The Influence of pH on Ice Nucleation by α-alumina

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Heterogeneous ice nucleation refers to ice nucleation initiated by an ice nucleating particles (INPs). Important INPs include mineral dust and biological particles. Cloud conditions, such as pH, significantly affect ice nucleation. Clouds are generally acidic but can have a range of pH values, depending on their compositions. Studies have shown that α -alumina is an efficient INP in both laboratory experiments and Molecular Dynamics (MD) simulations. The (0001) plane of α-alumina is covered by hydroxyl groups in aqueous solutions; therefore, the surface is expected to undergo dual protonation (acidic conditions) and deprotonation (basic conditions). We investigate the effect of pH on the ice-nucleating efficiency of the α-alumina (0001) plane in MD simulation. Multiple surface proton coverages are considered, and we relate the surface proton coverage to pH through pK_a values reported in the literatures. Among all possible surface proton coverages, the mono-protonated surface, which dominates under neutral condition, appears to be most efficient in nucleating the basal plane ice. For dual-protonated and deprotonated surfaces, the ice bilayer above the surface becomes less ice-like, leading to less efficient ice nucleation. Our MD results suggest that the (0001) plane of α-alumina is most efficient in nucleating ice under neutral condition, and less efficient under acidic and basic conditions.