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DoE News:

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## NREL & NIST Start Making Doped Nano-materials With Big H2 Storage Potentials

**GOLDEN, CO/GAITHERSBURG, MD** Working independently of each other, scientists at two Federal research institutions have come up with theoretical, similar, pathways that may lead to novel materials for onboard hydrogen storage with capacities about 50% higher than what the Energy Department would like to achieve five years from now.

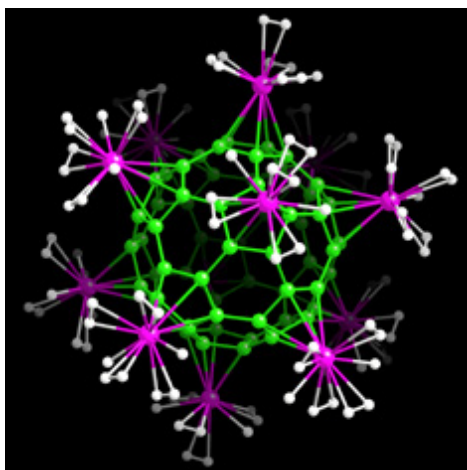
In fact, both teams have told H&FCL that they have already begun work on actually making samples of these types of materials.

Both the five-member team at the National Renewable Energy Laboratory (NREL) and two researchers at the National Institute of Standards and Technology (NIST) and at Bilkent University, Ankara, Turkey, calculate these materials could achieve almost 9 and 8% hydrogen storage by weight, respectively.

Two papers reporting this work appeared within two weeks of each other in the scholarly journal *Physical Review Letters*.

Storage targets laid down by the U.S. Energy Department's Hydrogen Program are 6% by weight (2kWh/kg) by 2010 and 9% by weight (3 kWh/k) by 2015.

If these materials can be made and live up to these projections they would go a long way towards attaining the so far elusive goal of a 300 mile range for fuel cell vehicles.



*An NREL lab image of a buckyball doped with scandium with attached hydrogen atoms.*

The key ingredient in both developments is the use of doped carbon nano-materials. The 5 NREL scientists led by Michael J. Heben propose the use of so-called organometallic buckyballs (the other members of the NREL group are Yufeng Zhao, Yong-Hyun Kim, Anne C. Dillon, and S. B. Zhang). The best carbon buckyballs would be doped with scandium, described in the *Illustrated Oxford Dictionary* as a rare, soft, silver-white metallic element occurring naturally in lanthanide ores.

A British website describing the elements says scandium is never found as a free metal: Scandium is apparently a much more abundant element in the sun and certain stars than on earth. However, it is widely distributed, being present in very small amounts in nearly a thousand

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different minerals.....Most scandium is recovered from thortveitite or is extracted as a by-product from uranium production plants.

The group reports one scandium-doped buckyball can bind as many as 11 hydrogen atoms to each metal atom, and the theoretical maximum reversible hydrogen storage density is about 9% weight (*H&FCL June 05, DoE Review story*).

### **NREL: Large Reversible Capacities**

NIST's Taner Yildirim, of the Center for Neutron Research, and his colleague S. Ciraci at Bilkent University, suggest the use of titanium-decorated single-walled carbon nanotubes (SWNTs). Their paper says that at high titanium coverage, a single SWNT can adsorb up to 8% weight hydrogen. Titanium is also a transition metal.

Heben and his colleagues say in their paper, *Hydrogen Storage in Novel Organometallic Buckyballs*, the observation that a trace amount of transition metal can lead to an enhanced capacity with a moderate binding energy caused us to explore the ways in which carbon and metals could be combined to construct new adsorbents capable of storing large amounts of hydrogen.

The team's theoretical studies predict that this large storage capacity can be achieved at room temperature and near ambient pressure, and that the process is reversible, obviously a key consideration in any on-board fueling system. Concluding, the authors say they believe that a new class of nanoscale organometallic materials even beyond the buckyballs could be synthesized that may charge and discharge hydrogen reversibly without degradation of the host.

Without going into details, Heben told H&FCL that work on actually making these materials has already started at NREL with some of our partners in the DoE Center of Excellence on carbon-based hydrogen storage materials. Heben heads the center which is being coordinated by NREL.

