III.F.2 Metal Hydride Center of Excellence (New Project)

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Oak Ridge National Laboratory
Savannah River National Laboratory
Stanford University
University of Hawaii
University of Illinois at Urbana-Champaign
University of Nevada, Reno
University of Pittsburgh in partnership with Carnegie Mellon University
University Of Utah

The Metal Hydride Center of Excellence involves seven universities, three industrial companies, and six federal laboratories. The Metal Hydride Center focuses on the development of advanced metal hydride materials, including lightweight, high-capacity complex hydrides; destabilized binary hydrides; intermetallic hydrides; modified lithium amides; and other onboard reversible hydrides. The Metal Hydride Center has two main objectives: (1) develop improved lightweight, high-capacity hydride-based materials for vehicular applications, and (2) pursue systems engineering science for the ultimate integration and demonstration of these advanced materials into a complete hydrogen storage and delivery system.

The Metal Hydride Center proposes to develop an advanced hydrogen storage system based on parallel research in four classes of hydride-based materials. These include 1) advanced complex hydrides of the light elements Li, Na, Mg, Ti, Ca, B, Al, Si; 2) destabilized binary hydrides (e.g., Li-Si destabilized H_2 release from LiH); 3) novel intermetallic hydrides (e.g., Mg-M-H alloys); and 4) other onboard reversible hydride materials, such as lithium amides, that demonstrate promising hydrogen storage properties.

The following paragraphs are brief summaries of the work proposed to be completed by each Metal Hydride Center team member.

Metal Hydride R&D for Hydrogen Storage

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Sandia National Laboratory-Livermore (SNL) will play a major role in the Metal Hydride Center to help coordinate research among the partners in addition to its role in materials discovery and engineering science. For materials discovery, SNL will lead coordination of a team that proposes to focus on complex hydrides and other hydride-based materials such as the lithium amides. SNL plans to explore the modification of sodium alanates to obtain higher capacity without a loss in hydrogen sorption kinetics, look for new hydrides, develop low-temperature reversible lithium amides, and investigate novel materials synthesis methods and processes. SNL will also conduct a parallel effort in safety and engineering sciences for the design of a lightweight, high-capacity hydrogen storage system. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Synthesis of Novel Metal Hydrides for Automotive Applications

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Brookhaven proposes to develop and test a new series of aluminum hydrides that have the potential to meet DOE's 2010 and 2015 system performance targets. The research plan includes investigation of sample synthesis and preparation, sample characterization, sample decomposition and regeneration of α-aluminum hydride and other aluminum hydride phases. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage

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The California Institute of Technology (CalTech) proposes to synthesize nanophase metals and hydride precursors to improve hydride kinetics and to investigate the thermodynamics of nanoscale systems. The hydrogen sorption properties of these nanophase materials will be measured and evaluated. CalTech will use a novel preparation technique to synthesize Li- and Mg-based hydrides that will enable a decoupling of size-related surface effects from grain boundary effects. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Lightweight Intermetallics for Hydrogen Storage

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GE Global Research proposes to discover and develop a high-capacity (> 6 wt.%) lightweight hydride that is practical and inexpensive for reversible vehicular hydrogen storage and delivery systems and capable of meeting or exceeding the 2010 DOE/FreedomCAR targets. GE will be using internally developed high-throughput, combinatorial techniques for materials discovery and characterization. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage

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HRL Laboratories proposes to develop and to implement hydride destabilization methods for thermodynamic control of reactions in light metal hydrides with gravimetric storage capacities greater than 6 wt. % hydrogen. The research will identify, synthesize and characterize nanoscale hydride materials and catalysts having the requisite dimensions and structural properties to promote hydrogen dissociation, diffusion and exchange at rates that greatly exceed those in bulk materials. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

High-Throughput Combinatorial Chemistry Development of Complex Hydrides

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Intematix proposes to implement high-throughput combinatorial techniques for new multi-element complex metal hydrides in order to deliver suitable on-board reversible hydrogen storage materials that meet or exceed DOE/FreedomCAR targets for 2010 and 2015. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage

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The Jet Propulsion Laboratory (JPL) proposes to develop and demonstrate a safe and cost-effective light-metal hydride materials system that meets or exceeds the DOE/FreedomCAR goals for on-board hydrogen storage. JPL plans to characterize and validate storage capacity and hydrogen sorption reversibility in the destabilized hydrides developed by partners under practical operating conditions. JPL will also develop lightweight and thermally efficient hydride storage vessels to reduce storage system mass and experimentally demonstrate their compatibility with appropriate complex and destabilized nano-phase hydrides. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Neutron Scattering Characterization and Thermodynamic Modeling of Advanced Metal Hydrides for Reversible Hydrogen Storage

