

Scientists Create And Manipulate Nanoscale "Water Wires"

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Upton, NY — Scientists working at the U.S. Department of Energy's Brookhaven National Laboratory have caused tiny strands of water, each less than one nanometer (a billionth of a meter) in width, to form inside a common mineral. These nanoscale "water wires" give the scientists a new opportunity to study the properties of very small quantities of water, such as that found inside cells, which behave differently than water at the macro-scale. The results are published in the March 17, 2004 issue of Nano Letters.

Brookhaven physicist Tom Vogt led the research, performed with collaborators Yongjai Lee of Brookhaven Lab; Joe Hriljac of the University of Birmingham, United Kingdom; and C. Dave Martin and

John B. Parise, both of Stony Brook University.

“Water in cells is distinct from bulk water as we know it,” explained Vogt. “For instance, it can take the form of long chains of single water molecules, which we call ‘water wires’ or ‘water polymers.’ But scientists know very little about water in this form.”

They do know, however, that water wires are responsible for proton transport across cell membranes, which is one step in the fundamental process by which most organisms produce energy. Scientists understand how proton conduction occurs in bulk water, but not yet in water at the nanoscale. Studying water wires may shed light on the mechanism.

“In order to understand the biological role of water wires, we must relate their structure to the properties they display, such as their stability and how they transport protons,” Vogt said. “Confining very small amounts of water inside minerals and glasses is a good way to model and thus learn about water polymers.”

Lee and Martin placed a sample of the mineral natrolite inside a diamond anvil cell, a device that applies very high pressure to a sample using the polished faces of two diamonds. In this case, the pressure was applied after the researchers first surrounded the natrolite sample with a water/alcohol solution. As the high pressure altered the natrolite structure, it also forced water molecules into its empty spaces – a process called pressure-induced hydration. Like tennis balls inserted into a canister, the water molecules nestled one-by-one within the structural framework, forming water wires.

As pressure was continually applied, it nudged the oxygen atoms in adjacent water molecules closer together than oxygen atoms in bulk water. This suggests that the wires may be good proton conductors, since protons travel in water by “hopping” from one molecule to the next,

choosing the path of least water-to-water distance.

Next, Vogt and his group heated the sample to 200 degrees Celsius. Under pressure and heat, the natrolite structure expanded non-uniformly – more in one direction than the other. As a result, some water molecules moved closer together while others moved farther apart. This shifted the direction of the shortest water-to-water distance, creating a new preferred hopping route for protons. Because the direction of proton hopping is what defines the water wires, this shift also changed the wires' orientation.

Understanding proton transport at the nanoscale in water wires could be useful in the development of applications such as hydrogen fuel cell technology, which also involves proton transport. It may also help scientists better understand biological processes that depend on proton transport, such the production of adenosine triphosphate, the compound that provides the energy for many cellular functions.

The scientists followed the natrolite's structural changes at the National Synchrotron Light Source facility at Brookhaven, which produces infrared, ultraviolet, and x-ray light for research. They focused a beam of x-rays at the sample as they increased the diamond anvil cell pressure. The x-rays entered the sample, bounced off its atoms, and emerged in a distinct pattern, creating a “signature” of the sample. By analyzing its changing signature, the scientists tracked the sample's changing structure.

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