First observation of how water molecules move near a metal electrode

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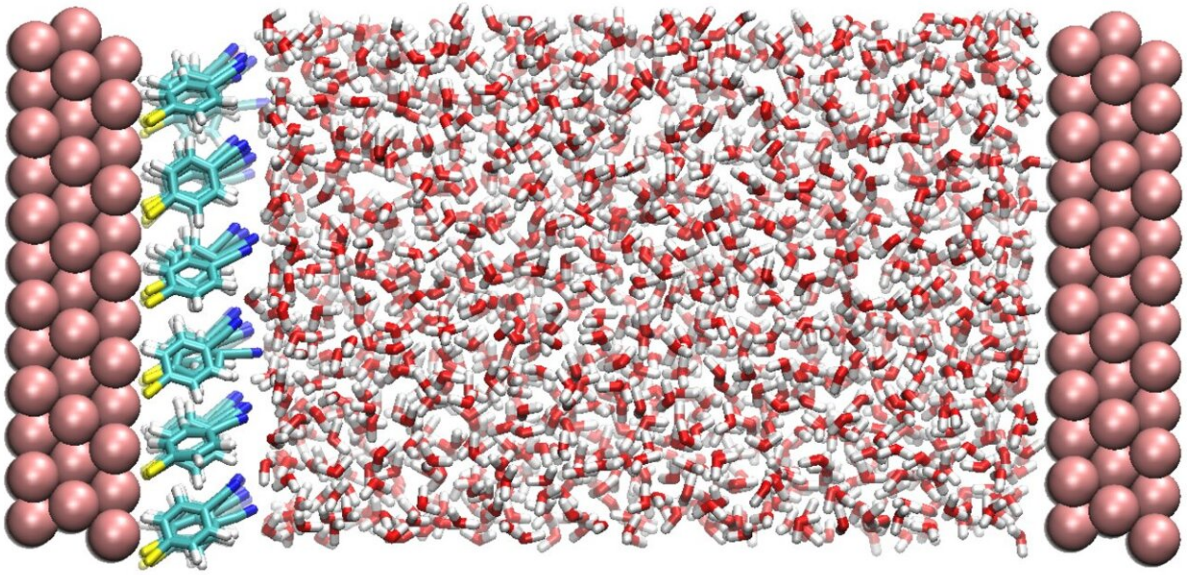


A snapshot taken from the computer simulation model of the system in this study. On both sides are three layers of gold atoms representing the metal electrode with adsorbed organic molecules on the left electrode. The space between the electrodes is filled with water molecules. Credit: Institute for Basic Science

A collaborative team of experimental and computational physical chemists from South Korea and the United States has made an important discovery in the field of electrochemistry, shedding light on the movement of water molecules near metal electrodes.

This research holds profound implications for advancing next-generation batteries utilizing aqueous electrolytes.

In the nanoscale realm, chemists typically utilize laser light to illuminate molecules and measure spectroscopic properties to visualize molecules. However, studying the behavior of water molecules near metal electrodes proved challenging due to the overwhelming interference from metal atoms in the electrode itself.

Additionally, water molecules distant from the electrode surface also contribute to the response of the applied light, complicating the selective observation of molecules at the liquid-metal electrode interface.

Led by Professor Martin Zanni from the University of Wisconsin at Madison and Director CHO Minhaeng from the Center for Molecular Spectroscopy and Dynamics within the Institute for Basic Science (IBS) addressed this challenge with newly developed spectroscopic techniques coupled with computer simulations.

To minimize the interference from the metals, the authors coated the surface of the electrode with specially designed organic molecules. Then, surface-enhanced femtosecond (10^{-15} second) two-dimensional vibrational spectroscopy was employed to observe the changes in the movement of water molecules near the metal electrode.

