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# Characterizing Key Features in the Formation Mechanisms of Ice

*Tuesday, January 9, 2018 10:50 AM (45 minutes)*

Ice crystallization is ubiquitous in nature and has numerous important roles, technological applications and implications. Yet, the ordering processes associated with the nucleation and growth of ice crystals have proven difficult to study directly with experiments, in part due to their stochastic nature of the underlying molecular processes. Consequently, a complete molecular-level picture of the details of ice formation has yet to emerge. Molecular simulations have afforded an excellent opportunity to investigate crystal nucleation and growth of ice at a molecular level, since they are able to probe directly the microscopic environment of a crystal during its nucleation or the interface of a growing crystal. In this presentation I will begin with a brief review of some key issues around simulations of crystallization, considering the attributes and limitation of various models and methods. I will describe some of the approaches that have been developed and utilized for the simulation of the formation and growth of crystals, both in the homogeneous and heterogeneous contexts. While specific results for ice will be a focus, the "simpler"case of gas clathrate hydrates will also be examined and compared. I will present results that will demonstrate that the process of crystallization is characterized by collective phenomena involving many molecules, where the organization can be seen to occur in stages. The nature of the structural topology and fluctuations that characterize a solid/liquid interface will be examined. I will show that defects can play key roles in observed behaviours. The lifetimes and transitions of specific structures will also be briefly discussed. Finally, I will consider how rugged funnel-shaped potential energy landscapes can provide a lens for understanding aspects of the phenomenological differences in the crystal nucleation of ice and gas hydrates.

## Significance statement

This is an invited presentation

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