Heben says while he and his fellow NREL scientists have done a lot of research on single- and multi-walled nanotubes in the past (*H&FCL April, June 00*), we chose to use C60 (buckyballs) for the calculations since we felt, due to the smaller number of atoms to be considered, the calculations could go farther, be more accurate, and tell us more than if we were to theoretically model the nanotubes.

Heben says his team has explored nearly all of the eight so-called First-Row transition metals, looking for trends to help guide the design of the materials. The group then focused on scandium because the capacity and energetics are calculated to be the best. Scandium, he added, is not too expensive but for large-scale deployment we may need to look for cheaper materials.

He particularly credits his colleague Dr. Shengbai Zhang as being principally responsible for developing the theoretical underpinnings for these new materials. We are probably among the first to realize the need to explore novel, relatively unknown physical interaction between H and its host by accurate first-principles theory in order to piece together the various experimental puzzles, Zhang told H&FCL by e-mail. As such, H storage in organometallic nanomaterials is fundamentally different from other known systems. There will be initial obstacles to synthesize them, but I see no reason why they can not be overcome.

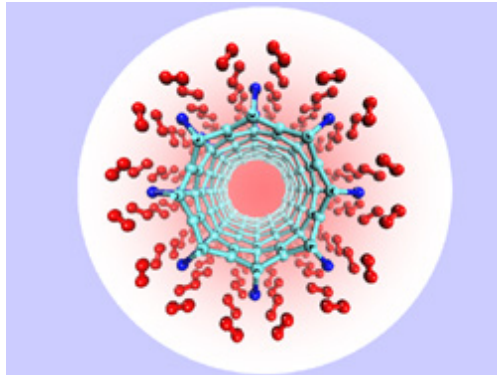
The attention that both of these efforts - NREL's and also NIST's - have gotten recently in both scholarly and general readership journals is sweet vindication for NREL, says Heben who recalls that various publications trashed their earlier research into nanotubes. DoE stuck with us in the

face of poor opinion, he recalled. It was that kind of support which allowed us to make this recent breakthrough. These efforts have created for the long term an entire new field that has exploded, Heben added. It's safe to say that all of the work in this area, including NIST's, is derivative from DoE's support of NREL's work.

NIST's Dr. Yildirim and Dr. Ciraci note in the introduction of their paper, Titanium-Decorated Carbon Nanotubes as a Potential High-Capacity Hydrogen Storage Medium, that the current state of the art is at an impasse in providing any material that meets a storage capacity of 6 wt % or more required for practical applications - a situation that led to DoE's decision two years ago to set up the storage Grand Challenge via storage Centers of Excellence (*H&FCL July 03*).

### **NIST: Remarkable and Unanticipated Results**

Their first-principles computation of the interaction between hydrogen molecules and transition metal atoms adsorbed on carbon nanotubes produced results that are quite remarkable and unanticipated, they wrote. We found that a single Ti atom adsorbed on a single-walled nanotube can strongly bind up to four hydrogen molecules, an unusual and complex bonding....generated by the concerted interaction among H, Ti and SWNT.



.....and another image from NIST of a titanium-decorated carbon nanotube with attached hydrogen molecules.

A high-temperature quantum molecular dynamics simulation also showed that these systems are stable and indeed exhibit associative desorption of H<sub>2</sub> upon heating, another requirement for reversible storage, they added.

Yildirim said in an e-mail to H&FCL that he and his colleague have started to try to make these materials: in addition to theoretical work reported in PRL, we also do experimental work at the NIST Center for Neutron Research. We have several ideas to realize our predictions.

We are also doing more calculations to see if we can identify other nanostructures that we can decorate with light-transition metals to test our predictions.

Concluded Yildirim and Ciraci, These results advance our fundamental understanding of dissociative and molecular chemisorption of hydrogen in nanostructures, a fundamental step towards novel materials needed for hydrogen production, storage, and consumption in the fuel cells. They also suggest a possible method of engineering new nanostructures for high-capacity storage and catalyst materials.

Adds Heben, there is a lot of excitement in the area these days, and high surface area and nano-structured adsorbents are viewed as having great potential.

*Sources/Contacts: Physical Review Letters, weeks ending April 22 and May 6, 2005.*

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