A watershed moment in understanding how H2O conducts electricity

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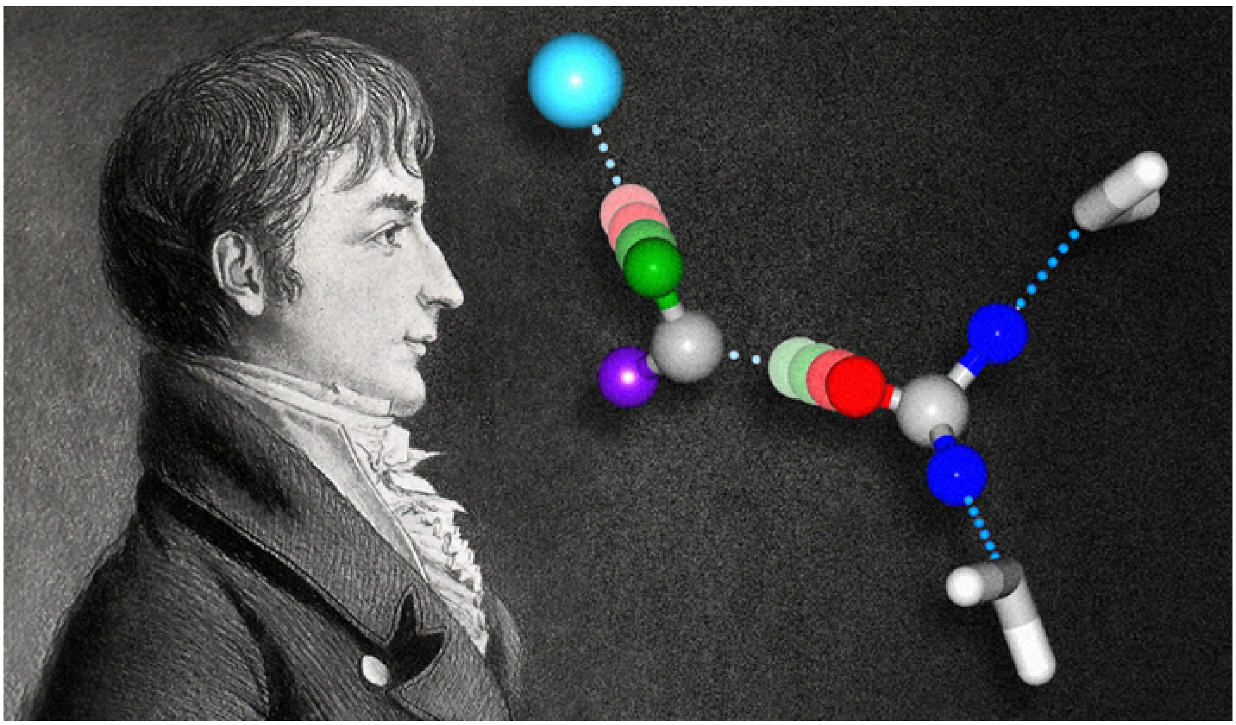

Researchers have taken spectroscopic snapshots of the passage of extra protons from one water molecule to another during conductivity, a mechanism first described by chemist Theodor Grotthuss. Credit: Grotthuss image courtesy of Wikipedia

Scientists have taken spectroscopic snapshots of nature's most mysterious relay race: the passage of extra protons from one water molecule to another during conductivity.

The finding represents a major benchmark in our knowledge of how water conducts a positive electrical charge, which is a fundamental mechanism found in biology and chemistry. The researchers, led by Yale chemistry professor Mark Johnson, report their discovery in the Dec. 1 edition of the journal *Science*.

For more than 200 years, scientists have speculated about the specific forces at work when electricity passes through water—a process known as the Grotthuss mechanism. It occurs in vision, for example, when light hits the eye's retina. It also turns up in the way fuel cells operate.

But the details have remained murky. In particular, scientists have sought an experimental way to follow the structural changes in the web of interconnected water molecules when an extra proton is transferred from one oxygen atom to another.

"The oxygen atoms don't need to move much at all," Johnson said. "It is kind of like Newton's cradle, the child's toy with a line of steel balls, each one suspended by a string. If you lift one ball so that it strikes the line, only the end ball moves away, leaving the others unperturbed."

Johnson's lab has spent years exploring the chemistry of water at the molecular level. Often, this is done with specially designed instruments built at Yale. Among the lab's many discoveries are innovative uses of electrospray ionization, which was developed by the late Yale Nobel laureate John Fenn.

Johnson and his team have developed ways to fast-freeze the chemical process so that transient structures can be isolated, revealing the contorted arrangements of atoms during a reaction. The practical uses for these methods range from the optimization of alternative energy technologies to the development of pharmaceuticals.

In the case of the proton relay race, previous attempts to capture the process hinged on using infrared color changes to see it. But the result always came out looking like a blurry photograph.

"In fact, it appeared that this blurring would be too severe to ever allow a compelling connection between color and structure," Johnson said.

The answer, he found, was to work with only a few molecules of "heavy water"—water made of the deuterium isotope of hydrogen—and chill them to almost absolute zero. Suddenly, the images of the proton in motion were dramatically sharper.

"In essence, we uncovered a kind of Rosetta Stone that reveals the structural information encoded in color," Johnson said. "We were able to reveal a sequence of concerted deformations, like the frames of a movie." Johnson's lab was assisted by the experimental group of Knut Asmis at the University of Leipzig and the theory groups of Ken Jordan of the University of Pittsburgh and Anne McCoy of the University of Washington.

One area where this information will be useful is in understanding chemical processes that occur at the surface of water, Johnson noted. There is active debate among scientists regarding whether the surface of water is more or less acidic than the bulk of water. At present, there is no way to measure the surface pH of water.

More information: "Spectroscopic snapshots of the proton-transfer mechanism in water" *Science*, science.sciencemag.org/cgi/doi … 1126/science.aaf8425

Provided by Yale University

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