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Molecular simulation of confined water among mineral grains

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Clays and clay minerals together with zeolites, are major mineral components in the earth's surface environment. These minerals interact with the atmosphere, natural water, inorganic and organic components in soils, etc. The physicochemical processes in the surface region are complex and difficult to understand because of the complicated "molecular" structures and the ambient conditions under wet circumstances.
We have investigated the structure and properties of the mineral - surrounding gasses and liquids systems by means of molecular simulation methods, molecular dynamics and Metropolis Monte Carlo methods. Swelling of smectite, adsorption of gasses molecules in zeolites, etc. are simulated and analyzed the atomic and molecular processes.
We have developed atomic and molecular interaction models for the use of molecular simulations. The model composed of electrostatic, short range repulsive, van der Waarls, and covalent (radial and angular) terms for all the elements appeared in the mineral-water systems.
Using the model for H2O molecule, structure and physical properties, such as density, diffusion coefficients, etc. of ices and water are well reproduced. Alkaliharide aqueous solutions and gas hydrates and their solutions also reasonably simulated.
clay mineral - water interactions are particularly important to understand the mechanical and chemical processes in the environments and to develop nano-composit materials, and also to use clays in engineering applications. the absorption and swelling are the most remarkable properties of clay minerals, specially smectite. We have investigate these properties by means of molecular simulation methods. The swelling curves, the relation between humidity and basal spacings were reproduced, and nano-scopic structural and dynamic properties of interlayer aqueous solutions ware obtained.
Wetting of clay mineral surfaces determine the mechanical properties of clays, soils, and sedimentary rocks. We investigate the wetting properties of smectite, kaolinite, pyrophyllite, brucite, etc. The wetness of these minerals were quite different each other. The origin of the difference have been demonstrated by molecular simulations.
One of our main purpose of studying clay nano-properties are to know the fundamental nano-mechanics of clays, and to apply the nano-properties to predict long term behavior of clay-based materials, such as engineering barrier for radioactive waste disposal. For this purpose, unified nano-micro-macro approaches should be established.

Keywords: water and aquaous solution, crustal fluid, intermineral grain, molecular simulation, molecular dynamics method, interatomic potential model