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The National Institute of Standards & Technology (NIST) proposes to provide expertise and capabilities in neutron metrology and Calphad thermodynamic modeling as part of the DOE Metal Hydride Center of Excellence. The support includes fundamental, physicochemical property characterization of hydrogen-storage materials using neutron metrology techniques. NIST will also combine experiment and Calphad thermodynamic modeling to aid in critical assessments of hydrogen content, heats of reaction, and phase-reaction sequences during hydrogen charge-discharge cycling of materials. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Novel Synthetic Approaches for the Preparation of Complex Hydrides for Hydrogen Storage

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The hydrogen storage development work at ORNL has as its objective to achieve the DOE/FreedomCAR system storage targets for 2010. Central to this effort is the development of new methods of preparation of a suitable variety of high-content hydrogen compounds. The ORNL team has expertise in the synthesis of organo-metallic compounds by solution-based synthetic methods, and they will apply this knowledge to prepare Ti-catalyzed $NaAlH_4$ and other complex hydrides by solution methods. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Hydrogen Storage R&D at Savannah River

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SRNL will concentrate its efforts on looking at a new electrochemical process for charging aluminum to aluminum hydride, or alane. The SRNL process is currently being patented. Alanes have a 10 wt.% hydrogen storage capacity. Recent results by other researchers indicate that alanes can be decomposed at reasonable conditions with the addition of the proper catalyst or dopant. The biggest challenge, however, will be in recharging the material. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and Kinetics of Nanoparticle and Model System Materials

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Stanford proposes to develop an understanding of the dynamics of hydrogen diffusion and phase transformations during hydrogenation/dehydrogenation in nanoscale materials using real-time in-situ synchrotron x-ray diffraction. They also plan to develop model nanostructured materials systems using the flexibility of physical vapor deposition to engineer atomic-level structural and chemical features. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Fundamental Studies of Advanced High-Capacity Reversible Metal Hydrides

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The University of Hawaii proposes to determine the chemical nature of the titanium species responsible for the enhanced dehydrogenation and re-hydrogenation processes in Ti-doped $NaAlH_4$ and elucidate the mechanism of action of the dopants. They also plan to explore reversible hydrogen storage materials based on complex aluminum hydrides as well as "thermodynamically tuned" binary hydrides, each with at least 7 wt.% materials-based gravimetric capacity with potential to meet DOE 2010 system-level targets. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Metal Hydride-based Hydrogen Storage Materials – Structure, Chemistry, and Electronic Structure

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The University of Illinois plans to determine the structural, chemical and bonding changes occurring during the hydriding/dehydriding cycles for candidate complex hydrides, other lightweight hydride materials, and destabilized binary hydrides through combining advanced characterization tools including controlled-environment transmission electron microscopy and multiple-scattering density-function-based methods. Determination of the role of impurities and contaminants on charging/discharging properties is planned as well. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Effect of Trace Elements on Long-Term Cycling and Aging Properties of Complex Hydrides

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The University of Nevada proposes to determine the effect of contaminants during hydrogen cycling and aging and observe any degradation in the hydrogen storage properties of complex hydrides, including Li amides. They also plan to develop complex hydrides and to characterize the hydrides using elastic and inelastic neutron scattering, in-situ neutron work using a portable Sievert's apparatus, and in-situ X-ray diffraction. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems

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The University of Pittsburgh plans to use Density Functional Theory methods coupled with Monte Carlo techniques to predict the heats of formation and finite temperature phase stability information for a variety of metal hydrides of interest. They plan to calculate the structure, interfacial energies, work of separation, and electronic properties of a number of different alanate interfaces and study the role of Ti doping of the Na_3AlH_6 phase on the dehydrogenation and transport reactions. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Chemical Vapor Synthesis of Nanocrystalline Binary and Complex Metal Hydrides for Reversible Hydrogen Storage

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The University of Utah proposes to develop a chemical vapor reaction process for synthesis of nanosized complex metal hydrides that meet reversibility and kinetics requirements with at least 7 wt.% materials-based gravimetric capacity and 50 g H_2/L materials-based volumetric capacity, with potential to meet DOE 2010 system-level targets. They also plan to demonstrate the feasibility and economical viability of the synthesis process. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*