Motion of a Water Cluster inside and around SWNTs

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The fact that some of the expanding prospective applications of carbon nanotubes involves aqueous environment has motivated extensive research concerning the interaction of water and carbon nanotubes. On considering the specific applications such as biomedical device for cell manipulators, nanopipettes for DNA sequencing and nanometer-scale capillary for material fabrications, the transport phenomena of liquid is of particular importance.

In the current work, by means of classical molecular dynamics simulations, we investigate the motion of a water droplet adsorbed on both internal and external walls of single wall carbon nanotubes (SWNTs) by imposing a longitudinal temperature gradient with phantom temperature control. The water molecules are modeled with the SPC/E water model whereas the carbon-carbon interaction is expressed using Brenner potential [1]. The carbon-water interacts through simple Lennerd-Jones potential.

Two systems with clusters of 96 water molecules inside and outside of SWNTs are shown in Fig. 1 and Fig. 2, respectively. For both systems, SWNTs are typically 63nm long with the chiral index of (10, 10). The simulations are initiated by placing a water droplet at the room temperature inside/outside the SWNTs prepared in advance to exhibit the temperature gradient. In case of the external-wall adsorption, the water molecules are stably placed in a grove formed by a tube-tube junction. By utilizing these two aqueous systems, the dynamic behavior of the water cluster will be discussed.

[1] D. W. Brenner., *Phys.Rev B*, **42** (1990) 9458.

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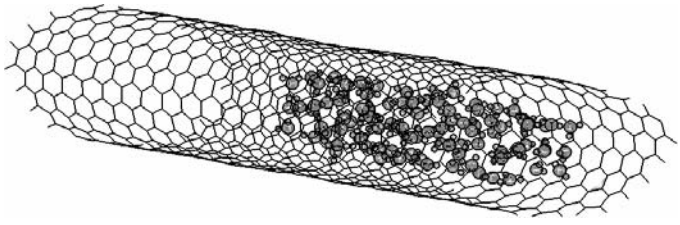

Fig. 1. An oblique slice of a (10, 10) SWNT confining a water cluster.

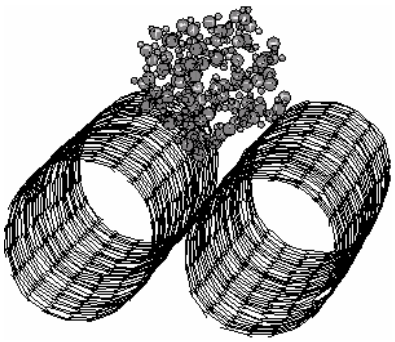

Fig. 2. Water cluster adsorbed in a groove formed by tube-tube junction of (10,10)-SWNTs.