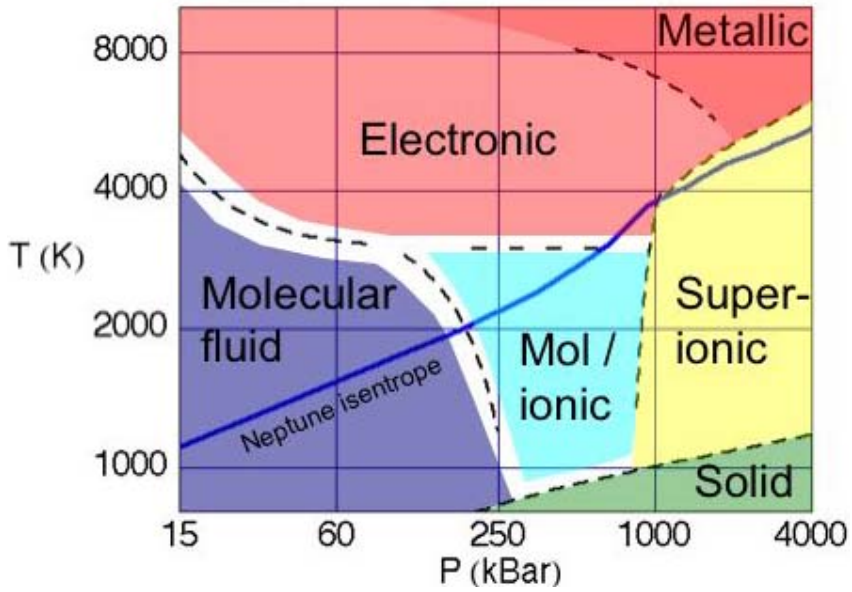
T. Mattsson Press Release

Water on giant planets gets a new look

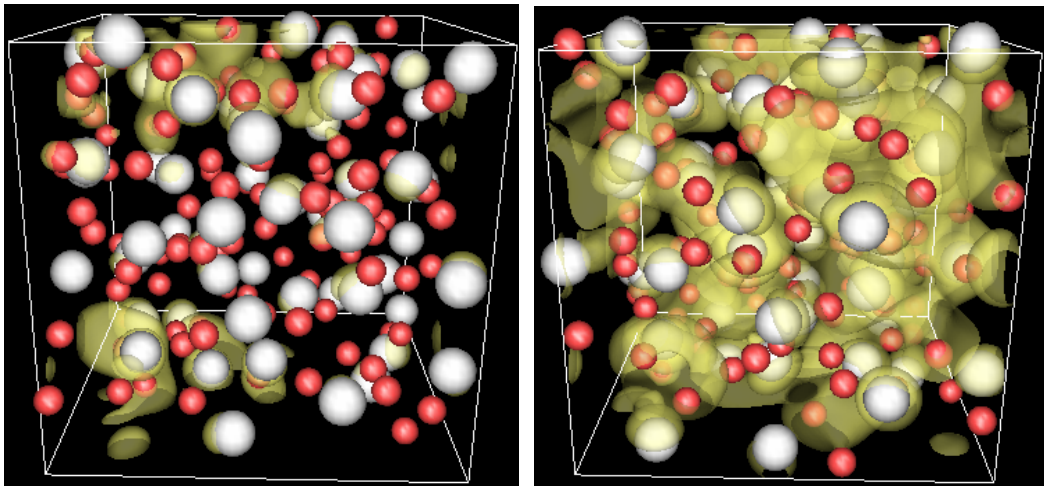
Quantum simulations of water at high energy densities leads to a revised phase diagram

Scientists at Sandia National Laboratories have significantly altered the theoretical phase diagram of water at high energy densities. Their computational study shows that an electronically conducting phase of water could occur at a temperature of 4000 K and a pressure of 100 GPa, which is significantly lower than the previous estimates (7000 K and 250 GPa, respectively). In addition, the superionic phase of water (with frozen oxygen atoms and mobile hydrogen atoms) is demonstrated to extend to higher temperatures than previously concluded and, on a pressure versus temperature phase diagram, directly borders the conducting phase. Importantly, these revisions are in the region of the phase diagram that corresponds to conditions that exist inside giant planets like Neptune and could have significant consequences for planetary models.



Theoretical pressure/temperature phase-diagram for water from first-principles simulations, together with a calculated Neptune isentrope. The isentrope is found to traverse four different phases.

The calculations were performed using first principles molecular dynamics based on a quantum mechanical description known as density functional theory. The key difference between these calculations and earlier attempts to describe water under these conditions is the statistical modeling of the electron states. In contrast to the earlier work, which effectively treated the electrons as cold when the ions were hot, these new calculations treat the electrons with Fermi statistics in thermal equilibrium with the ions. This small change from a computational point of view, has big consequences for the physics.



Two snapshots from the quantum simulations of water at 4000 K and 100 GPa, showing a constant electron density surface (gold) from a conduction band along with oxygen atoms (white) and hydrogen atoms (red). The change in electronic structure from modeling cold electrons (left) to warm electrons (right) enables electrical conduction.

The motivation driving the research is the desire to better understand, from basic physics principles, conditions on Sandia's large pulsed-power Z machine which uses water as both an insulator and a breakdown dielectric for switching. The study significantly expands the range where water's electrical conductivity is known, enabling more accurate simulations of the extreme environments (short-lived high-temperature, high-pressure) encountered during operation of the Z accelerator. The Z machine is currently in the process of being upgraded, a large project which is to be completed in July 2007. With new capacitors, the expected amperage sent through the machine to a target placed at its hub is expected to rise from 20 million to 26 million amps. Compression of Z's amperage in time is the cause of its huge power – equivalent to 50 times the electrical production of all the generating plants on Earth, albeit for a few nanoseconds.

Contact:
Thomas Mattsson, Sandia National Laboratories, (505) 844-9215, trmatts@sandia.gov
Mike Desjarlais, Sandia National Laboratories, (505) 845-7273, mpdesja@sandia.gov

[QO3.00012] Density Functional Theory simulations of water: phase-diagram and electrical conductivity
Abstract: http://meetings.aps.org/Meeting/DPP06/Event/52718
November 1, 2006
Wednesday, 4:12 pm–4:24 pm
Session QO3: High-Energy-Density Science
Philadelphia Marriott Downtown - Grand Salon KL

Further information: Thomas R. Mattsson and Michael P. Desjarlais, "Phase Diagram and Electrical Conductivity of High Energy-Density Water from Density Functional Theory", *Physical Review Letters* **97**, 017801 (2006)