Advanced molecular simulations and methods to study self-assembly processes

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Self-assembly of colloidal particles and biological molecules are often activated processes. This presents a challenge to their studies using molecular simulations since the waiting time to observe the process (or transition) is large. This means that most of the computational effort is wasted on waiting for the process rather than in sampling the transition. Sarupria group focuses on using advanced sampling methods in combination with molecular dynamics to study such activated processes. Sarupria has studied nucleation – that is the onset of a new phase from a metastable phase – in Lennard-Jones liquid, water and aqueous solutions extensively using these techniques. Specific interest has focused on the liquid-to-solid transition. Using the advanced sampling techniques in conjunction with molecular dynamics simulations we have sampled hundreds and thousands of nucleation events. In my talk, I will discuss key results obtained for homogeneous nucleation in Lennard-Jones-like liquids and in aqueous solutions. The latter specifically focuses on nucleation of clathrate hydrates of water soluble guest molecules. I will also discuss the limitations of the current methodologies and our approaches to improve the efficiency of the advanced sampling techniques. We have developed novel sampling methods that have the potential to be more efficient in sampling activated processes thereby, making studies of phenomena such as nucleation more viable and accessible. This work has relevance to the EPSCoR Made in SC project in several ways. For example, the techniques developed here are well-suited to study colloidal assembly in the presence of external fields such as magnetic fields. We will discuss such avenues in the talk.