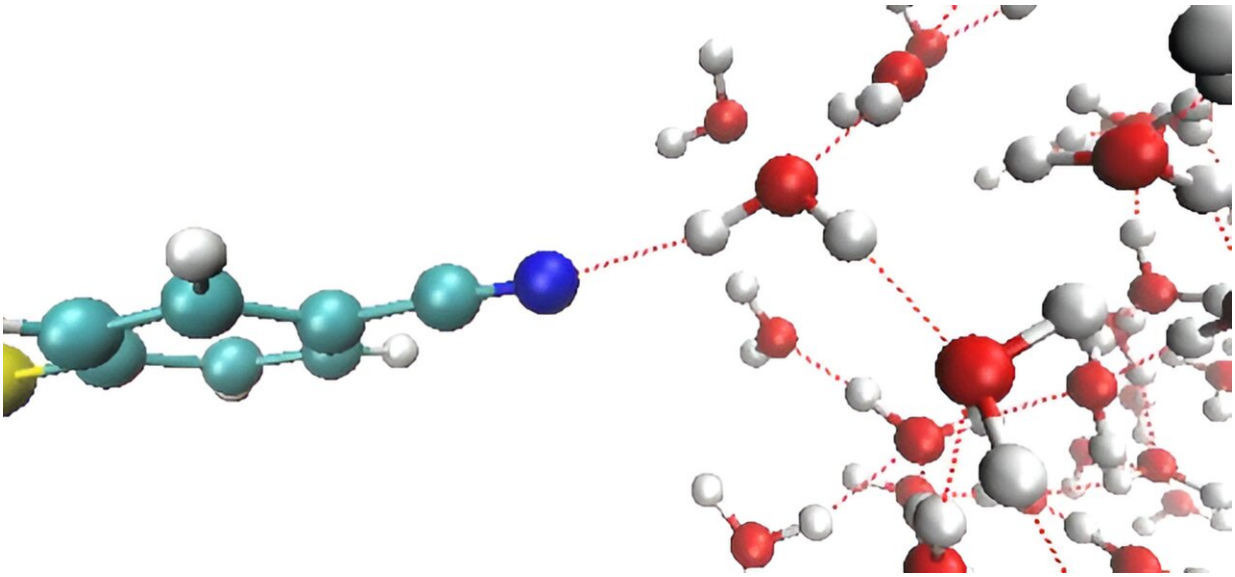


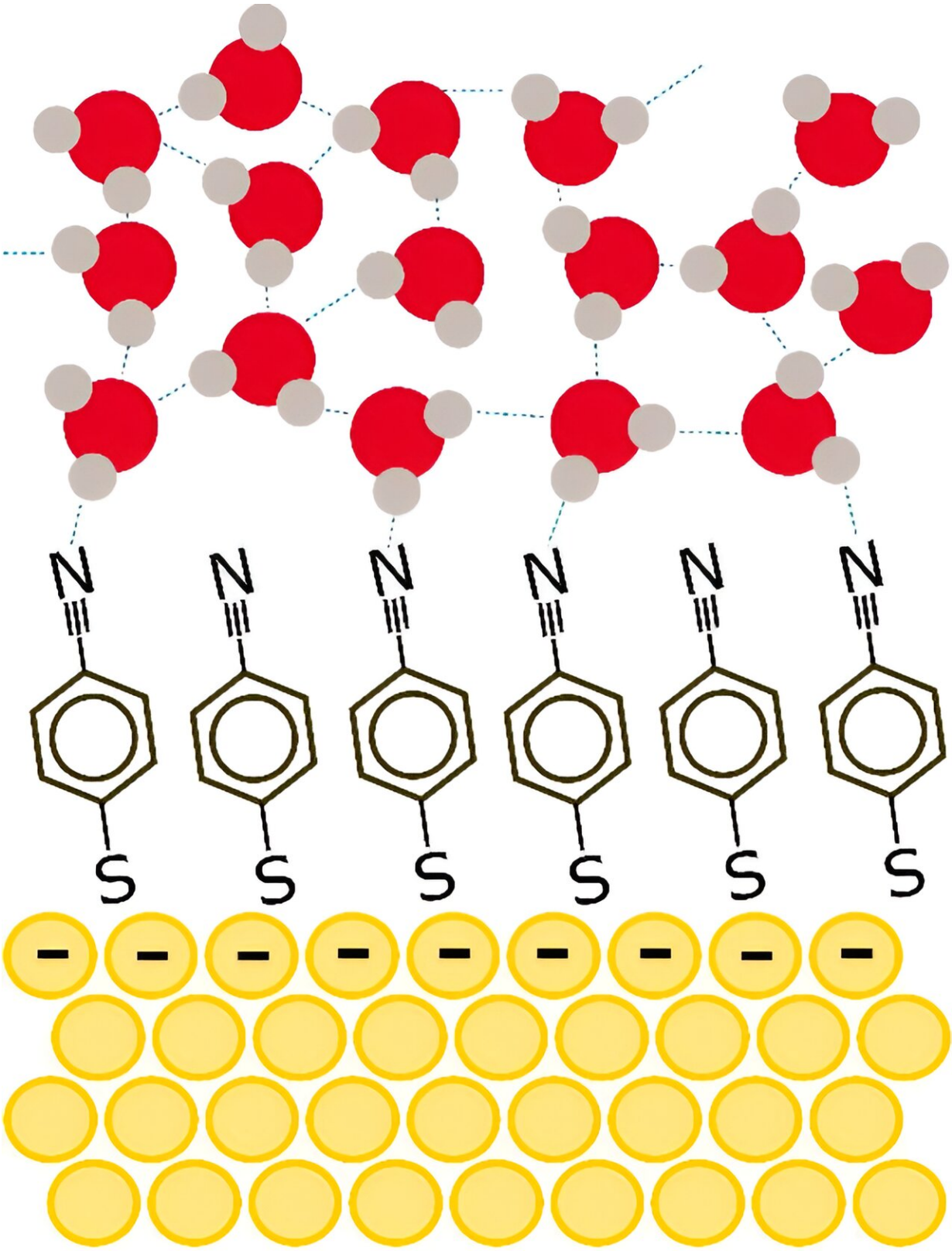
Figure representing the hydrogen bonding interaction between water molecules and an adsorbed organic molecule. Credit: Institute for Basic Science

Depending on the magnitude and polarity of the applied voltage on the metal electrode, the researchers observed, for the first time, either deceleration or acceleration of the motion of water molecules near the electrode.

"When a positive voltage is applied to the electrode, the movement of nearby water molecules slows down. Conversely, when a negative voltage is applied, the opposite is observed both in femtosecond vibrational spectroscopy and in computer simulations," explains Dr. Kwac.

"The results of this study provide crucial information for understanding electrochemical reactions, offering essential physical insights necessary for the research and development of aqueous electrolyte batteries in the future," comments Director CHO Minhaeng of the IBS Center for

Molecular Spectroscopy and Dynamics, a corresponding author of the study.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Schematic figure representing the organic molecules adsorbed on a gold surface and water molecules near the gold electrode. Credit: Institute for Basic Science

This outcome implies a close relationship between electrochemical reactions involving water on the surface of electrodes and the dynamics of interfacial water molecules. It is expected to not only advance our understanding of fundamental electrochemical processes but also pave the way for the design of more efficient and sustainable battery technologies.

This research was published in the *Proceedings of the National Academy of Sciences*.

More information: The hydrogen-bonding dynamics of water to a nitrile-functionalized electrode is modulated by voltage according to ultrafast 2D IR spectroscopy, *Proceedings of the National Academy of Sciences* (2023). DOI: 10.1073/pnas.2314998120. doi.org/10.1073/pnas.2314998120

Provided by Institute for Basic Science