Molecular simulations of mineral-water/solution systems

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Interaction between clay minerals, zeolites, etc. and gas/water/aqueous solutions have impotant rolls in the earth's surface environments. The physicochemical processes are generally complex and often difficult to understand because of the complicated molecular structures/texture and the ambient conditions under wet circumstances. We have investigated the structure and physical/dynamical properties of the mineral-gas/liquid systems by means of molecular simulation methods; molecular dynamics (MD) and Metropolis Monte Carlo (MC) methods. We have investigated adsorption, diffusion, hydration, interface properties, etc. of those systems.

We have developed atomic interaction models of inorganic systems. The models compose of Coulomb, short range repulsive, van der Waals and covalent (radial and angular) terms with respect to all the elements appeared in the mineral-water systems. MD simulations were performed with full degree of freedom of atom motions. Using the model for H_2O molecule, the structure and physical properties such as density, diffusion coefficients, etc. of ice polymorphs and water are well reproduced. Alkali haride aqueous solutions and gas hydrates and their (hydrophobic) solutions are also reasonably simulated.

We discuss in my presentation on :

1) effective and transferable atom/molecule models for molecular simulations: model forms and parameter determinations,

2) relaxation/equilibration of some systems in MD simulations,

3) possibility of large/complex simulations of the earth's surface environments based of atoms,

4) extension to macro systems and meso-scale modeling,

5) others.