Uncovering Heterogeneous Ice Nucleation using Advanced Molecular Simulations

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Heterogeneous ice nucleation is relevant to a broad range of fields from atmospheric chemistry to food and transportation industries. In principle, because molecular simulations can access molecular length scales, they are ideal to study nucleation. However, since nucleation is a rare event in molecular simulations, straightforward simulation techniques cannot be used to sample statistically significant nucleation events. In our research, we have addressed this challenge by using the advanced sampling technique called forward flux sampling (FFS). Further, we have developed a software platform called SAFFIRE to enable large scale FFS calculations in a high performance computing environment with computational and user efficiency. In this talk, we will discuss the results obtained from molecular dynamics and large scale FFS studies of heterogeneous ice nucleation performed using SAFFIRE. We studied ice nucleation on silver iodide (AgI) and kaolinite-like surface. Both these surfaces are considered to be good ice nucleating agents and have a good lattice match with the ice lattice. Traditionally, lattice match has been used as a governing parameter to determine the ice nucleating efficiency of the surface. Our extensive calculations show that the rates of ice nucleation on AgI and the modified kaolinite surface are different. Our results clearly demonstrate that lattice spacing is not a sufficient measure of ice nucleating efficiency. Exhaustive calculations of committor probability further enables us to comment on the difference in the nucleation mechanisms and role of surface properties in determining ice nucleating efficiency. To the best of our knowledge, these studies are the largest scale FFS calculations of heterogeneous ice nucleation using an all-atom water model.