III.F.3 Chemical Hydrogen Storage Center of Excellence (New Project)

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The Chemical Hydrogen Storage Center of Excellence focuses on three "tiers" of R&D for chemical hydrogen storage. The Center involves two national laboratories, seven universities, and four industrial companies.

Tier 1, Borohydride/Water, concentrates on the chemistry required for facile reaction of borohydride, BH_4^-, compounds such as $NaBH_4$ with water to release hydrogen, and for lowering the cost of converting the resulting borates back to BH_4^-. The overall goal of Tier 1 is to develop new chemistry to remove barriers to implementation of $NaBH_4$ technology for hydrogen generation.

Tier 2, Novel Boron Chemistry, addresses the possibility that the expense of converting B-O bonded species back to BH_4^- could remain unacceptably high, and focuses on chemical processes that release hydrogen from other B-H bonded species that may be less energy-intensive and less expensive to regenerate than borohydride itself. The overall goal of Tier 2 is to design and develop new boron-hydride chemistry with improved thermodynamics for regeneration of spent material after hydrogen generation.

Tier 3, Innovation Beyond Boron, examines materials comprising light elements other than boron that could satisfy non-toxicity and mass/volume-storage requirements for serving as useful sources of hydrogen, while at the same time requiring minimal energy cost of recycling/regenerating. The overall goal of Tier 3 is to identify and develop new compounds and materials for chemical hydrogen storage.

The following pages contain brief summaries of the work proposed to be completed by each Chemical Hydrogen Storage Center of Excellence team member.

Chemical Hydrogen Storage

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Chemical hydrogen storage involves systems in which hydrogen is chemically bonded to molecules or materials and therefore requires a chemical reaction (likely involving catalysis) to release hydrogen. Regeneration of chemicals after the hydrogen has been released constitutes the major technical challenge for chemical hydrogen storage systems. LANL proposes to develop borohydrides, novel boron chemistry, and related materials beyond boron for use as chemical hydrogen storage. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Combinatorial Synthesis and High-Throughput Screening of Effective Catalysts for Chemical Hydrides

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Intematix proposes to provide combinatorial capabilities for discovering new heterogeneous catalysts for releasing hydrogen from known and new hydrogen storage materials. They plan to perform high-throughput screening of thousands of candidate catalysts for hydrogen release from boron-hydrogen and other chemical hydrogen storage materials, and identify the most promising solid catalysts for use in hydrogen storage systems for transportation. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Development of Advanced Chemical Hydrogen Storage and Generation System

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Millennium Cell proposes to develop improved capability to store and generate hydrogen with concentrated sodium borohydride by focusing on reactor and system development. They plan to develop a hydrogen fuel system that will meet the system-based storage capacity of 1.2 kWh/L (36 g H_2/L) and 1.5 kWh/kg (4.5 wt.%). *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Safety Analysis and Applied Research on the Use of Borane-Amines for Automotive Hydrogen Storage

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Northern Arizona University proposes to provide guidance for safe handling of borane-amine compounds throughout the Chemical Hydrogen Storage Center, and to evaluate the hydrogen on-board generation and off-board regeneration capability and capacity of borane-amines to determine if a laboratory-scale system can be

developed that safely meets the DOE 2015 target of 9 wt.% hydrogen. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Chemical Hydrogen Storage

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PNNL will investigate several routes to lower the energy cost of regenerating BH_4^- from BO_2^-, including the development of suitable catalysts and development of transfer hydrogenation processes to provide hydrogen from another molecule to recharge $NaBH_4$ at a lower energy cost. PNNL also plans to perform life cycle analyses including efficiency, cost, and environmental impact for off-board regeneration. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Electrochemical Hydrogen Storage Systems

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Pennsylvania State University proposes to explore the feasibility of electrochemically affecting changes in the formal oxidation states of elements in complex boranes as a means of reducing B-O to B-H and for the reversible storage of hydrogen. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides

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Rohm and Haas proposes to define and evaluate novel chemistries and processes to produce chemical hydrides for hydrogen storage, with emphasis on low-cost routes to sodium borohydride. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Main Group Element Chemistry for Hydrogen Storage and Activation

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The University of Alabama proposes to provide computational chemistry support (thermodynamics, kinetics, properties prediction) to the experimental efforts of the Center to reduce the time to design and develop new materials. They also plan to develop and implement imidazolium-based H_2 activation chemistry, develop systems based on polyhydrides of heavier main group elements, and investigate cyanocarbon systems for H_2 storage. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Novel Boron Chemistry/Innovation Beyond Boron

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The University of California-Davis proposes to develop amine and hydrogen-capped light main group element alloy nanoparticles and boron complexes, or other main group compounds with diradical character, that have sufficient reversible hydrogenation/dehydrogenation capability to meet DOE 2010 system-level targets. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Chemical Hydrogen Storage Using Polyhedral Borane Anion Salts

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The University of California, Los Angeles proposes to evaluate the utility of polyhedral borane anions for chemical hydrogen storage applications. Specifically, they plan to develop efficient catalysts for the hydrolysis of polyborane anions with controlled hydrogen release, synthesize compounds for electrochemical studies to be conducted by other partners in the Center of Excellence for Chemical Hydrogen Storage, and synthesize polyhedral borane-amine complexes and ammonium salts for catalytic dehydrogenation studies with other Center partners. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Amineborane Hydrogen Storage

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The University of Pennsylvania will investigate efficient routes for the dehydrogenation of amineboranes and regeneration of the B-N products back to amineboranes. The objectives are to develop new ways of inducing amineborane dehydrogenations and elucidating the important controlling factors in these reactions, and to develop efficient methods for the regeneration of ammoniaborane or other hydrogenated amineborane species from boron nitride or amorphous $[BHNH]_x$ materials. Metal-catalyzed B-H dehydrogenation and amineborane precursors to boron nitride preceramic polymers will be investigated. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Solutions for Hydrogen Storage: Hydrogenation/Dehydrogenation of BN Bonds

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The University of Washington, Seattle proposes to develop an understanding of the dehydrogenation/hydrogenation of amineborane derivatives and to use this insight to develop catalysts exhibiting satisfactory rates of hydrogenation/dehydrogenation of amineborane derivatives to allow for efficient hydrogen storage. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Background Studies on Boron Hydrides

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US Borax has a library of declassified reports on government-funded research on boron hydrides that was conducted for an advanced aviation fuel program in the 1950-1960's timeframe. US Borax will compile and evaluate this unique information, which may be vital for developing new chemical hydrogen concepts. *(Note: US Borax did not request government funding for their work.)*