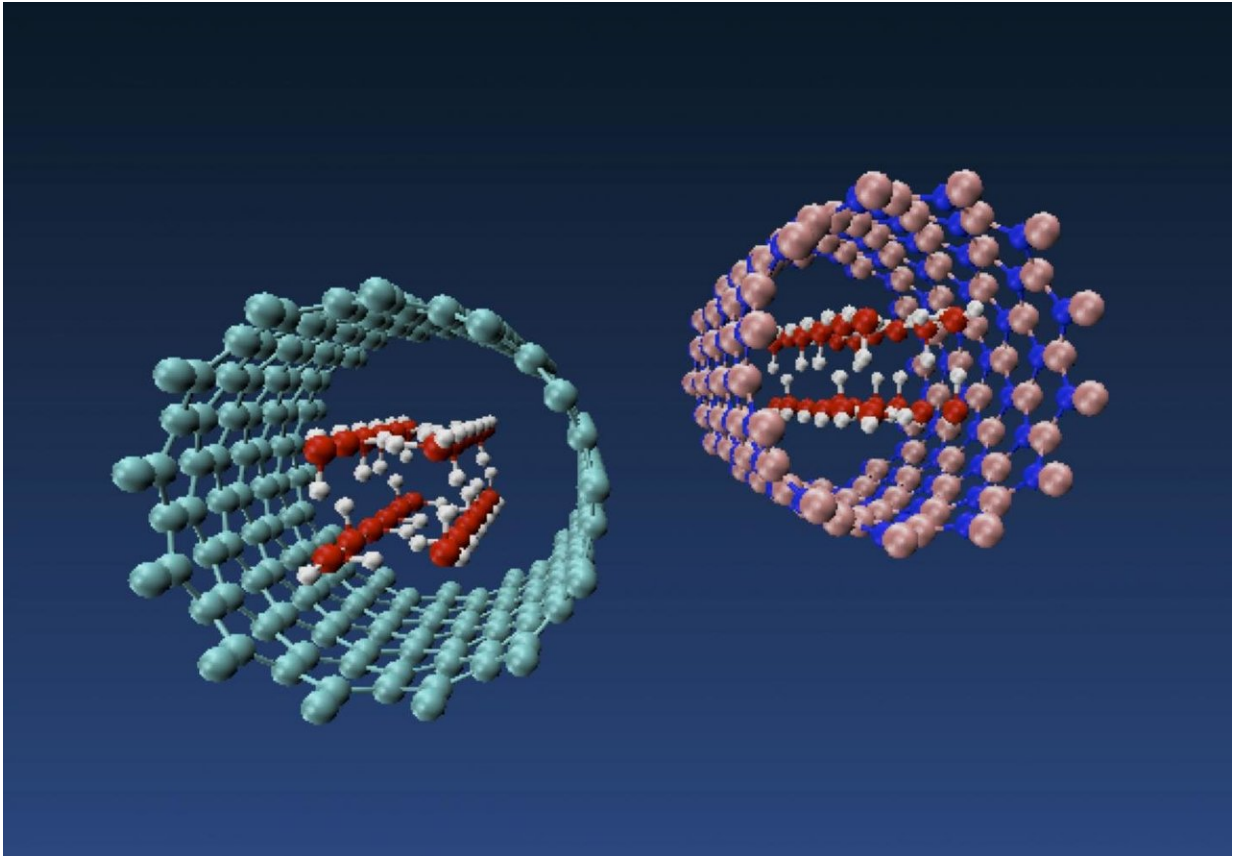


Nanotubes change the shape of water

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Molecular models of nanotube ice produced by engineers at Rice University show how forces inside a carbon nanotube at left and a boron nitride nanotube at right pressure water molecules into taking on the shape of a square tube. The phenomenon is dependent upon the diameter of the nanotube. Credit: Multiscale Materials Laboratory/Rice University

First, according to Rice University engineers, get a nanotube hole. Then insert water. If the nanotube is just the right width, the water molecules will align into a square rod.

Rice materials scientist Rouzbeh Shahsavari and his team used molecular models to demonstrate their theory that weak van der Waals forces between the inner surface of the nanotube and the [water molecules](#) are strong enough to snap the oxygen and hydrogen atoms into place.

Shahsavari referred to the contents as two-dimensional "ice," because the [molecules](#) freeze regardless of the temperature. He said the research provides valuable insight on ways to leverage atomic interactions between nanotubes and [water](#) molecules to fabricate nanochannels and energy-storing nanocapacitors.

A paper on the research appears in the American Chemical Society journal *Langmuir*.

Shahsavari and his colleagues built molecular models of carbon and [boron nitride nanotubes](#) with adjustable widths. They discovered boron nitride is best at constraining the shape of water when the nanotubes are 10.5 angstroms wide. (One angstrom is one hundred-millionth of a centimeter.)

The researchers already knew that [hydrogen atoms](#) in tightly confined water take on interesting structural properties. Recent experiments by other labs showed strong evidence for the formation of nanotube ice and prompted the researchers to build density functional theory models to analyze the forces responsible.

Shahsavari's team modeled water molecules, which are about 3 angstroms wide, inside carbon and boron nitride nanotubes of various chiralities (the angles of their atomic lattices) and between 8 and 12

angstroms in diameter. They discovered that nanotubes in the middle diameters had the most impact on the balance between molecular interactions and van der Waals pressure that prompted the transition from a square water tube to ice.

"If the nanotube is too small and you can only fit one water molecule, you can't judge much," Shahsavari said. "If it's too large, the water keeps its amorphous shape. But at about 8 angstroms, the nanotubes' van der Waals force starts to push water molecules into organized square shapes."

He said the strongest interactions were found in boron nitride [nanotubes](#) due to the particular polarization of their atoms.

Shahsavari said nanotube ice could find use in molecular machines or as nanoscale capillaries, or foster ways to deliver a few molecules of water or sequestered drugs to targeted cells, like a nanoscale syringe.

More information: Farzaneh Shayeganfar et al, First Principles Study of Water Nanotubes Captured Inside Carbon/Boron Nitride Nanotubes, *Langmuir* (2018). [DOI: 10.1021/acs.langmuir.8b00856](https://doi.org/10.1021/acs.langmuir.8b00856)

Provided by Rice University

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