Researchers solve decade-old mystery of hydrogen storage material

Environmentally friendly hydrogen gas fueled vehicles can dramatically reduce greenhouse gas emissions and lessen the country's dependence on sources of fossil fuel. Though several hydrogen vehicles exist on the market today, there is still much room for improvement in the way that hydrogen is stored on-board the vehicle. With current technologies, hydrogen gas storage tanks have to be as large as or larger than the trunk of a car to carry enough gas to travel only one to two hundred miles.

While liquid hydrogen is denser and takes up less space, it is very expensive and difficult to produce. It also reduces the environmental benefits of hydrogen vehicles. Widespread commercial acceptance of these vehicles will require finding the right material that can store hydrogen gas at high volumetric and gravimetric densities in reasonably sized light-weight fuel tanks.

Researchers at the UCLA Henry Samueli School of Engineering and Applied Science, with the use of molecular dynamics simulations, have solved a decade old mystery that could one day lead to commercially practical designs of storage materials for use in hydrogen gas fueled vehicles. The study appears on the *Proceedings of the National Academy of Sciences* web site on February 27.

In 1997, it was discovered that adding a small amount of titanium to a well-known metal hydride, sodium alanate, not only lowers the temperature of hydrogen release from the material but also allows for an easy refueling and storage of high density hydrogen at reasonable pressures and temperatures. In fact, the weight percent of stored hydrogen was instantly doubled in comparison with other inexpensive materials.

"Nobody really understood what the titanium did. The chemical processes and the mechanisms were really a mystery," said Vidvuds Ozolins, associate professor of material science and engineering, a member of the California NanoSystems Institute, and lead author of the study.

With computers and the power of basic physics, chemistry and quantum mechanics, Ozolins' group decided to take a step back and analyze the sodium alanate in its pure form, without added titanium. The group analyzed the atomic processes occurring in the material and what happens to the chemical bond between the hydrogen and the material at the temperatures of hydrogen release. The computation gave the researchers information that would have been very difficult to obtain experimentally.

The computation suggested a reaction mechanism that is essential for the extraction of hydrogen from the material which involves diffusion of aluminum ions within the bulk of the hydride. By comparing the calculated activation energies to the experimentally determined values, Ozolins' group found that aluminum diffusion is the key rate limiting process in materials catalyzed with titanium. Thus, titanium facilitates processes in the material that are essential for turning on this mechanism and extracting hydrogen at lower temperatures.

"This method and this knowledge can now be used to analyze other materials that would make for better storage systems than sodium alanate. We are still on the fundamental end of the study. But if we can figure this out computationally, the people with the technology in engineering can figure out the rest," said Hakan Gunaydin, a UCLA graduate student in Ozolins' lab and another one of the study's authors.

"Sodium alanate in itself is a prototypical complex hydride with a reasonable storage density and very good kinetics. Hydrogen goes in and comes out quickly but it wouldn't be practical for a car simply because it doesn't contain enough hydrogen. So that's why we are so interested in understanding how the hydrogen comes out, what happens exactly and how we can take this to other materials," said Ozolins.

What Ozolins' group, along with UCLA chemistry and biochemistry professor Kendall Houk, also a member of the California NanoSystems Institute, hopes to do now is to apply the methods and lessons learned to those materials that would make for a commercially practical hydrogen gas storage system. They hope their findings will one day facilitate the design and creation of an affordable and environmentally friendly hydrogen vehicle.

Source: University of California - Los Angeles