

Chemists to develop new materials for hydrogen storage in vehicles

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Berkeley Lab scientist Jeffrey Long co-leads a project to develop novel materials for hydrogen storage. Credit: Roy Kaltschmidt/Berkeley Lab

(PhysOrg.com) -- The biggest challenge with hydrogen-powered fuel cells lies in the storage of hydrogen: how to store enough of it, in a safe and cost-effective manner, to power a vehicle for 300 miles? Lawrence Berkeley National Laboratory (Berkeley Lab) is aiming to solve this problem by synthesizing novel materials with high hydrogen adsorption capacities.

The U.S. Department of Energy recently awarded Berkeley Lab a three-year, \$2.1 million grant for the project, which will also include contributions by the National Institute of Standards and Technology

(NIST) and General Motors (GM). The grant was part of more than \$7 million awarded by DOE last month for [hydrogen](#) storage technologies in [fuel cell](#) electric vehicles.

“We’re working on materials called metal-organic frameworks to increase the capacity of hydrogen gas in a pressure cylinder, which would be the fuel tank,” said Jeffrey Long, a Berkeley Lab scientist who co-leads the project along with Berkeley Lab chemist Martin Head-Gordon. “With these materials, we’re working on storing the hydrogen without the use of very high pressures, which will be safer and also more efficient without the significant compression energy losses.”

Metal-organic frameworks (MOFs) are three-dimensional sponge-like framework structures that are composed primarily of carbon atoms and are extremely lightweight. “What’s very special about these materials is that you can use synthetic chemistry to modify the surfaces within the materials and make it attractive for hydrogen to stick on the surface,” Long explained.

Separately, Long is also using MOFs in a carbon capture project, in which the material would selectively absorb carbon dioxide over nitrogen. For the fuel cell project, the trick lies not in getting the MOF to select hydrogen out of a mixture but to store as much hydrogen as possible.

Currently, vehicles using hydrogen fuel cells can achieve a range of close to 300 miles—but only if the hydrogen is stored at extremely high pressures (600 to 700 bar), which is expensive and potentially unsafe. It is also energy intensive to pressurize the hydrogen.

So far Long has succeeded in more than doubling hydrogen capacity, but only at very low temperatures (around 77 Kelvin, or -321 Fahrenheit). “It’s still very much basic research on how to create revolutionary new

materials that would boost the capacity by a factor of four or five at room temperature,” he said. “We have an idea of what kinds of frameworks we might make to do this.”

Long’s approach is to create frameworks with lightweight metal sites on the surface, making it attractive for hydrogen molecules to bind to the sites. “Our approach has been to make some of the first metal-organic frameworks that have exposed metal cations on the surface,” he said. “Now we need to figure out ways of synthesizing the [materials](#) so that instead of one hydrogen molecule we can get two or three or even four hydrogen molecules per metal site. Nobody’s done that.”

This is where Head-Gordon, a computational chemist, comes in. He will work on theoretical understanding of MOFs so that he can try to predict their [hydrogen storage](#) properties and then instruct Long’s team as to what kind of material to synthesize. “He can do calculations on a lot of different target structures and say, here’s the best one for you guys to spend time trying to make, because synthetic chemistry is very cost and labor intensive,” Long said.

The scientist at GM will aid in providing accurate high-pressure measurements. The NIST scientist is an expert in neutron diffraction and neutron spectroscopy, which will allow Long and his team to pinpoint where exactly the hydrogen is going and verify that it is binding to the metals.

Provided by University of California - Berkeley

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