Potential energy surfaces of water mapped for the first time

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Water is certainly the best-known liquid in the world. It plays a crucial role in all biological and many chemical processes. The water molecules themselves hardly hold any secrets. In school we learn that water consists of one oxygen atom and two hydrogen atoms. We even know the typical obtuse angle that the two O-H legs form with each other. In addition, we know when water boils or freezes and how these phase transitions are related to pressure.

But between facts on individual molecules and a deeper understanding of the macroscopic phenomena, there is a wide area of uncertainty: Only statistical information is known about the behavior of the individual molecules in normal liquid water. The water molecules in the liquid phase form a fluctuating network of hydrogen bonds, disordered and dense, and their interactions are not at all as well understood as in the gaseous state.

Pure liquid water examined

Now, a team led by HZB physicist Dr. Annette Pietzsch has taken a closer look at pure liquid water at room temperature and normal pressure. Using X-ray analysis at the Swiss Light Source of the Paul Scherrer Institute and statistical modeling, the scientists have succeeded in mapping the so-called potential energy surfaces of the individual water molecules in the ground state, which come in a large variety of shapes depending on their environment.

Oscillations and vibrations measured

"The special thing here is the method: we studied the water molecules on the ADRESS beamline using resonant inelastic X-ray scattering. Simply put, we nudged individual molecules very carefully and then measured how they fell back into the ground state," says Pietzsch. The low-energy excitations led to stretching oscillations and other vibrations, which—combined with model calculations—produced a detailed picture of the potential surfaces.

"This gives us a method to experimentally determine the energy of a molecule as a function of its structure," explains Pietzsch. "The results help to enlighten the chemistry in water, for example to understand better how water behaves as a solvent."

The results were published in *Proceedings of the National Academy of Sciences*.

Outlook: METRIXS at BESSY II

The next experiments are already planned at the BESSY II X-ray source at HZB. There, Annette Pietzsch and her team have set up the METRIXS measuring station, which is designed precisely for investigating liquid samples with RIXS experiments. "After the summer shutdown due to maintenance work on BESSY II, we will start with the first tests of our instruments. And then we can move on."

More information: Annette Pietzsch et al, Cuts through the manifold of molecular H_2O potential energy surfaces in liquid water at ambient conditions, *Proceedings of the National Academy of Sciences* (2022). DOI: 10.1073/pnas.2118101119

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