IV.A.4 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: June 30, 2009

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 entire year was spent trying to get the High Throughput Synthesis System operational. A critical piece of the system, a powder doser, had not operated properly. The piece was redesigned several times by the vendor, but ultimately it could not carry out the tasks it was designed for. Since we are now two years past the original closing date of this project and there is no progress making the High Throughput Synthesis System functional, a decision was made to shut down the project as of June 30, 2009.

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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

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 fraction of a 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. Several new incarnations of the powder dosing tool is looked promising, but to date, none have operated reliably. Hence, after a two year extension, the project has now been shut down.

Conclusions and Future Directions

The project is now concluded, since we have failed to make the High Throughput Synthesis System operational. 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 the extended portion of the project, we tried to use the high throughput synthesis in concert with the high throughput assay. Unfortunately we never overcome the hurdle presented by our powder dosing tool. As of June 30, 2009, the project is ended.