Structure and Dynamics of Water on Forsterite Surface

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Olivine-water interaction has broad implications ranging from chemical weathering to water formation on rocky planets. The behavior of water on the mineral surface is the key to understanding numerous complex geochemical processes. This work details molecular dynamics (MD) simulations and quasi-elastic neutron scattering (QENS) experiments as a complementary tool to study the structure and dynamics of water on forsterite (Mg- end member of olivine) surface at 270 K. We employed a fully hydroxylated forsterite(010) surface in the simulation to mimic the mineral at ambient conditions. The water structure on the hydroxylated surface is composed of a well-ordered immobile first layer that interacts with both the OH and H groups, a second continuous strong layer that interacts with the first layer and the OH groups, and a more mobile top layer. Because the calculated tranlational and rotational motions have energies that are observable within the instrument's energy range, we calculated the intermediate scattering function (ISF) that integrates both motions. A combination of three different QENS instruments was used to study the dynamics of water on forsterite surface to probe several dynamical processes occuring at different time scales. The experimental data were fitted using two Lorentzian fucntions that represent two different time scales of motion. Time scales of three dynamical processes observed in the simulation match with those observed with QENS in a satisfactory manner. The slow, intermediate, and fast motions of the water molecules span a dyanmic energy range from a few to hundreds of μeV. The three components represent three different diffusive motions contributed by all the surface water molecules. MD simulations further show that the rotational motion of water molecules is non-isotropic due to the confined environment. Furthermore, both translational and rotational motions of water molecules on the forsterite(010) surface are found to be suppressed compared to bulk water. Water molecules closest to the forsterite(010) surface exhbit preferred orientations.