Vibrations flit along water's fast lane

With its starring role in the history of Earth and the planet's inhabitants, water has long attracted intense scrutiny from scientists. Studies have revealed that water, despite its apparent simplicity, acts in fascinating, sometimes surprising, ways.

Now, scientists studying vibrations in water molecules have witnessed yet another moving performance: The vibrational energy in water's oxygen-hydrogen (OH) bonds appears to skip quickly from one molecule to the next.

This surprising sleight of hand suggests that molecules dissolved in water—for example, many biological molecules—may exchange energy via a previously unknown fast track through the solvent. If so, the researchers say, this transfer mechanism might illuminate water's role in chemical reactions and important biological processes such as protein folding (SN: 2/20/93, p. 121).

Adding to the drama, the speed of the energy leaps is "enormously fast," says Huib J. Bakker of the FOM Institute for Atomic and Molecular Physics in Amsterdam. Their swiftness may enable vibrational energy to jump among many water molecules before it dissipates. The fast moves also leave in the dust the current theory of how such transfers take place, he and his FOM colleague Sander Woutersen, now at the Max Born Institute in Berlin, conclude in the Dec. 2 NATURE.

In an accompanying commentary, Abraham Nitzan of Tel Aviv University predicts that the new results "may force us to re-examine some of our notions" about energy transfers from molecule to molecule.

John C. Tully of Yale University finds the new observations "both exciting and surprising."

Researchers investigating molecular vibrations often use laser pulses to set bonds in motion (SN: 10/10/92, p. 238). When struck with a laser pulse, OH bonds start to vibrate at a characteristic frequency, Bakker explains. The vibration creates an oscillating electric field that can stimulate the electric field of an OH bond in a nearby water molecule, causing that bond to jitter in turn.

In the new experiment, the FOM team fired polarized infrared laser pulses lasting about 200 femtoseconds (fs) into water samples, exciting OH bonds that happened to lie parallel to the pulse's electric field. Picoseconds later, the experimenters measured vibrations having orientations different from those originally excited.

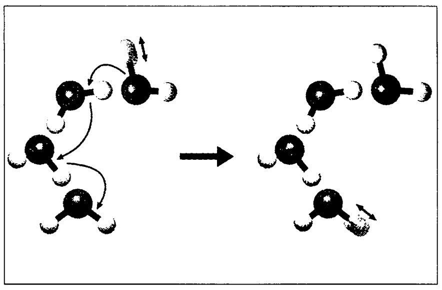
They did this by scanning their samples with a weaker laser beam polarized at 45 degrees relative to the initial pulse. An increase of excitations at the different angles indicates that energy had jumped to bonds in neighboring molecules.

The team first studied thin films of ordinary water mixed with so-called heavy water. Heavy water contains deuterium, a heavy form of hydrogen. Because the deuterium-oxygen bond behaves differently from the OH bond, deuterium can act as a spacer between water molecules in experiments on OH-bond interactions.

With decreasing heavy water concentrations, and therefore less separation on average between OH bonds of neighboring molecules, the scientists found that the rate of energy transfer increases. Their measurements support a leading theory attributing vibration transfers to excitation of one electric field by another.

"We have determined for the first time that the energy in the OH bond definitely hops from one [water] molecule to another," Bakker says.

To the FOM researchers' surprise, when they eliminated the heavy water altogether, the rate of vibration transfer leapt ahead of theoretical predictions by at least a factor of two.



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Vibrations in bonds between oxygen (red) and hydrogen (white) pass from one randomly oriented water molecule to another. Researchers have tracked such transfers by monitoring the changing orientation of the vibrations.

Unknown mechanisms in pure water probably play a role along with the electric field interaction, Bakker says. Because their instruments could not clock transfers briefer than 100 fs, the researchers don't know exactly how quickly these energy movements took place. —*P. Weiss*

Mutation causes rare gum disease

In most people, a squadron of enzymes and immune cells works around the clock to keep teeth and gums healthy—even when their host is too busy to brush. For people with Papillon-Lefèvre syndrome, however, the teamwork breaks down and healthy gums become an elusive dream. Most lose their permanent teeth in their teens.

These people make a faulty version of cathepsin C, a key player in the gum-protection brigade, an international team of researchers reports in the December NATURE GENETICS. They find that individuals with Papillon-Lefèvre syndrome have a mutation on chromosome 11 at the site of the gene, called *CTSC*, that encodes cathepsin C.

While the full role of this protein remains unknown, the findings establish that an abundance of properly functioning cathepsin C deters infection in the vulnerable spaces where teeth meet gums, says study coauthor Nalin S. Thakker, a dentist and geneticist at St. Mary's Hospital in Manchester, England.

Thakker and his colleagues, including scientists from Egypt and Australia, analyzed blood samples from eight families from Egypt, Pakistan, and Lebanon. Each family has at least one member with Papillon-Lefèvre syndrome. Although the parents of affected individuals have reduced cathepsin C activity, none have severe gum disease, or periodontitis, Thakker says.

In each case, however, both parents carried a recessive mutation in *CTSC*, and the children who had inherited one copy from each parent were burdened with Papillon-Lefèvre syndrome. All these parents had married someone within their extended family—often a cousin.

In contrast, the mutations didn't appear at all in 100 Egyptians, 50 Europeans, and 50 South Asians chosen randomly from other families.

Billions of microbes lurk in the mouth, and only a thin layer of skin called the epithelium protects gums from the onslaught. When bacteria lodge between the teeth and gums, many cells in the region make cathepsin C. Also, immune cells called neutrophils rush to the gums.

Thakker and his colleagues investigated cathepsin C because it's necessary for the normal function of neutrophils. He suggests that neutrophils use the protein to activate other enzymes, which fight bacteria. "It would seem logical to conclude that the neutrophils' function is altered in these patients," he says.

The study "helps to further underline the importance of neutrophils in terms of host defense" against periodontitis, says Christopher A. McCulloch of the University of Toronto. Eventually, findings such as these may help scientists devise compounds that make neutrophils more effective at killing bacteria, he adds.

Meanwhile, it remains unclear whether a person's genetic makeup may lead to other types of gum disease, Thakker says. Roughly 15 percent of people lose teeth to periodontitis in middle age.

"Lowered activity of cathepsin C might not cause full-blown Papillon-Lefèvre syndrome, but it might cause periodontitis—with less-efficient cleaning up of the plaque bacteria," he says. —*N. Seppa*