New engineering model advances prospect of alternative-fuel vehicles

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Researchers at the UCLA Henry Samueli School of Engineering and Applied Science have developed a model that could help engineers and scientists speed up the development of hydrogen-fueled vehicles by identifying promising hydrogen-storage materials and predicting favored thermodynamic chemical reactions through which hydrogen can be reversibly stored and extracted.

The new method, published online in the peer-reviewed journal *Advanced Materials*, was developed by Alireza Akbarzadeh, a UCLA postdoctoral researcher in the department of materials science and engineering; Vidvuds Ozolins, UCLA associate professor of materials science and engineering; and Christopher Wolverton, professor of materials science and engineering at Northwestern University in Illinois.

Because of global environmental changes associated with man-made carbon dioxide emissions and the limited resources of fossil fuels, developing alternate and renewable energy sources is important for a sustainable future. Hydrogen is a potential source of clean energy for future use in passenger vehicles powered by cheap and energy-efficient fuel cells, but its widespread adoption has been hindered by the need to store it on-board at very high densities.

A promising solution to this problem involves storing hydrogen within a material in the form of a chemically bound hydride, for example lithium hydride (LiH). Unfortunately, simple binary hydrides, in which hydrogen combines with light elements such as lithium, sodium,

magnesium or others, do not adequately satisfy the requirements for on-board storage, as the hydrogen-yielding reaction requires heating the material to impractically high temperatures.

Because of this, researchers have turned to multicomponent hydride mixtures with higher volumetric and gravimetric densities, better operating temperatures and improved reaction rates for practical hydrogen storage. However, this flexibility comes at the price of drastically increased complexity associated with the large number of competing reactions and possible end-products other than hydrogen. Thus, predicting desirable hydrogen storage with multicomponent mixtures has proved difficult. For example, the recently studied lithium hydride compound Li4BN3H10 was found to have as many as 17 hydrogen-release reactions, of which only three were found to be feasible — and none were in the desired range of temperatures and hydrogen pressures for practical on-board storage in hydrogen-powered vehicles.

The research team used modern quantum mechanical theories and high-powered computers to develop an algorithm that can automatically and systematically pinpoint phases and reactions that have the most favored thermodynamic properties — that is, those that can release hydrogen at ambient temperatures using the waste heat from a proton exchange membrane (PEM) fuel cell. The team tested the method on the well-studied Lithium-Magnesium-Nitrogen-Hydrogen system, predicting all experimentally observed pathways in the system. The researchers say this method can also be applied to other multicomponent hydrogen systems.

“The development of an algorithm that goes beyond chemical intuition and finds all hydrogen storage reactions ‘in silico’ is crucial and will help the scientific and engineering community to develop revolutionary new hydrogen-storage materials,” Akbarzadeh said. “This is a major

achievement in the field, which can boost up the search for the best reversible solid-state hydrogen storage."

"We are steadily approaching the moment when we will be able to theoretically design materials with desired properties, just like a tailor makes a suit to fit the customer's needs," Ozolins said. "This will bring in a qualitatively new era of collaboration between theory and computation, experiment and technology development."

Source: University of California - Los Angeles