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Title: Replica-exchange molecular dynamics simulation study on phase behavior of quasi-one-dimensional water inside carbon nanotube

Abstract:
Phase transition is a fundamental ubiquitous phenomenon from science and engineering to nanotechnologies. The most popular examples of phase transition are freezing and boiling of water. It is known that water forms 18 crystalline and 3 amorphous phases. If water is confined to nano pore, such as nanotube and nanoslit, it freezes into various crystalline phases which are not shown in bulk. The structures of confined water change depending on characteristic length of nano pore, such as diameter of nanotube or width of nanoslit. As nano pores can serve as an indispensable tool to control characteristics of confined materials, the researches on the fundamental knowledge of confined system have been done in many research fields for many applications, however, the whole phase diagram of confined water is still not unveiled due to the wide phase diagram which has not only temperature and pressure but also characteristic length as an axis. An efficient method to search wide range of conditions is essential.

Replica-exchange method, an extended ensemble method, enables to sample wide phase space at many temperature-pressure conditions and to avoid the replicated systems getting trapped into metastable state for long time. In addition, physical properties which are difficult to calculate, such as free energy surface or entropy, can be computed with replica-exchange method.

In this talk, I report the result of the replica-exchange molecular dynamics simulation of quasi-one-dimensional water inside carbon nanotube at the diameter of 12.5 angstrom. To perform the simulation over wide-range temperature and pressure region, graphics processing unit (GPU) was adopted to accelerate the simulation. The phase equilibrium condition among the quasi-one-dimensional hexagonal and heptagonal ice nanotubes and liquids was determined by computing the temperature and pressure dependence of physical quantities, such as enthalpy and specific heat. The radial distribution function along the cylindrical axis of carbon nanotube and density distribution function for radial direction indicate the presence of high-density and low-density liquid phases separated by the hexagonal ice nanotube solid phase. The solid-liquid critical point between heptagonal ice nanotube phase and liquid phase was determined by the calculation of free energy surface and Challa-Landau-Binder parameter of volume and entropy. The free energy surface calculation also showed the empty hexagonal ice nanotube gradually changes into partially filled hexagonal ice nanotube with the increase of pressure.