III.F New Hydrogen Storage "Grand Challenge" Projects

III.F.1 Carbon-based Materials Center of Excellence (New Project)

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The Center of Excellence on Carbon-based Materials focuses on developing high-surface-area sorbents and carbon-based materials for vehicular hydrogen storage systems that are reversible on-board. Through parallel efforts, the Center proposes to determine the limits of performance for specific material systems and extract general mechanistic information that can be used for further design and optimization. A key effort is to determine the relationship between nanoscale structure and the energetics of hydrogen binding using a variety of experimental and theoretical tools and well-defined nanostructured materials. Materials of interest include single-wall carbon nanotubes, graphite nanofibers, multi-walled nanotubes, alkali metal intercalated carbons and nanotubes, carbon nanohorns, chemomechanically processed (ball-milled) materials, metal catalyst-decorated and substitutionally doped versions of these, conducting polymers, and metal-organic frameworks. The Center involves seven universities, one industrial company, and four federal laboratories. *(Note: Subject to congressional appropriations, work on the Center of Excellence is anticipated to begin in FY 2005.)*

The following pages contain brief summaries of the work proposed by each Center team member.

Research and Development of Carbon-based Materials for Hydrogen Storage

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The National Renewable Energy Laboratory proposes to identify an efficient and cost-effective carbon-based technology that can meet DOE's RD&D Plan goals for on-board vehicular hydrogen storage applications. This will be accomplished through mechanistic studies and materials design and discovery, development of carbon materials, and materials measurement and analyses. NREL plans to determine the adsorption mechanism that allows for hydrogen to be stabilized on carbon materials with higher binding energies than physisorption. NREL will lead the initiative to understand hydrogen adsorption mechanisms in advanced carbon-based materials such as metal-organic frameworks and various forms of nanostructured carbons. Systems analyses, including life cycle analyses, will also be conducted. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Designing Microporous Carbons for Hydrogen Storage Systems

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Air Products and Chemicals proposes to develop and demonstrate reversible carbon-based hydrogen storage materials 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 plan to develop novel reversible H_2-sorbent materials that are tailored for optimal binding energy, storage capacity and other parameters, such as charging rates and discharge kinetics. An integral component of the work is theoretical modeling, including predictive modeling of enhanced hydrogen physisorption. A novel high-throughput screening technique for hydrogen storage measurements will be investigated. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Enhanced Hydrogen Dipole Physisorption

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The California Institute of Technology's efforts focus on increasing the strength of physisorption onto carbon surfaces and edges to enable high-surface-area materials to meet DOE hydrogen storage targets. The proposed plans are to develop high potential local charge sites using (i) alkali metal intercalation in single-walled nanotubes and (ii) the design of high edge potential sites by incorporating new organic linkers in metal-organic framework structures. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Growth of Uniform Carbon Nanotubes Using Molecular Clusters as Catalysts

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Duke University proposes to explore the use of molecular nanoclusters with identical sizes for the growth of uniform carbon nanotubes with controlled diameters. Long-term goals are to produce nanotubes with specific diameters for hydrogen storage applications at kilogram-scale production with low cost and high quality. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Metal-Containing Organic and Carbon Aerogels for Hydrogen Storage

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LLNL proposes to produce metal-loaded aerogel materials as sorbents for hydrogen storage. These materials should be well-suited for hydrogen adsorption due to their extremely high surface area (~500-800 m^2/g based on N_2 adsorption) and the presence of the metal centers, which catalyze the formation of graphitic structures in the carbon materials. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Neutron Characterization of Carbon-Based Materials for Hydrogen Storage

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NIST plays an important role in materials characterization for the Center of Excellence. The plans are to perform neutron-scattering measurements to probe the amount, location, bonding states, dynamics, and morphological aspects of hydrogen in carbon-based materials such as polymers, metal-organic frameworks, and carbonaceous materials such as carbon nanotubes. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Synthesis and Processing of Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports

