New details of atomic structure of water under extreme conditions found

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Scientist from Dortmund, Helsinki, Potsdam, and the ESRF have revealed details of the microscopic atomic structure of water under extreme conditions. The results have now been published in the *Proceedings of the National Academy of Sciences* of the USA.

Liquid water remains a mystery even after decades of dedicated scientific investigations and researchers still struggle to fully describe its unusual structure and dynamics. At high temperatures and high pressures, water is in the so called supercritical state and exhibits a number of peculiar characteristics that are very unlike from water at ambient conditions. In this state water is a very aggressive solvent, enabling chemical reactions impossible otherwise, e.g. the oxidization of hazardous waste or the conversion of aqueous biomass streams into clean water and gases like hydrogen and carbon dioxide.

High temperature and high pressure conditions can also be found inside the Earth, in its lower crust and upper mantle. Here, the unique properties of supercritical water have been believed to play a key role in the transfer of mass and heat as well as in the formation of ore deposits and volcanoes. Supercritical water is even thought to have contributed to the origin of life.

Knowledge of the structural properties of water on an atomic scale under these extreme conditions of high temperature and high pressure may become very helpful in understanding these processes, says Christoph Sahle, from the Department of Physics at the University of Helsinki and a member of the research team behind the new results.

Spectroscopic investigations confirm previous theoretical model

Now, a research team of scientists from the Technische Universität Dortmund, Germany, the University of Helsinki, Finland, the Deutsches GeoForschungsZentrum in Potsdam, Germany, and the European Synchrotron Radiation Facility (ESRF), Grenoble, France, have used x-ray spectroscopy to study the structural properties of water in the supercritical state.

Conventional spectroscopic analyses can provide key insights into the atomic structure of a substance, however, these techniques are not well suited to studying water under supercritical conditions because of the complicated sample environments in which supercritical water has to be contained. Using the intense x-ray radiation from the ESRF for inelastic x-ray scattering spectroscopy and a new technique that makes it possible to look at the chemistry of water inside a complex environment together with a quantum mechanical modeling framework known as density functional theory, the group of scientists has made these spectroscopic investigations of water at high temperature and high pressure feasible.

The researchers found that the measured inelastic x-ray scattering spectra evolve systematically from liquid-like at ambient conditions to more gas-like at high temperatures and pressures. To learn more about the local atomic structure of water at the tested conditions, theoretical inelastic x-ray scattering spectra from computer simulations were calculated and compared to the experimental data. All features found in the experimental data and the systematic changes of these features as a function of temperature and pressure could be reproduced by the calculation.

Based on this close resemblance of the calculated and measured data, the authors extracted detailed information about the atomic structure and bonding. They could show that, according to the theoretical model, the microscopic structure of water remains homogeneous throughout the range of examined temperatures and pressures.

The presented findings also implicate means to study unknown disordered structures and samples under extreme conditions on an atomic scale in depth even when other structural probing techniques fail.

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