Molecular Simulation of water and aquaous solution in the vicinity of mineral surfaces

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We investigated the structure and physical properties of water and aquaous solution in the vicinity of mineral surfaces by means of molecular simulation methods. The minerals are smectite, quartz, periclace, rock salt etc. we investigated the structure as the orientation of water molecules of the function of distance from the surface. Physical properties are density, diffusivity, viscosity etc.

We investigated the structure and physical properties of water and aquaous solution in the vicinity of mineral surfaces by means of molecular simulation methods. The methods are mainly molecular dynamics method with the interatomic and intermolecular potential models which were developed by ourselves.

The minerals are smectite (Beidellite,

molecular surface and edge), quartz (covered by Si-O-H's), periclace(MgO, (100)), rock salt (NaCl, (100)) etc.

We investigated the local structure as the orientation of water molecules of the function of distance from the surfaces. Physical properties are were investigated as density, diffusivity, viscosity etc.