Chemists take a closer look at the spot where water meets air

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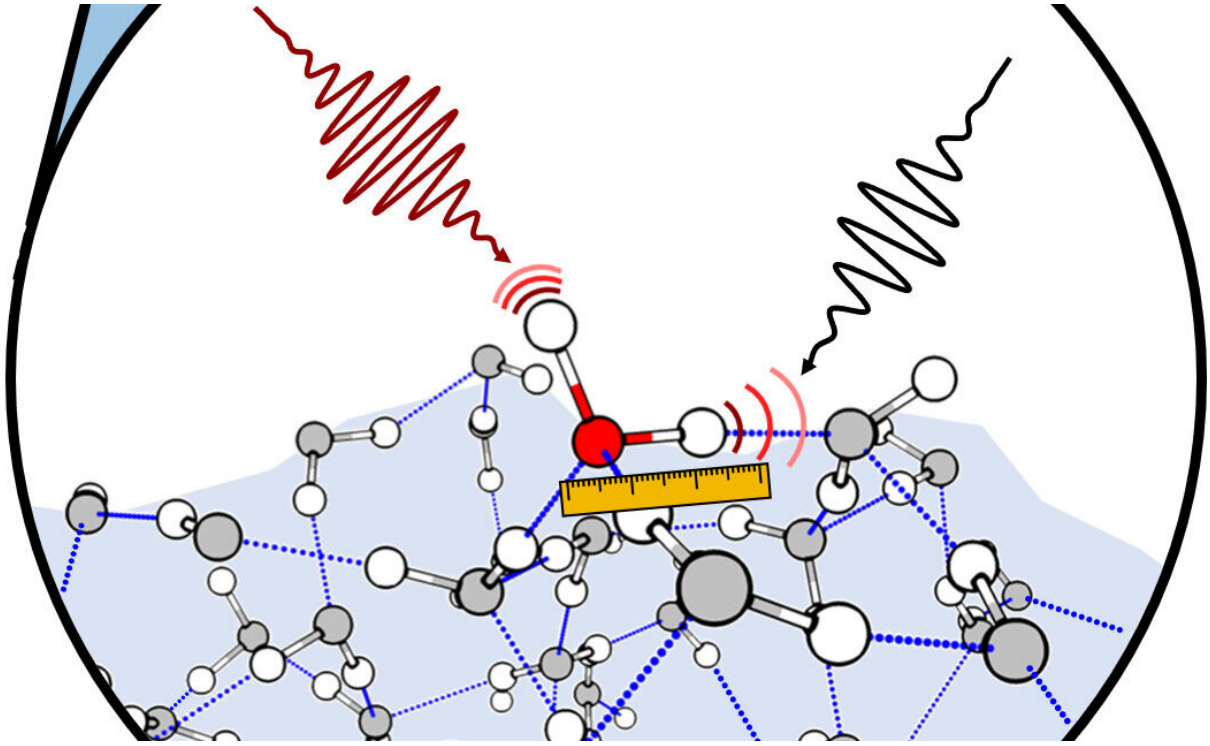

Schematic of water surface where the spectral signature of one isotopically labeled water molecule is isolated with two infrared lasers. Credit: Nan Yang

Water, despite its central place in so many processes vital to life on Earth, remains a chemical mystery in many respects. One of those mysteries is the nature of water at the exact point where it comes into contact with air.

A study from the laboratories of Yale chemistry professor Mark Johnson and University of Washington chemistry professor Anne McCoy offers a new level of observation and analysis.

They provide the first direct measurement of variations in frequency and complexity associated with bonded oxygen and hydrogen (OH) atoms perched on the surface of water—when one of the OH groups is sticking out of it. The researchers also offer the first measurement of how these OH groups are coupled together on the surface plane of water.

"Our work is really a fundamental science contribution. Its importance lies in the fact that elementary mechanics and chemical properties of water are important in many fields, and many researchers are involved in simulating this behavior from first principles. We provide a quantitative benchmark upon which to calibrate such simulations," said Johnson, who is the Arthur T. Kemp Professor of Chemistry at Yale.

Johnson's work has highlighted a number of the chemical properties of water—often using instruments designed and 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, and ways to fast-freeze chemical processes in water to reveal the contorted arrangements of atoms during a reaction.

The new study appears in the April 18 online edition of *Science*. The first author of the study is Nan Yang and co-authors are Chinh Duong and Patrick Kelleher—all from Yale.

More information: N. Yang el al., "Deconstructing water's diffuse OH stretching vibrational spectrum with cold clusters," *Science* (2019). science.sciencemag.org/cgi/doi … 1126/science.aaw4086

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