

## Structure and Dynamics of Water on Muscovite Mica Surface

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Investigating the properties of water-mineral interfaces is crucial in geology, mineral science, and environmental study. Adsorption of water molecules and ions on mineral surfaces often drastically changes the physical properties of rocks composed of mineral aggregates. Adsorbed water and ions on minerals directly affect the frictional strength of rocks in fault zones, transport properties of radioactive waste, and partitioning of trace elements in water. These changes are accompanied by the characteristic structure and dynamic properties of water molecules at the liquid-solid interface.

Here we performed molecular dynamics (MD) simulations to understand the physical properties of water molecules above the muscovite mica (001) surface and discussed the interfacial structures and dynamics by comparing our results with those of X-ray reflectivity measurements and surface forces apparatus (SFA). We prepared a cleaved mica surface with remaining K<sup>+</sup> ions on the surface (named K-mica) to investigate the structure and dynamics of pure water around the cleaved mica surface. The controversial issue of desorption of K<sup>+</sup> ions from the cleaved mica surfaces on immersing it in pure water is discussed using our results and X-ray reflectivity measurements for pure water and aqueous KCl solution on mica (Cheng et al., 2001; Schlegel et al., 2006).

X-ray reflectivity profiles highly reflecting the interfacial structure are directly calculated and compared with those of experiments. Their good correspondence has validated our simulations of the interfacial structure of the mica-water system. We observed five distinguished peaks in the density profile of oxygen of water molecules, and these peaks are attributable to the water molecules directly adsorbed on mica, hydrated to K<sup>+</sup> ions on the mica surface, and ordered due to hydrogen bonds between hydrated K<sup>+</sup> ions. The hydrated K<sup>+</sup> ions make an inner-sphere complex and have an explicit first hydration shell with a radius of 3.6 angstrom and a hydration number of 2.9. The viscosity of water located within 1 nm from mica surface increases by a factor of ca. 2-3 relative to that of bulk water. This feature is in good agreement with a recent experimental study in which shear measurement was conducted using SFA.