Resolving water's electrical properties

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Scientists at Pacific Northwest National Laboratory and Lawrence Livermore National Laboratory provided a consistent interpretation of the different measurements. Their work graces The Journal of Physical Chemistry B cover. Credit: American Chemical Society.

An old confusion about the electrical properties of water's surface has ended, thanks to scientists at Pacific Northwest and Lawrence Livermore National Laboratories. The conflict arose because two types of measurements gave two radically different interpretations of what was happening at the surface of water. The team showed, through careful analysis, that the measurements weren't wrong, but rather the behavior of water's electrons influenced one measurement more than the other. The team's results provided a consistent interpretation of the different

measurements and grace *The Journal of Physical Chemistry B* cover.

"This could change how we think about water," said Dr. Gregory Schenter, a chemical physicist at PNNL who worked on the study.

While most people may not think of water as having electrical properties , when the behavior and movement of the electrons in this ubiquitous liquid comes into play in designing alternatives to today's fossil fuels, water is often part of the conversation. The electrical forces that exist in water, a simple V-shaped molecule made from two hydrogen atoms and an oxygen atom, are vital to understanding and controlling how molecules, ions, and other chemical components move and behave. For example, understanding water is necessary to convert agricultural waste into bio-fuels. Further, water's behavior impacts work on storing energy from solar cells, wind turbines, and other renewable sources, allowing more flexibility in designing energy strategies.

In chemistry, the simple approach that assigns a positive charge to a hydrogen atom and a negative charge to an oxygen atom can be very powerful. This simple model can work when it comes to understanding the forces that move molecules around in water. In other cases, it doesn't work.

When taking measurements with certain instruments, the simple model matches experimental results quite well. But, when using other techniques, the model differs wildly from what's measured. Theoretical chemists at PNNL and LLNL were the first to figure out what was happening.

They found that to measure electrical properties occurring at the molecular scale, where the length scales are measured in billionths of a meter, the models need to consider that the protons are in the nucleus and the electrons are everywhere else.

"It comes down to understanding where in the molecule you are making the measurements," said Dr. Shawn Kathmann, a chemical physicist at PNNL who worked on the study.

Complex descriptions of matter, referred to as ab initio electronic structure calculations, that focus on identifying electrons location and electron holography experiments showed that the conflict was caused by where you were measuring the surface potential in the molecules. If you determined the surface potential right next to the protons, you got one answer. If you determined the potential in the void between molecules, you get a different answer. And, finally, if you took measurements close to the electrons, you got still another answer.

"When you treat the electrons and protons appropriately, you get more accurate results," said Kathmann.

This research is part of ongoing work at PNNL to fundamentally understand the forces inside water and other molecules. The goal is to push past the existing knowledge frontiers regarding ions and interfaces. The team is working on developing models that more accurately and appropriately represent electrons. They are also striving to isolate the effects of electrons in driving matter at interfaces as well as the electrical stresses inside aqueous electrolytes.

More information: Kathmann SM, et al. 2011. "Understanding the Surface Potential of Water." *The Journal of Physical Chemistry B* 115, 4369-4377. DOI: 10.1021/jp1116036

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https://phys.org/news/2011-05-electrical-properties.html