Nanotube-confined liquids: water and methanol

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Carbon nanotube-confined simple hydrogen-bonded liquids, water and methanol, are studied based on molecular dynamics simulations.

Hydrogen bonding is of importance in nature. Its ‘moderate’ strength (i.e., substantially weaker than covalent bonds and stronger than van der Waals bonds) allows of bond making/breaking to bring hydrogen-bonded materials structural flexibility. Water and methanol are prototypical, familiar examples from nonorganic and organic hydrogen-bonded materials, respectively.

What if these tiny molecules are confined in nanospace such as the interior of carbon nanotubes? We focus on natural filling of the interior of uncapped carbon nanotubes that are immersed in the liquid reservoir [1, 2]. A variety of rearrangements of hydrogen bonds are observed depending on the diameter size of the carbon nanotube. Correspondingly, drastic changes in transport properties are also observed.

The results from these confined liquids not only improve our general knowledge of the hydrogen bonded liquids, but also are suggestive of links to future applications of carbon nanotubes in terms of making the most of their hydrophobic interior.