Formation of Ice Nanotubes with Hydrophobic Guests

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The carbon nanotube provides a well-defined nanoscale cylindrical pore which serves to prepare quasi-one-dimensional materials. Water is known to be confined in the carbon nanotube, but its properties in the quasi-one-dimensional space have been as little studied as or even less studied than those of other substances in spite of the fact that water itself has been more studied than the others. However, recent theoretical studies on water confined in the carbon nanotube and the experimental studies followed have demonstrated that the confined water freezes into crystalline structures that have never been found in the bulk counterpart and exhibits continuous and discontinuous freezing transitions [1]. A composite ice nanotube inside a carbon nanotube has been explored by molecular dynamics (MD) and grandcanonical Monte Carlo (GCMC) simulations [2]. It is made from an octagonal ice nanotube whose hollow space contains hydrophobic guest molecules such as neon, argon, and methane. It is shown that the attractive interaction of the guest molecules stabilizes the ice nanotube. The guest occupancy of the hollow space is calculated by the same method as applied to clathrate hydrates. We have found that the octagonal ice tube is formed with coexistence of hydrophobic molecules in its interior by MD simulation. The occupancy by guest molecules is calculated from the approximate theory, which we found agrees well with the GCMC simulations for guest argon and methane but does not for neon. Stability of the ice nanotube relies on the attractive interaction with the guest molecules.

[1] K. Koga, G. T. Gao, H. Tanaka, and X. C. Zeng, *Nature*, **412**, 802 (2001).
[2] H. Tanaka and K. Koga, *J. Chem. Phys*. **123**, 94706 (2005).