

Phase Transitions by Molecular Simulations: Some Recent Examples in Adsorption, Bubble Nucleation and Crystallization

Donguk Suh

Department of Mechanical Engineering, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Molecular simulations have become a powerful tool in understanding the underlying mechanism in phase transitions. The constant increase in computational capacity has made rare event simulations possible and the scale of the simulations, which started from nanoscale have moved into micro order and beyond. In this talk, I will present some recent simulations that have been conducted for adsorption and nucleation. The first example of adsorption will be on understanding the physics of cylindrical nanopore filling using Grand Canonical Molecular Dynamics and Grand Canonical Monte Carlo simulations [1]. The nanopores examined have different hydrophilicity arrangements. The second example is water adsorption and imbibition in a metallic organic framework called MIL-100 (Cr). The aim is to understand how water fills the different pores within the framework. The water has also been frozen and understanding where freezing begins inside the pores is also a point of interest. For a different system, the mechanism in how surfactant molecules inhibit ice crystallization has been studied [2]. Finally, I will introduce some preliminary results on creating a nanoscale bubble using biphilic surfaces.

[1] K. Kashiwagi, D. Suh, J. Hwang, W.-L. Hsu, and H. Daiguji, "Molecular simulations of water adsorption and transport in mesopores with varying hydrophilicity arrangements" *Nanoscale* 10, 11657 (2018).

[2] N. Shimazu, D. Takaiwa, D. Suh, T. Kawaguchi, T. Fuse, T. Kaneko, K. Yasuoka, "Molecular Dynamics Simulation of Ice Crystal Growth Inhibition by Surfactant Molecules," *Langmuir* 34, 9330, 2018.