Physics Colloquium

Michigan Technological University

Tuesday May 19, 2015

2:00PM Fisher Hall 101

Nucleation of ice and hydrates: Moving beyond direct molecular simulations

Tianshu Li
Department of Civil and Environmental Engineering
George Washington University

Abstract: Ice and gas hydrates are the crystalline solids formed in aqueous environment upon freezing. Despite their apparent significance, the formation mechanisms of ice and hydrates remain poorly understood. In particular, acquiring the quantitative understanding of nucleation at the molecular level is still a formidable challenge. Direct molecular simulation has been serving as a major tool for providing the molecular insight of crystal nucleation, but it fails to acquire nucleation details with sufficient statistical sampling under realistic conditions. In this contribution, I will discuss our recent progress in developing the effective strategy for moving beyond the direct approach to model the nucleation of ice and gas hydrates. Our strategy integrates the forward flux sampling method and the coarse-grained water model, and incorporates the order parameter that we have developed based on the topological analysis of the tetrahedral network. Employing this strategy, we have gained the quantitative and molecular insights of the nucleation behaviors of ice and hydrates in both homogeneous and heterogeneous environments, under various thermodynamic conditions.

Bio: Dr. Tianshu Li obtained his Bachelor's and Master's degrees in Materials Science and Engineering from Tsinghua University in 1999 and 2001, respectively. He obtained his Ph.D. in Materials Science from University of California, Berkeley in 2005. From 2006 to 2010, Dr. Li continued his research as a post-doctoral associate in the Department of Chemistry at University of California, Davis. Dr. Li is now an assistant professor in the Department of Civil and Environmental Engineering at George Washington University. Dr. Li's research is focused on modeling materials' behaviors using classical and quantum approaches. His research interests include the nucleation in aqueous environment, computational design of 2D nano heterostructures, and mechanical behaviors of metals and alloys.

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