Unlocking hydrogen's fuel potential

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Hydrogen is being touted as the fuel of the future, a clean-burning, renewable and inexpensive replacement for petroleum. But a major stumbling block for hydrogen-powered vehicles is figuring out a way to carry enough hydrogen onboard to travel even moderate distances between refueling stops.

Researchers at the U.S. Department of Energy's Ames Laboratory will be investigating a possible solution to that problem thanks to $1.6 million in funding announced recently by DOE Secretary Samuel Bodman as part of a $64 Million Hydrogen Fuel Initiative.

"With compressed hydrogen gas, you simply can't carry a tank big enough to travel very far," Ames Lab senior scientist Vitalij Pecharsky said. "The answer is a hydrogen-rich, solid fuel that mimicks the hydrogen content of methane, where four hydrogen atoms encapsulate a single carbon atom."

So why not just use methane? According to Pecharsky, methane and similar hydrocarbon compounds have covalent bonds that keep the hydrogen atoms tightly "locked" in place. The energy required to break those bonds is very high compared to the energy you'd get from the hydrogen produced. Also, methane and other hydrocarbons that come from oil are not renewable. The ideal solution would be a hydrogen-rich solid material that would give up its hydrogen atoms easily, through moderate heating or by other means. These materials could also be "recharged" – absorbing "new" hydrogen atoms during refueling from a pressurized hydrogen gas source.

That's why Pecharsky and fellow Ames Laboratory scientists Marek Pruski, Victor Lin and Scott Chumbley are looking at some novel materials – light-metal alanates, borohydrides, amides, imides, and their derivatives – that have a total hydrogen content exceeding 10 percent by weight.

A key component in the research project is solvent-free mechanochemical processing, a technique Ames Laboratory researchers had shown back in 2002 to work well when applied to complex hydrides. The process uses variable energy milling to modify both the structure and properties of hydrides, and potentially, to make them easily rechargeable with hydrogen. Materials to be processed are placed in a hardened steel vial along with steel balls. The vial is vigorously shaken and mechanical energy transferred into the system alters the crystallinity of the solids and provides mass transfer, eventually breaking down the solids and releasing hydrogen, or combining the materials and hydrogen gas into new compounds.

"Processing these materials without the use of solvents is important," Pecharsky said, "because once a material is dissolved, its structure fundamentally changes. Creating these complex hydride compounds in solid state will allow us to look at the molecular structure to see if there are ways to more easily get the hydrogen back out of these systems."

Another ingredient the group will use is called nanostructuring. Ames Lab chemist Victor Lin has developed a way of using the nanoscale pores in a self-assembling polymer as "molds" to precisely control the size of the material particles going into the milling process. Smaller particles have higher surface energies and surface energy may be a decisive factor in shifting thermodynamic equilibrium. Lowering the size of particles to a few nanometers also reduces the distances over which the mass transport takes place, thus improving the kinetics – the rates of the reactions – of complex hydride-hydrogen systems.

Synthesizing various combinations and sizes of materials will provide samples to be studied and characterized using a variety of high-tech methods. Ames Lab scientist Scott Chumbley hopes that scanning and transmission electron microscopy will give researchers a close-up look at the structure of the processed materials. The team will also rely on the expertise of Ames Lab senior scientist Marek Pruski in using solid-state nuclear magnetic resonance. Earlier studies performed by Pruski's group proved that NMR is uniquely suited for the studies of complex phases resulting from the milling process. Coupled with X-ray powder diffraction, and other traditional materials characterization techniques, researchers hope to gain a fundamental understanding of the relationships between the chemical composition, bonding, structure, microstructure, properties and performance of these materials.

"We'll look at the rates of absorption and desorption of hydrogen as well as the cycling properties of these materials at various temperatures and pressures," Pecharsky said. "Furthermore, we plan to modify these nanoparticles with titanium and other transition metal catalysts and perform a full array of characterization and hydrogenation-dehydrogenation property tests on these metal-doped nanostructured hydrides."

Parallel with the materials' characterization, the group will work with physicist Purusottam Jena of Virginia Commonwealth University to develop first-principle theoretical models based on the experimental data. Those models will then be used to predict outcomes of further experiments. The predictions and actual results will be compared to see if the theory holds or needs further modification. Ultimately, the theoretical model will be used to help steer research toward the most promising compounds.

Funding for the project will be spread over three years. Ames Laboratory is operated for the Department of Energy by Iowa State

University. The Lab conducts research into various areas of national concern, including energy resources, high-speed computer design, environmental cleanup and restoration, and the synthesis and study of new materials.

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