Computational Science for Environmental Geochemistry

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Computational science has provided powerful methods for chemistry, physics, biology, and geoscience with the development of computational facilities and methods. Here we discuss atomic-scale simulations in computational science including *ab initio* calculations and molecular simulations using force fields. These atomic-scale simulations have developed in different way depending on research fields such as band calculations for understanding conductivity and magnetism of solids in physics, molecular orbital methods for reproducing weak molecular interactions and chemical reactions in chemistry, and molecular simulations for revealing the stable structure of large protein molecules in biology. A direction of computational science in geochemistry is the development of methods applicable to elevated temperature, pressure, and multi-component systems. In this presentation, we discuss perspectives of computational science for developing environmental geochemistry.

Keywords: ab initio calculation, Molecular simulation, Free energy, pH, Fluid, Solid-liquid interface

