IV.A.2 Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods

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Project Start Date: May 1, 2004
Project End Date: December 31, 2008

Objectives

Discovery of complex metal hydrides through molecular modeling and combinatorial methods which will enable a hydrogen storage system that meets DOE 2010 performance goals. The deliverables include:

- Optimized material
- Accompanying documentation

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume
(B) System Cost
(D) Durability/Operability
(E) Charging/Discharging Rates
(P Lack of Understanding of Hydrogen Physisorption and Chemisorption

Technical Targets

This project uses virtual high-throughput screening by computer modeling and combinatorial experimentation to identify promising metal hydrides for vehicular on-board hydrogen storage applications meeting DOE 2010 system targets:

- Useable, specific-energy from H_2: 2 kWh/kg
- Useable energy density from H_2: 1.5 kWh/L
- Storage system cost: $4/kWh net
- Cycle life: 1,000 cycles
- Minimum and maximum delivery temperature: -40/85°C
- System fill time: 3 minutes for a 5-kg hydrogen system.

TABLE 1. UOP Progress Toward Meeting DOE On-Board Hydrogen Storage Targets (data is based on material only, not system)

Storage Parameter	Units	2010 Target	$LiBH_4$-$LiNH_2$-MgH_2
Specific Energy	kWh/kg	2.0	1.1
Energy Density	kWh/L	1.5	0.8

Accomplishments

The project officially ended May 1, 2007 and was extended for UOP only to work on high throughput synthesis. Most of the year was spent working with the vendor of the high throughput synthesis system to make its powder dosing capabilities operational. The new tool is expected to be ready in September 2008. Synthesis and characterization of complex metal hydride hydrogen storage materials will then continue.

Introduction

Metal hydrides have the potential for reversible on-board hydrogen storage with hydrogen release at low temperatures and pressures. However, known hydrides are either too heavy (such as $LaNi_5H_6$), or require high temperature to release hydrogen (such as MgH_2). This project will systematically survey complex hydrides to

discover a material which would enable a hydrogen storage system that meets DOE's 2010 goals.

Approach

The team is applying combinatorial experimentation and molecular modeling to discover materials with optimum thermodynamics and kinetics for on-board hydrogen storage. Virtual high-throughput screening exploits the capability of molecular modeling to estimate the thermodynamics on the computer more quickly than can be measured in the laboratory. First-principles calculations are being used to predict thermodynamic properties of these new materials. Even more importantly, the coupling of combinatorial experiments with molecular modeling of structural and thermodynamic properties is providing insights into the underlying mechanisms of action in these complex materials, permitting the design of hydrogen storage materials which would never have been envisioned otherwise.

Results

High-Throughput Combinatorial Capability

The high throughput synthesis system has proven problematic in regard to the controlled transfer of finely ground powders. The small scale of the combinatorial experiments requires milligram accuracy of the powder dosing component of the high throughput synthesis system. This last year we have gone through several iterations with the vendor to develop a tool that can function accurately and reproducibly without any upsets. The new powder dosing tool is looking promising as it enters the final phases of testing and is expected to be ready by September 2008. This project was extended to get this instrument into a fully functional state. Once the new tool is installed, high throughput synthesis and characterization of complex metal hydrides will continue.

Conclusions and Future Directions

The focus of our future work will be high throughput synthesis. Our work over the course of this project included a high throughput assay to evaluate hydrogen storage capacities, but the synthesis was carried out one sample at a time with some parallel steps. For this extended portion of the project, we will use the high throughput synthesis in concert with the high throughput assay. This will start after we overcome our hurdle presented by our powder dosing tool. The chemistry to be pursued will address the methods used to synthesize the hydrogen storage materials. Many materials released hydrogen during traditional milling before they could even be tested. Softer synthetic methods such as solution or ionic liquid synthesis, and the addition of stabilizing components are strategies that would be part of our future work. Future directions in materials screening will also continue to focus on transition-metal modified borohydride-containing systems. The development of reversible borohydride components for a hydrogen storage system is important because of their gravimetric advantage. The general composition of these materials can be described as M-TM-BH_4-NH_2-AlH_4-H, where M is an alkali/alkaline earth metal and TM stands for transition metals. The goal here is to lower the desorption temperature and improve reversibility compared to the known alkali and alkaline earth borohydrides.

FY 2008 Publications/Presentations

1. "Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods," Gregory J. Lewis, J. W. A. Sachtler, John J. Low, David A. Lesch, Paul Dosek, Syed Faheem, Lisa M. Knight, Leon Halloran; *DOE Hydrogen Program Peer Review,* Washington, D.C., June 9, 2008.

2. "High Throughput/Combinatorial Screening of Hydrogen Storage Materials: UOP Approaches," Adriaan Sachtler; *DOE Meeting on High Throughput/Combinatorial Analysis of Hydrogen Storage Materials, June 26, 2007.*