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Structure of mica and calcite/water intefaces

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Mineral/liquid interfaces are ubiquitous in the Earth's surface and control a range of processes such as ion exchange, contaminant migration, biomineralization, oil reservoir, and many others. These processes occur in the atomic scale and therefore we need techniques having atomic scale resolution for observing and analyzing the interfaces. A combination of x-ray crystal truncation rods (CTR) method and molecular dynamics (MD) simulations are powerful methods for observing the structure and dynamics of these interfaces [1]. The pioneered works of X-ray CTR scattering measurements on the mineral/liquid interfaces by Fenter group [2] revealed the electron-density distribution of the interfaces with sub-angstrom resolutions. A limitation of the CTR scattering technique is the lack of identification of atomic species. The MD simulation is a candidate that overcomes this limitation by comparing the results with those of the X-ray CTR scattering measurements.

Here we talk about the recent results of mica/salt solutions and calcite/artificial sea water (ASW) interfaces. Mica is a good model mineral for clay minerals and the interaction with water should be important for understanding the frictional strength of faults. The X-ray CTR scattering and MD simulations revealed the structure of electrical double layer for mica/NaCl solution interface [3] and the presence of the hydrated Na^+ on the interface can be the high lubrication among mica surfaces [4]. Calcite is a biomineral preferred by many organisms and plays an important role in the carbon and oxygen cycles. It is the main constituent of chalk and limestone, which serve as hosts for oil reservoirs and water aquifers in Europe. The modification of the affinity of the surface for water and the attachment of organic molecules is critical for enhancing oil recovery and the crystal growth. Can dissolved ions in water change the affinity of the calcite surface? The X-ray CTR measurements may give some clues to understand the effects and the underlying mechanism.

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