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Oak Ridge National Laboratory proposes to synthesize and process single-walled carbon nanohorns (SWNHs) for evaluation as pure carbon hydrogen storage materials and as metal cluster catalyst supports for catalyst-assisted hydrogen storage media. A test apparatus for SWNH production is proposed for construction, and samples are planned for synthesis and delivery to other partners for testing. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Advanced Boron and Metal-loaded High-Porosity Carbons

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Penn State University proposes to explore new hydrogen storage materials that can form intermediate-strength bonds with molecular hydrogen. Ternary high-surface-area materials are emphasized that are constructed from boron-doped carbon and light element metals. These may be synthesized by pyrolysis, high-temperature chemical processing, and high-temperature vapor phase approaches. The plans are to determine the relationships between physical properties, hydrogen storage performance, pore size distribution and metallic character of the materials. The objectives are to measure such properties and correlate them with the local atomic chemistry and pore structure of various materials. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Cloning Single-Wall Carbon Nanotubes for Hydrogen Storage

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The focus of this project at Rice University will be on technology to reduce the cost of single-wall nanotubes (SWNTs) and to produce SWNTs of specific types that are best suited for hydrogen storage. Extensive experience in methods to prepare carbon nanotubes as well as cutting, doping, growth of seeds on supports and attachment of catalysts to cut tubes will be used in process development and optimization. A key objective is the evaluation of a scaled-up process that can be commercialized at a scale and cost with potential to meet DOE targets. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Optimization of SWNT Production and Theory of H_2-SWNT Systems for Hydrogen Storage

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This project focuses on single-wall nanotube (SWNT) synthesis approaches for low-cost, high-volume manufacturing. The objective is to take advantage of the tunability of the high-pressure carbon monoxide (HiPco™) synthesis process to produce SWNTs. Structure-capacity correlations will be theoretically derived to guide the experimental HiPco™ effort. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Characterization of Hydrogen Adsorption in Carbon-Based Materials by NMR

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The University of North Carolina proposes to support the Center of Excellence by developing nuclear magnetic resonance (NMR) techniques for the characterization of hydrogen storage in carbon-based materials. NMR signatures of adsorbed molecular hydrogen in carbon-based materials will be established to enable selectivity and quantitative measurement of hydrogen storage. The key objective is to develop a quantitative, and rapid NMR procedure to measure hydrogen adsorption capacity and identify adsorption mechanisms in carbon-based storage materials. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Examination of the Physical Aspects of Hydrogen Storage in MOFs

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Metal-organic frameworks (MOFs) are synthetic nanoporous crystalline materials composed of inorganic and organic building blocks. The work proposed in this project will elaborate on early work by Yaghi and coworkers to optimize the hydrogen affinity of MOFs. Key objectives are to optimize the performance of MOFs by testing and evaluating various structures, synthetic methods, and activation procedures. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Hydrogen Storage in Graphite Nanofibers and the Spillover Mechanism

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Graphite nanofibers can be synthesized using metallic catalysts and have exhibited the ability to store hydrogen. The focus of this effort will be on characterizing and enhancing hydrogen spillover using graphite nanofibers and other solid carbonaceous substrates to develop a viable storage system. A key objective of this work is to develop a better understanding of the spillover mechanism to enhance hydrogen storage capacities. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*

Conducting Polymers as New Materials for Hydrogen Storage

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It has been reported in the literature that nanoporous conducting polymers can store significant amounts of hydrogen. If true, this would constitute a new important class of hydrogen storage materials. In this effort, a primary objective is to confirm that approximately 8 wt.% (reversible) hydrogen gas storage in conducting polymers can be attained. Optimization and testing of various materials, such as doped (metallic) forms of organic conducting polymers ("synthetic metals"), polyaniline and polypyrrole, are planned. *(Note: Subject to congressional appropriations, work on this project is anticipated to begin in FY 2005.)*