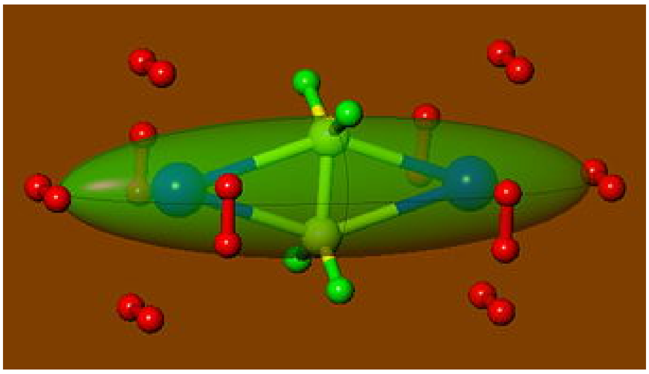
Ethylene Suggested for Hydrogen Storage



Results of modeling studies indicate that attaching titanium atoms (blue) to the ends of an ethylene molecule (yellow-green) will result in a capsule-shaped complex that absorbs 10 hydrogen molecules (red). The results open a new avenue in the pursuit of materials that will enable efficient solid-state storage of hydrogen. Credit: NIST

Ethylene, a ho-hum material that is the building block of the most common plastic, might have an exciting future in storing hydrogen, the hoped-for transportation fuel of the future. New research reported by scientists from the National Institute of Standards and Technology and Turkey's Bilkent University makes the surprising prediction that "ethylene, a well-known inexpensive molecule, can be an important basis in developing frameworks for efficient and safe hydrogen-storage media."

The team's calculations show that attaching titanium atoms at opposite ends of an ethylene molecule (four hydrogen atoms bound to a pair of carbon atoms) will result in a very attractive "two for" deal. The addition of the two metal atoms results in a net gain of up to 10 hydrogen molecules that can absorb onto the ethylene-titanium complex, for a total of 20 hydrogen atoms. As important, the engineered material is predicted to release the hydrogen with only a modest amount of heating.

The absorbed hydrogen molecules account for about 14 percent of the weight of the titanium-ethylene complex. That's about double the Department of Energy's minimum target of 6.5 percent for economically practical storage of hydrogen in a solid state material. Although significant challenges stand in the way, solid state storage is preferred to storing hydrogen as a liquid or compressed gas, both of which require large-volume tanks.

"The success of future hydrogen and fuel-cell technologies is critically dependent upon the discovery of new materials that can store large amounts of hydrogen at ambient conditions," explains Taner Yildirim, a theorist at the NIST Center for Neutron Research.

Yildirim and collaborators have been searching for routes to develop these needed materials. Their earlier research has pointed to several candidates, including carbon nanotubes coated with titanium atoms. Difficulties in securing bulk amounts of small-diameter nanotubes and other challenges have foiled efforts to create these materials in the laboratory.

The team anticipates that ethylene-based complexes, made with titanium or other so-called transition metals, will prove easier to synthesize and, then, to evaluate for their potential for high-capacity hydrogen storage.

Citation: E. Durgun, S. Ciraci, W. Zhou, and T. Yildirim. Transition-metal-ethylene complexes as high-capacity hydrogen-storage media. *Physical Review Letters*. 97, 226102 (2006)

Source: NIST