Pushing liquids to their limits with next-gen materials simulation methods

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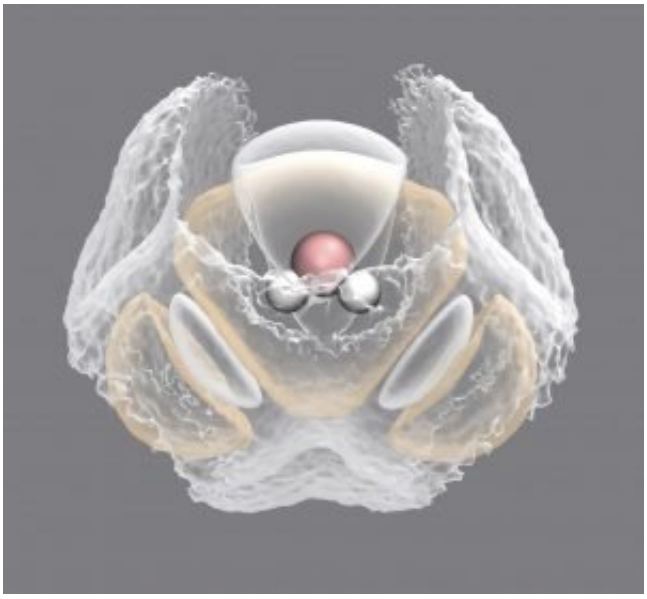

An illustration showing how water molecules are arranged in the liquid around a central reference molecule. The white areas show the highly directional organization of water density in the first and second structural “shells” arising from the hydrogen bonds – while the orange area shows the depletion region – where no water molecules can reside. The images are obtained using the quantum Drude oscillator model. Credit: IBM Blog Research

Materials in industrial and engineering applications, such as iron and steel, are often used at extreme pressures and temperatures or in complex environments where their properties may be very different from those found under normal circumstances.

Perhaps the most famous example of this in practice are the exterior tiles of the NASA Space Shuttle Columbia, which was covered in a combination of silica compounds and aluminum oxide to protect it against temperatures of up to 1,200 degrees F. Looking back now, it was an incredible engineering feat to achieve this considering they lacked the computational power we have today.

The ability to predict the properties of materials, such as with the tiles, far from the conditions encountered in common experience, and where experimental measurements are limited, is therefore a major advantage in materials design and discovery. This situation presents unique challenges for materials simulation as it requires models and their underlying assumptions to be applied in situations very different from those in which they were developed.

A team involving IBM Research and the UK Science and Technology Facilities Council's (STFC) Hartree Centre have developed a new class of materials simulation methods designed to improve predictive power and extend the range of conditions over which materials simulation models at the molecular scale can be applied with confidence. This is achieved by incorporating electronic responses into the molecular description. This innovation allows the simulated molecules to adapt to their environment in the way "real" molecules do and is efficient enough to be applied to relatively large, complex systems.

In a paper appearing today in *Nature Scientific Reports*, we address the celebrated challenge of liquid water as a model system exhibiting unusual and dramatic changes to physical properties depending on temperature – with particularly mysterious behaviour (such as a temperature of maximum density and negative thermal expansion) appearing near and below freezing.

Our team uses materials simulation to explore the structure and

properties of water at the extremes of its stability range as a liquid: At its high temperature limit when the liquid first condenses into small molecular-scale chains and droplets down to the lowest temperatures reachable for the highly structured "supercooled" liquid – which survives far below the normal freezing point; and into the unfamiliar "stretched" regime – where the liquid bonds support high tensile stresses before "breaking" to form vapour cavities. The work also reveals previously unrecognised relationships between the liquid structure and those of "glassy ices."

The agreement with available experimental evidence across such a wide range of conditions is powerful evidence that the electronic responses incorporated in the model capture the essential physics required to describe some of the mysterious properties of water and expose their molecular origins for the first time.

While in our paper we focused on water or liquids, it's also practical for solids, and we are currently developing for wider applications in industrial sectors such as in the life sciences through the Hartree Centre.

Thinking back to the engineers designing the Space Shuttle, they probably had months if not years of trial and error to develop the tiles to be heat resistant, yet light and not too brittle. By applying the technology discussed in our paper they could have tested hundreds of designs in minutes. Not to forget, we are doing virtual testing, which also is much less costly and safer when compared to physical testing.

I am confident that this materials simulation work will contribute to a new cognitive age of discovery.

More information: Flaviu Cipcigan et al. Structure and hydrogen bonding at the limits of liquid water stability, *Scientific Reports* (2018). DOI: 10.1038/s41598-017-18975-7

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