Nobel laureate puts the squeeze on hydrogen

October 14 2011, By Vivek Venkataraman

Nobel laureate Roald Hoffmann, professor emeritus of chemistry, recounts his work on putting hydrogen under pressure, as part of the Local Legends of Chemistry lecture series, Oct. 6. Jason Koski/University Photography

Hydrogen, normally a gas, may act like a metal when squeezed under extreme pressure. In that state, competing chemical and physical effects determine its properties, said Nobel laureate Roald Hoffmann, Cornell's Frank H.T. Rhodes Professor in Humane Letters and professor emeritus of chemistry.

Hoffmann recounted work done in collaboration with Neil Ashcroft, the Horace White Professor of Physics Emeritus, and Vanessa Labet, a former postdoctoral researcher, in a talk, "The First Element Under Pressure," part of the Local Legends of Chemistry lecture series, Oct. 6 in the Physical Sciences Building. Hoffmann and co-workers have recently submitted four papers to the Journal of Chemical Physics on the structure of high pressure solid hydrogen, building on previous theoretical work of British scientists Chris Pickard and Richard Needs.

Hydrogen is the lightest and by far the most abundant element in the universe, and it makes up 10 percent of our bodies, he said. It normally exists as two-atom molecules that can be thought of as two balls connected at the ends of a spring, which can vibrate by stretching and compressing.

Although hydrogen is not so abundant in the Earth's crust, it is the primary constituent of the outer planets Jupiter, Saturn, Uranus and Neptune. "We can study hydrogen in the lab at a pressure approaching that at the center of these planets," said Hoffmann. Hydrogen gas in a small vessel between two diamond pieces can be squeezed to 3.5 million atmospheres (1 atmosphere is the pressure of air felt on the surface of the Earth).

In 1935, it was calculated that mono-atomic hydrogen under high pressure would show metallic behavior. Ashcroft in 1968 proposed that hydrogen could become a high-temperature-superconductor at high pressures, enabling it to carry electric current without resistance. "At the highest pressures in the diamond anvil cell [experiments], hydrogen acquires color [like copper and gold] ... this is promising for metallicity," Hoffmann said.

Hydrogen at room temperature is expected to crystallize into an ordered lattice arrangement at about 50,000 atmospheres, he said. However, X-rays bouncing off highly pressurized hydrogen barely show any lattice signature. "Solid hydrogen doesn't form a nice molecular crystal ... it's an orientationally disordered rotational solid (containing freely rotating molecules)," explained Hoffmann. Infrared spectroscopy experiments show clear evidence of these rotational modes. At 1 million atmospheres, the highly pressurized hydrogen undergoes a phase transition, something akin to water turning into ice. At low pressures, infrared absorption is forbidden by the symmetry of the hydrogen molecule.

"As you turn up the pressure higher, you get this gigantic infrared activity (absorption)," Hoffmann said. "The infrared activity turns on [beyond 1 million atmospheres] because the two ends of the hydrogen molecule are no longer equivalent. At very high pressures [above 5 million atmospheres] hydrogen goes mono-atomic and is no longer molecular," he said. The metallic phase is expected to occur around 3.5-4 million atmospheres, while the solid is still somewhat molecular.

Extensive numerical simulations show that the distance between hydrogen molecules decreases with increasing pressure, while the distance between hydrogen atoms within each molecule roughly remains constant. Hoffman said this is because of two competing effects, one chemical and one physical. "There is a chemical effect of populating the anti-bonding orbital, which stretches the thing, but meanwhile it's being physically compressed."

Hoffmann shared the 1981 Nobel Prize in chemistry with Kenichi Fukui for their theories concerning the course of chemical reactions.

Provided by Cornell University

Citation: Nobel laureate puts the squeeze on hydrogen (2011, October 14) retrieved 28 April 2024 from https://phys.org/news/2011-10-nobel-laureate-hydrogen.html