Structural and Dynamical Response of Water on Mineral Surfaces Affects Surface Ice Nucleating Ability

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Abstract: Water, known as “matrix of life”, participates in events vividly from as small as cellular respiration in a single cell, to one of the largest energy exchange processes on earth, the hydrological cycle. Clouds, a mixture of water vapor, condensed liquid droplets, solid crystals and some aerosol particles, exert an importance on weather and climate via controlling the amount of precipitation and transportation of radiative fluxes. One of the major processes involved in clouds is heterogeneous ice nucleation, which is nucleation facilitated by the presence of mineral substrates. Understanding the role played by solid surfaces in influencing the structure and dynamics of water and thus regulating ice nucleation paves the road for forecasting long-term climate change and designing surfaces with customer-specified ice nucleation properties. The goal of our research is to be able to predict the nucleating ability of a surface based on the interfacial water structure and dynamics. To investigate this problem, we focus on mica, which has a molecularly smooth nature to begin with, thus eases out the complexity of dealing with surface defects. By combining molecular dynamics (MD) simulations with Fourier-transform infrared spectroscopy (FTIR), we are able to probe the change in interfacial water arrangement, spatial correlation and dynamics on mica surface. The interplay of ion-water, ion-surface, and surface-water interactions are found to affect the interfacial water arrangement along with the hydrogen bond network. The surface affinity of water altered by substituted ions will impact the propensity of observing heterogeneous ice nucleation on a given surface.