

Researchers clarify properties of 'confined' water within single-walled carbon nanotube pores

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This global temperature-diameter (T-D) phase diagram of water inside SWCNTs shows that, depending on the water content, hollow or filled ice will form. On the right, hollow- and filled-ice nanotubes can be calculated at low temperature for SWCNTs with diameters indicated with (a) and (b) in the lower portion of the phase diagram. Credit: Yutaka Maniwa

Water and ice may not be among the first things that come to mind when you think about single-walled carbon nanotubes (SWCNTs), but a Japanbased research team hoping to get a clearer understanding of the phase behavior of confined water in the cylindrical pores of carbon nanotubes zeroed in on confined water's properties and made some surprising discoveries.



The team, from Tokyo Metropolitan University, Nagoya University, Japan Science and Technology Agency, and National Institute of Advanced Industrial Science and Technology, describes their findings in the American Institute of Physics' <u>Journal of Chemical Physics</u>.

Although <u>carbon</u> nanotubes consist of hydrophobic (water repelling) graphene sheets, experimental studies on SWCNTs show that water can indeed be confined in open-ended carbon nanotubes.

This discovery gives us a deeper understanding of the properties of nanoconfined water within the <u>pores</u> of SWCNTs, which is a key to the future of <u>nanoscience</u>. It's anticipated that nanoconfined water within carbon nanotubes can open the door to the development of a variety of nifty new nanothings—nanofiltration systems, molecular nanovalves, molecular water pumps, nanoscale power cells, and even nanoscale ferroelectric devices.

"When materials are confined at the atomic scale they exhibit unusual properties not otherwise observed, due to the so-called 'nanoconfinement effect.' In geology, for example, nanoconfined water provides the driving force for frost heaves in soil, and also for the swelling of clay minerals," explains Yutaka Maniwa, a professor in the Department of Physics at Tokyo Metropolitan University. "We experimentally studied this type of effect for water using SWCNTs."

Water within SWCNTs in the range of 1.68 to 2.40 nanometers undergoes a wet-dry type of transition when temperature is decreased. And the team discovered that when SWCNTs are extremely narrow, the water inside forms tubule ices that are quite different from any bulk ices known so far. Strikingly, their melting point rises as the SWCNT diameter decreases—contrary to that of bulk water inside a largediameter capillary. In fact, tubule ice occurred even at room temperature inside SWCNTs.



"We extended our studies to the larger diameter SWCNTs up to 2.40 nanometers and successfully proposed a global phase behavior of water," says Maniwa. "This phase diagram (See Figure) covers a crossover from microscopic to macroscopic regions. In the macroscopic region, a novel wet-dry transition was newly explored at low temperature."

Results such as these contribute to a greater understanding of fundamental science because nanoconfined water exists and plays a vital role everywhere on Earth—including our bodies. "Understanding the nanoconfined effect on the properties of materials is also crucial to develop new devices, such as proton-conducting membranes and nanofiltration," Maniwa notes.

Next up, the team plans to investigate the physical properties of confined <u>water</u> discovered so far inside SWCNTs (such as dielectricity and proton conduction). They will pursue this to obtain a better understanding of the molecular structure and transport properties in biological systems.

Provided by American Institute of Physics

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