More Evidence for a Revolutionary Theory of Water

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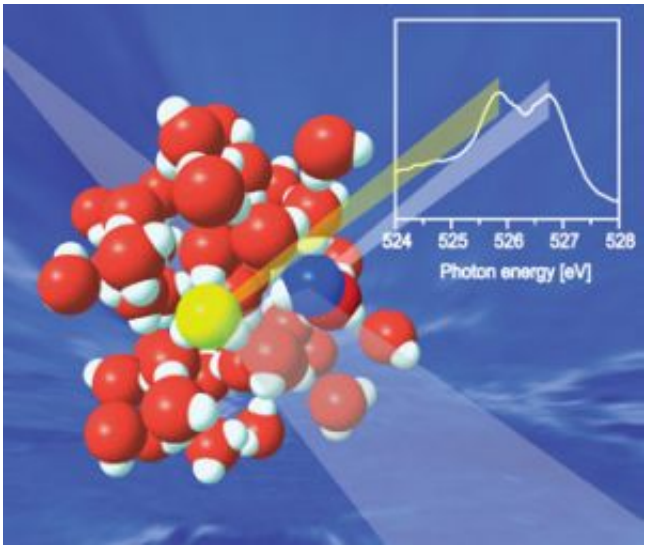

Recent X-ray Spectroscopy studies have revealed that modern theories of the structure of liquid water are incorrect. (Courtesy: Stanford Linear Accelerator Center)

The traditional picture of how liquid water behaves on a molecular level is wrong, according to new experimental evidence collected by a collaboration of researchers from the Department of Energy's Stanford Linear Accelerator Center (SLAC) in California, RIKEN SPring-8 synchrotron and Hiroshima University in Japan and Stockholm University in Sweden.

The team, involving SLAC scientist Anders Nilsson, used advanced X-

ray spectroscopy techniques to create a more detailed picture of water's molecular behavior. Published as the cover story in the June 30 edition of the journal *Chemical Physics Letters*, the findings could soon help overturn the established orthodoxy surrounding the substance most essential to life.

Water, by any measure, is strange stuff. It behaves unlike any other liquid. It has a tremendous capacity for carrying heat—which is why the Gulf Stream keeps Europe warm. Water's solid phase —ice— is less dense than the liquid, which is why ice floats; life on Earth could never have formed if oceans and lakes froze from the bottom up. Water also has unusually strong surface tension—a property essential for the capillary action at work in the roots of plants and within our cells. These strange properties are what make water such an essential substance to the existence of life.

But despite its prevalence and importance, liquid water is not well understood, and its molecular structure has been the subject of intense debate for decades. Ice, whose structure was long ago well established, forms a tight "tetrahedral" lattice of molecules each binding to four others. The prevailing model of liquid water holds that as ice melts, the molecules loosen their grip but remain generally arranged in the same tetrahedral groups.

In the recent study, Nilsson and colleagues probed the structure of liquid water using X-ray Emission Spectroscopy and X-ray Absorption Spectroscopy. These techniques use powerful X-rays, generated by a synchrotron light source, to excite electrons within a water molecule's single oxygen atom. Tuning the X-rays to a specific range of energies can reveal with tremendous precision the location and arrangement of the water molecules. In this way Nilsson's team found that water is indeed made up of tetrahedral groups, but clear evidence also emerged for the dominance of a second, less defined structure in the mix.

The idea that liquid water is made up of two structures is not new. German physicist Willhelm Conrad Röntgen, who discovered X-rays in the late 19th century, published a paper proposing that liquid water comprised two different structures—one tetrahedral "ice-like" structure, and another more loosely arranged structure, which helped explain why water behaves in such unusual ways. Now, more than a century later, the current study is giving new life to Röntgen's "two structure" model.

"It is amazing that the modern usage of X-rays demonstrates that Röntgen, more than 100 years ago, was on the right path," said Nilsson. "Water is still not fully understood, although it is the basis of our existence. I expect more surprises to be discovered in the future."

Settling the debate about water's molecular structure holds tremendous importance for a range of fields including medicine, chemistry and biology. Current molecular dynamics models, which are used to understand chemical and biological processes, are notoriously limited in their ability to predict water's behavior.

The current study is the most recent addition to a growing body of evidence for a new theory about the structure of liquid water. In 2004, Nilsson and colleagues sparked controversy with a paper published in Science that suggested the tetrahedral model of water was incorrect. Nilsson agrees that the debate is far from settled and that much work remains before a clear picture of liquid water emerges.

"Over the last decade or so we have discovered that materials once considered homogeneous exhibit complex nanoscale order," said Stanford Synchrotron Radiation Laboratory director Jo Stöhr. "In my view, the work on water is yet another example of the actual complexity of matter, this time within a simple liquid. Modern X-ray work appears to be triggering a new understanding of liquids and we may have only seen the beginning of a paradigm shift in our understanding."

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Source: Stanford Linear Accelerator Center

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