now a Distinguished Member of the Technical Staff. He also spent two years as an Assistant Professor in the Geology Department at the University of Illinois. His research interests are in geochemistry and materials science, and include kinetics, chemical diffusion, mineral dissolution, adsorption, shock metamorphism, and molecular simulation. He is a Centennial Fellow of the College of Earth and Mineral Science at Pennsylvania State University and a Fellow of the Mineralogical Society of America.

