

Computational Investigations of Complex Aqueous Solutions and Heterogeneous Ice Nucleation

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This talk is divided into two parts. In the first part, we will discuss recent results for complex aqueous solutions such as mixtures of water and 2-butoxyethanol. These solutions are complex because the solutes tend to associate even at very low concentrations, giving structures on mesoscopic length scales. We will discuss the nature and origin of such structures in light of molecular dynamics simulations on very large systems (up to 32,000 molecules), that are necessary to explore mesoscopic behavior. Results for different systems and models will be described, and where possible comparisons will be made with experimental data.

The second part of the talk will describe surface induced ice nucleation. Heterogeneous ice nucleation is very important in many physical situations, being particularly important for cloud formation in the upper atmosphere. We will show that some particular surface-fields that extend only a short distance ($\sim 10\text{\AA}$) from the surface can effectively cause ice to nucleate and grow in undercooled water.