Liquid water molecules are inherently asymmetric: New insight into the bonds between water molecules

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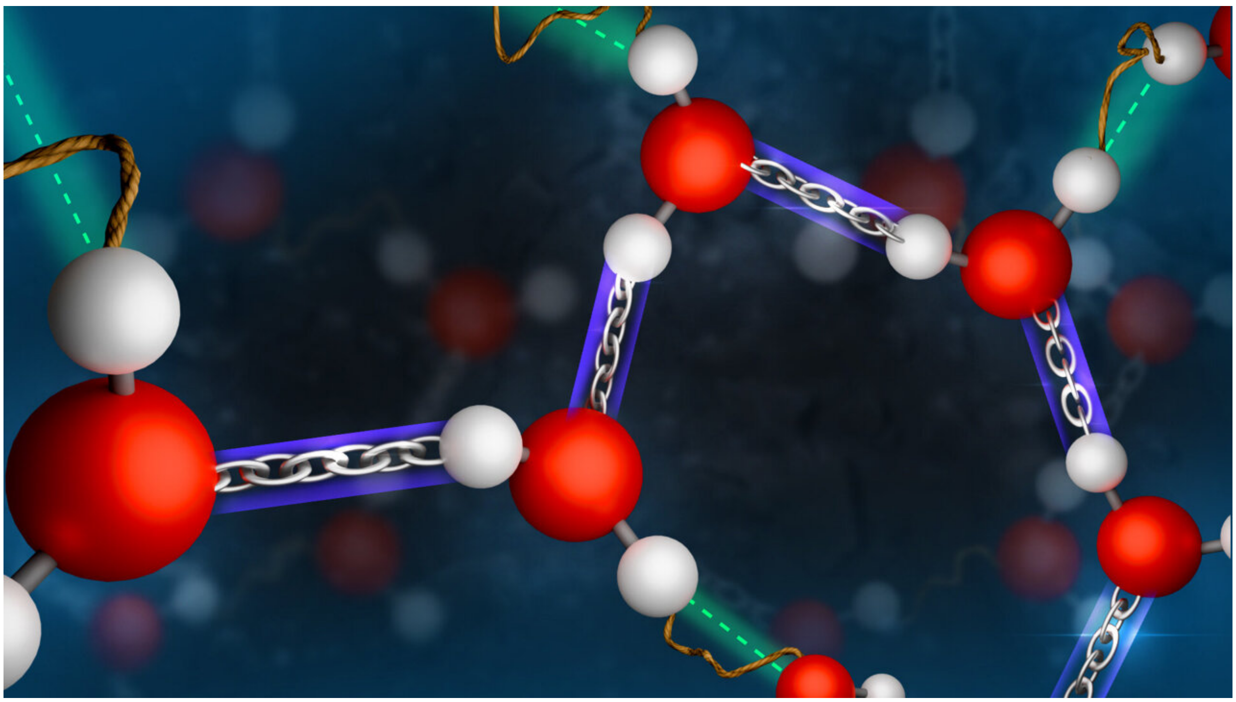


The bonds between neighboring water molecules are not purely randomly distributed: Each water molecule forms a strong and a weak bond. This could be a key to explain anomalies of water. Credit: Max Planck Society

Icebergs float on water because the underlying liquid water has a higher density than the iceberg. Liquid water itself has its highest density at

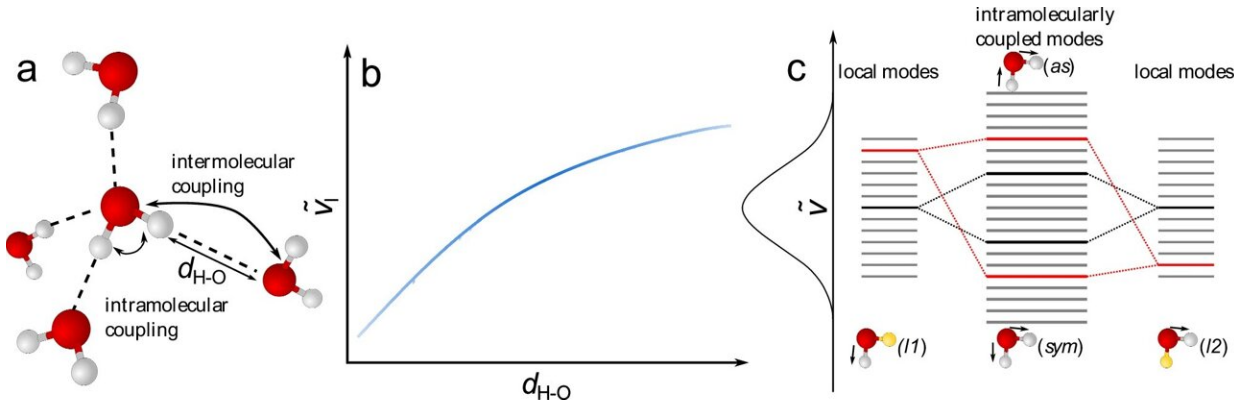
4°C—one of the so-called anomalies of water, i.e. properties of liquids that are rarely observed for other liquids.

The origins of these anomalies have long been the subject of scientific research. Researchers at the Max Planck Institute for Polymer Research have now discovered another piece to the puzzle to explain the special behavior of water.

Many of the anomalous properties of water can be traced to the special interactions between the individual water molecules—the so-called hydrogen bonds. Each water molecule can donate two of these bonds—one from each hydrogen atom—and accept two of them from other, neighboring molecules.

Unlike in ice, these bonds are broken and re-formed on average 1 trillion times per second in liquid water, so that the water molecules can be packed closer together and move very quickly. Due to the rapid movement of the water molecules in the liquid, one might assume that the strength of the individual bonds to its neighbors is purely random.

However, the team led by Johannes Hunger has discovered that the hydrogen bond distances are not simply random, but that two bonds of a molecule have different strengths: If one bond is very strong—i.e. the first neighboring water molecule is very close—the second hydrogen bond is weak—i.e. the second neighboring water molecule is further away.



H-bonding and vibrational structure of water. Credit: *Nature Communications* (2024). DOI: 10.1038/s41467-024-54804-y

These alternating bond distances lead to structuring of the nominally disordered liquid: if you move from one water molecule to the next and to the one after that, there is always a strongly bonded neighboring molecule. As a result, structures such as rings or chains of water molecules can form in the liquid. The structure of liquid water is therefore not just a random arrangement of individual water molecules but follows certain rules.

To obtain these results, the scientists diluted water with a solvent so that they could examine isolated water molecules. They made individual atoms of the water molecules vibrate with the help of lasers and investigated how the vibrations influence each other. This allowed them to measure the strength of individual hydrogen bonds and the strength of the neighboring bond at the same time.

The study, now published in the journal *Nature Communications*, contributes to a comprehensive understanding of the anomalies of water at a molecular level.

More information: Lucas Gunkel et al, Dynamic anti-correlations of water hydrogen bonds, *Nature Communications* (2024). DOI: 10.1038/s41467-024-54804-y

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