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Materials' increased capacity, efficiency could lower the bar for hydrogen technology

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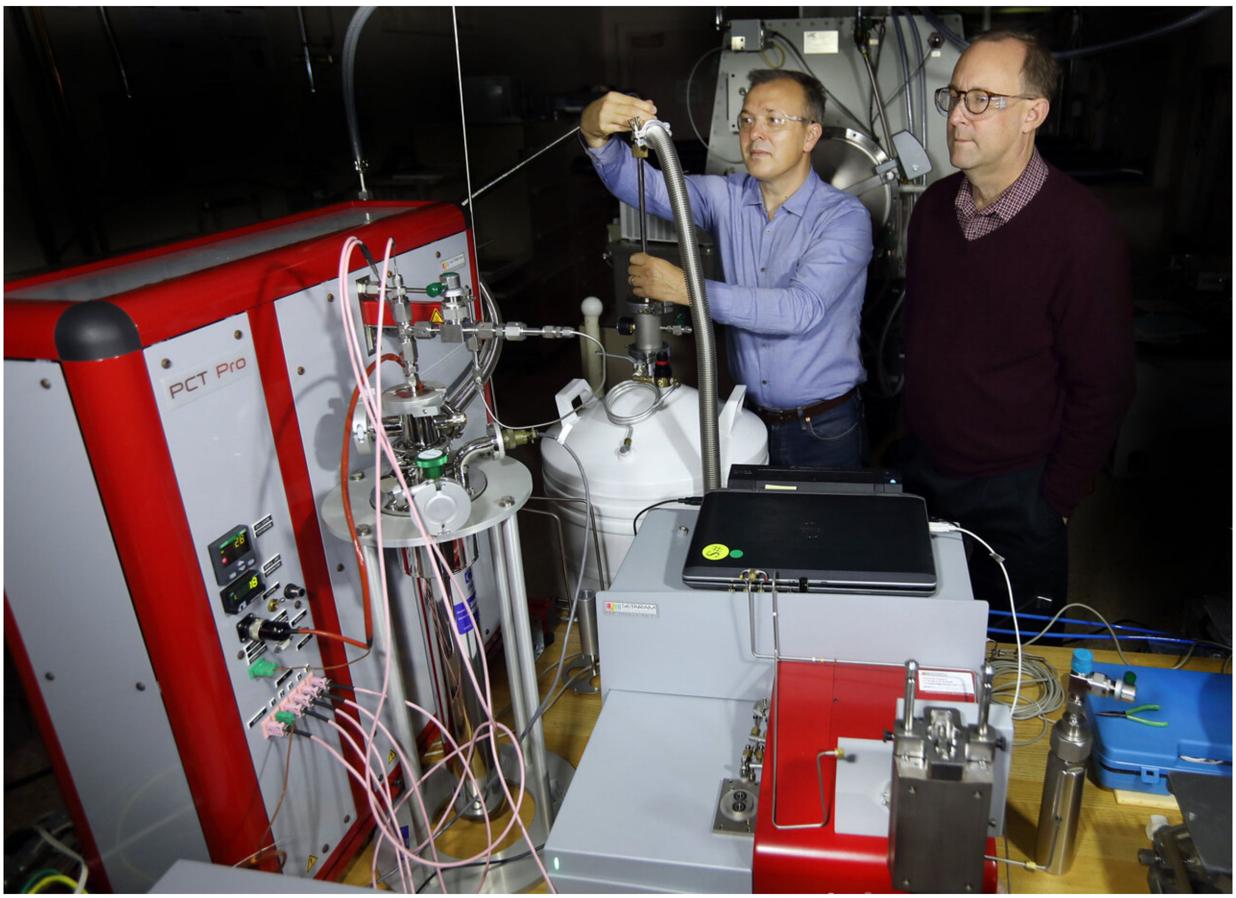

Sandia researchers Vitalie Stavila, left, and Mark Allendorf are part of a multilab consortium to advance storage materials for future hydrogen powered transportation. Credit: Dino Vournas

Hydrogen as a carbon-free energy source could expand into a variety of sectors, including industrial processes, building heat and transportation. Currently, it powers a growing fleet of zero-emission vehicles, including trains in Germany, buses in South Korea, cars in California and forklifts worldwide. These vehicles use a fuel cell to combine hydrogen and oxygen gases, producing electricity that powers a motor. Water vapor is their only emission.

For hydrogen to continue to grow and change sectors across the economy, new infrastructure is needed. Hydrogen-powered cars store hydrogen gas onboard at a pressure 700 times greater than atmospheric pressure to drive as far as conventional gasoline vehicles. While this technology has enabled hydrogen-powered cars to be commercialized, it cannot meet the challenging energy density targets set forth by the U.S. Department of Energy.

With the support of DOE's Energy Efficiency and Renewable Energy Office's Fuel Cell Technologies Office, the Hydrogen Materials Advanced Research Consortium (HyMARC), a multilab collaboration, is developing two types of hydrogen storage materials to meet those federal targets. In the first phase of its work, the group identified strategies and did foundational research to increase the storage capacity of metal-organic frameworks and increase the storage efficiency of metal hydrides.

