Quantum simulations uncoverhydrogen's phase transitions

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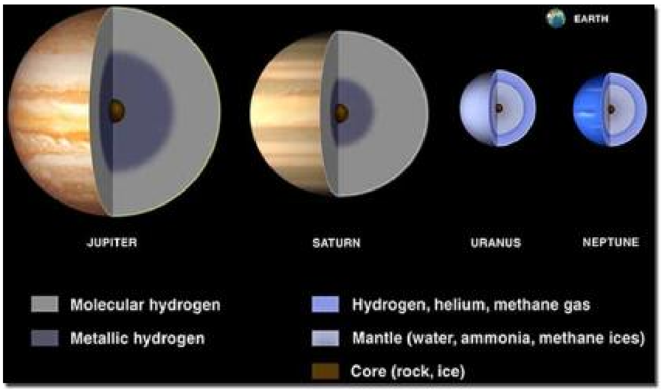

As indicated in the graphic, the gas giant planets of our solar system - Jupiter, Saturn, Uranus and Neptune - are mostly composed of hydrogen. Image courtesy of NASA

Hydrogen is the most abundant element in the universe and is a major component of giant planets such as Jupiter and Saturn.

But not much is known about what happens to this abundant element under high-pressure conditions when it transforms from one state to another.

Using quantum simulations, scientists at the Lawrence Livermore National Laboratory, the University of Illinois at Urbana-Champaign and the University of L'Aquia in Italy were able to uncover these phase transitions in the laboratory similar to how they would occur in the centers of giant planets.

They discovered a first order phase transition, a discontinuity, in liquid hydrogen between a molecular state with low conductivity and a highly conductive atomic state. The critical point of the transition occurs at high temperatures, near 3100 degrees Fahrenheit and more than 1 million atmospheres of pressure.

"This research sheds light on the properties of this ubiquitous element and may aid in efforts to understand the formation of planets," said LLNL's Eric Schwegler.

The team used a variety of sophisticated quantum simulation approaches to examine the onset of molecular diassociation in hydrogen under high-pressure conditions. The simulations indicated there is a range of densities where the electrical conductivity of the fluid increases in a discontinuous fashion for temperatures below 3100 degrees Fahrenheit.

There is a liquid-liquid-solid multiphase coexistence point in the hydrogen phase diagram that corresponds to the intersection of the liquid-liquid phase transition, according to Miguel Morales from the University of Illinois and lead author of a paper appearing online in the Proceedings of the National Academy of Sciences for the week of June 21-25.

Provided by Lawrence Livermore National Laboratory