

The Two Faces of Supercooled Water

Computations support the 30-year-old idea that supercooled liquid water can undergo a transition between high- and low-density states.

By **Ryan Wilkinson**

Water has many remarkable features. For instance, it is the only substance that exists in nature as a solid, a liquid, and a gas. In 1992, scientists suggested that water might have another unusual attribute: they proposed that it could transition between high- and low-density liquid forms when it is supercooled—quickly chilled to a temperature below which it would normally freeze. Now Thomas Gartner and his colleagues at Princeton University have found the strongest computational verification to date for such a liquid–liquid transition [1]. They hope that their work will inspire others to use similar computational approaches to tackle additional longstanding problems in chemistry and physics.

The existence of this high- to low-density transition could explain some anomalous features of liquid water, such as the sharp increase in the substance’s heat capacity and compressibility when it is cooled at ambient pressure. But the transition is difficult to experimentally detect because supercooled water solidifies before the necessary

measurements can be made. Given this challenge, Gartner and his colleagues instead conducted an extensive computational study of supercooled water. Their work combined state-of-the-art molecular simulations, electronic-structure calculations, and machine learning.

The researchers obtained definitive computational evidence for a liquid–liquid transition in supercooled water. In addition to improving our understanding of the physical chemistry of this substance, the team says that the findings could have wider implications: liquid–liquid transitions are often used in industrial separation processes and are thought to have pivotal roles in cellular function.

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REFERENCES

1. T. E. Gartner III *et al.*, “Liquid-liquid transition in water from first principles,” *Phys. Rev. Lett.* **129**, 255702 (2022).



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