Events

Current Events
Lectures
Events Archive

Other

Probing Long Time-Scale Events with Advanced Simulation Techniques

Bin Chen, LSU

Material World Adjunct Faculty Position

Johnston Hall 338
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Abstract:

Among the greatest challenges for molecular simulation are the limited time and spatial scales that can be afforded using the current computer technology and simulation algorithms, especially when applied to complex biochemical problems. As a first step to wards the goal of enabling molecular simulation as a tool in probing the long time-scale events, we aimed at a prototypical example of such phenomena: nucleation. The sampling difficulties for this problem (and also for many other long time-scale events) are caused not only by the large free energy barrier that can be used to characterize the rate-determining step (i.e., formation of a transition complex, such as a critical nucleus in nucleation) but also by the inherent micro-heterogeneity of the phase space. For example, for vapor-liquid nucleation the micro-heterogeneity arises from the presence of a spectrum of micro-phases (e.g., monomers and clusters). These micro-phases differ to a great extent on both energetic and entropic factors, which makes particle transfers (condensation and evaporation) between these micro-phases rather slow. In other words, the challenge to molecular simulation imposed by this problem arises from the presence of a multitude of slow events that span over a wide range of time-scales, many of which are far outside the boundary of conventional simulation methods. Correspondingly, many of the current free-energy based methods including umbrella sampling (US) that focus only on the time-determining step would become insufficient as a separate approach is still required to deal with the other slow kinetics. The simulation method developed by us that has led to recent success in vapor-liquid nucleation hinges on the synergism of the several advanced simulation techniques that are able to surmount the multitude of sampling bottlenecks encountered in the nucleation study. In particular, an approach called aggregation-volume-bias Monte Carlo (AVBMC) is specifically designed to deal with the slow diffusive/evaporative motions involved in nucleation. This talk will showcase the success of using a combination of AVBMC, US, configurational-bias Monte Carlo, histogram-reweighting, and density of states methods to study nucleation phenomena for complex systems.

Speaker's Bio:

Bin Chen is an Associate Professor of Chemistry at LSU. He received his B.S. from Peking University in 1996, and his Ph.D. from the University of Minnesota in 2001. His research studies the relationships between the microscopic structures/interactions and the macroscopic properties for systems of chemical, biological, and environmental interest. His research tool is computer simulation empowered by different levels of theory (from abinitio to classical). Research topics include: development of transferable potentials and efficient algorithms for phase equilibrium calculations; novel computational methods for long time-scale events; vapor-liquid nucleation; peptide/protein folding; protein
crystallization; ab initio study of reactive chemical systems in condensed phases; and de novo design of biomimetic materials. Some of his
work has been featured by Chemical & Engineering News, the Pittsburgh Supercomputing Center, and as cover pages of the February 20, 2004 issue of Angewandte Chemie International Edition, the March 2, 2006 issue of Journal of Physical Chemistry B, and both June 14, 2007 and January 28, 2008 issues of Physical Chemistry Chemical Physics, and both June 18, 2009 and September 2, 2010 issues of Journal of Physical Chemistry C.

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