Now, the newly expanded collaboration is using the most promising strategies to optimize the materials for future use in vehicles, potentially offering more compact onboard storage systems, reduced operating pressures and significant cost savings.

"Those benefits could help get more fuel cell vehicles on the road by enabling a driving experience similar to that of conventional vehicles," said Mark Allendorf, a researcher at Sandia National Laboratories and co-director of the HyMARC consortium.

The consortium is now exploring ways to strip hydrogen reversibly from molecules, such as ethanol. These molecular hydrogen carriers would be easier to transport to fueling stations than hydrogen gas, increasing the efficiency of fuel delivery and reducing the cost of hydrogen-powered vehicles as well as other applications. Breakthroughs in advanced hydrogen storage materials coming out of HyMARC will also support DOE's H2@Scale initiative to enable affordable large scale hydrogen production, storage, transport and utilization across multiple sectors.

Consortium continues

Since 2015, researchers at Sandia, Lawrence Berkeley and Lawrence Livermore national laboratories have focused on two primary types of hydrogen storage materials to learn how their shape, structure and chemical composition affects their performance. The HyMARC consortium has added researchers at the National Renewable Energy Laboratory, Pacific Northwest National Laboratory, SLAC National Accelerator Laboratory and the National Institute of Standards and Technology.

The expanded group recently received a second round of funding from the DOE Energy Efficiency and Renewable Energy Office to address performance issues that prevent the most promising materials from reaching the federal targets for hydrogen storage. To do that, the researchers have identified the most relevant challenges that slow the pace of hydrogen storage material innovation. They then develop tools to tackle those challenges, including reliable ways to make the materials, new computer models to predict material properties that influence their storage performance and novel measurement methods to accommodate some materials' high reactivity with moisture and oxygen. "HyMARC makes these tools available to other labs that apply them to specific materials," Allendorf said. "We also collaborate with them to facilitate their research."

Taming temperature

The first class of materials of interest to HyMARC is called sorbents. These materials have tiny pores that act like sponges to adsorb and hold hydrogen gas on their surfaces. These pores create a material with a high surface area, and thus storage space. One gram of material can have as much surface area as an entire football field.

That leads to an unexpected practical effect: porous materials can theoretically hold more hydrogen than a high-pressure fuel tank, said Vitalie Stavila, a Sandia chemist. Yet because hydrogen gas interacts weakly with the pore walls, much of that storage space goes unused. These materials work best at cryogenic temperatures too low for practical use.

The best performing sorbents are materials called metal-organic frameworks, or MOFs. In these materials, rigid linkers made from carbon atoms connect individual metal ions like the bars in a playground jungle gym. To increase the amount of hydrogen stored in the materials, the consortium recommends adding hydrogen-grabbing elements like boron or nitrogen into the carbon linkers that form the pore walls.

Team members also have developed MOFs in which more than one hydrogen molecule can stick to a metal ion in the framework. Along with increased storage capacity, these materials interact with hydrogen more strongly. Practically, this means the gas sticks to the pore walls at higher temperatures.

Nanostructures increase storage efficiency

The second class of promising hydrogen storage materials is metal hydrides, a material that Sandia researchers have been making for decades. In these materials, metal ions hold hydrogen with chemical bonds. Breaking these bonds allows hydrogen gas to be released for use in a fuel cell.

However, these materials form strong bonds with hydrogen, and energy is required to release stored gas. Reducing the size of hydride particles from macroscopic grains to nanoclusters more than ten thousand times smaller than the width of a human hair makes the material much more reactive, allowing it to release hydrogen at lower temperatures. Stavila and his colleagues use porous materials, such as a MOF or porous carbon, as templates to control cluster size and prevent them from clumping together.

"We learned during the first phase of HyMARC that making nanostructured metal hydrides allows us to tune the strength of the bonds formed with hydrogen and change how quickly hydrogen attaches to and leaves the surface," Stavila said. "This means less energy is needed to release the gas."

The researchers are testing the nanoscale hydrides for features, such as storage reversibility and usable storage capacity, that are important for future applications. "We are building confidence that nanoscale hydrides can be practical storage materials," Stavila said.

The group also is using a computer science technique called machine learning to rapidly identify the physical properties of these storage materials that correlate to the performance necessary to reach the federal targets. Their approach allows them to understand how the computer identified its predictions. "We are generating scientific insight to create new intuition of how these materials behave," Allendorf said.

"Identifying hydrogen storage materials that can meet all of the DOE targets is an essential step toward transitioning to a future hydrogen economy," he said.

For hydrogen-powered vehicles, meeting those targets for storage materials means such vehicles could have driving ranges, refueling times and fuel costs similar to conventional vehicles.

"Although the technical challenges are great," Allendorf said, "the HyMARC team is highly motivated by the importance of its role and by its recent discoveries that point the way to successful materials."

Provided by Sandia National Laboratories

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