Report on Hydrogen Storage Panel Findings in DOE-BES Sponsored Workshop on Basic Research for Hydrogen Production, Storage and Use

A follow-on workshop to BESAC-sponsored workshop on "Basic Research Needs to Assure a Secure Energy Future"

Workshop dates: May 13-15, 2003
Anticipated date of final report: August 2003

Harriet Kung

Program Manager
Office of Basic Energy Sciences
Office of Science
Department of Energy

Basic Research for Hydrogen Production, Storage and Use Workshop

Workshop Chair:	**Millie Dresselhaus**	**(MIT)**
Associate Chairs:	**George Crabtree**	**(ANL)**
	Michelle Buchanan	**(ORNL)**

EERE Coordination:

Pre-Workshop Briefings

- **JoAnn Milliken (Hydrogen Storage)**
- **Nancy Garland (Fuel Cells)**
- **Mark Paster (Hydrogen Production)**

Workshop Plenary Presentation

- **Steve Chalk (President's Hydrogen Initiative)**

Charge: To identify fundamental research needs and opportunities in hydrogen production, storage, and use, with a focus on new, emerging and scientifically challenging areas that have the potential to have significant impact in science and technologies. Highlighted areas will include improved and new materials and processes for hydrogen generation and storage, and for future generations of fuel cells for effective energy conversion.

Hydrogen Storage and Distribution Team

Co-Chairs: Kathy Taylor (GM, Retired) and Puru Jena (VCU)

Speakers

Scott Jorgensen (GM)
Key Issues

Robert Bowman (JPL)
Metal and Compound Hydrides

Karl Johnson (Univ. Pittsburgh)
Theory and Computation

Thomas Klassen (GKSS-Research Center, Germany)
Nanostuctured Hydrides

Peter Eklund (Penn State Univ)
Carbon related materials

Panelists

Mike Baskes (LANL)

Seiji Suda (Kogakun Univ, Japan)

John Wolan (Univ S Florida)

James Ritter, Univ S Carolina)

Hannes Jonsson (Univ of Wash)

BjÖrgvin HjÖrvarsson (Uppsala Univ, Sweden)

George Thomas (SNL (Retired))

Vitalij Pecharsky (Ames Lab)

Hydrogen Storage and Distribution

Current Status, Technology Goals and Scientific Challenges

Target Applications

- Transportation– on board vehicles and non-transportation applications for hydrogen production/delivery

System Requirements

- Demand compact, light-weight, affordable storage.
- System requirements set for FreedomCAR: 4.5 wt% for 2005, 9 wt% for 2015.
- No current storage system or material meets all targets. (Currently: Solid Storage $\leq$ 3%; Liquid and Gas Storage $\leq$ 4%)

Current Technology

- Focus mainly on tanks for gaseous or liquid hydrogen storage.
- Progress demonstrated in solid state storage materials: metallic hydrides, light metal hydrides, complex (chemical) hydrides, novel nanostructured materials.

Future Technology Needs

- Basic research to identify new materials and to improve the properties of existing materials before they can be considered viable candidates.
- Theory and computation to understand the mechanisms, electronic structure, dynamics and energetics of hydrogen in materials.

Summary of Major Findings/Research Directions

Focus Areas:

- Hydrides
  - Metal Hydrides
  - Complex Hydrides
- Nanoscale and Other Novel Materials
- Theory and Simulation

Metal Hydrides

- Understand lifetime degradation issues
- Understand the role of processing/dopants/catalysts in improving kinetics
- Understand the role of surfaces in hydrogen storage
- Explore nanostructured composites of metal hydrides with complex hydrides
- Understand hydrogen-promoted mass transport
- Understand thermophysical properties

Complex Hydrides

- Initiate interdisciplinary basic research program to study broad class of complex hydrides
- Generate reliable information about structural, thermodynamic, physical and chemical properties
- Couple experiment with first principle theory and semi-empirical modeling
- Develop effective (e.g. solvent-free) synthesis approaches
- Understand the role of processing/dopants/catalysts in improving both thermodynamics and kinetics
- Understand mass transport in phase transformations
- Understand the role of surfaces in hydrogen storage
- Explore nanostructured composites of complex hydrides with metal hydrides

Nanoscale and Other Novel Materials

– **Exploit**
  - **Finite size and shape effects on electronic states and resulting thermodynamics**
  - **Heterogeneous compositions and structures**
  - **Catalyzed dissociation and interior storage phase**
  - **Curvature, shape and pore-size to affect surface chemistry and binding**

Theory and Computation

- Develop more general approaches for integrating disparate time & length scales
- Develop more accurate and faster first principles methods applicable to condensed phases
- Experiments on model systems for benchmarking against calculations at all length scales

Hydrogen Storage and Distribution

Priority Research Areas

- Initiate a broadly based research program to explore and further the potential of complex hydrides for hydrogen storage
- Exploit computational methods to predict trends, guide experiments, and to identify new promising materials for hydrogen storage & catalysis
- Utilize fundamentally different physical and chemical properties at the nanoscale in the design of new storage materials

Crosscutting Issues

- Catalysis
- Membranes and Separations
- Nanostructured / Novel Materials
- Sensors, Characterization and Measurement Techniques
- Theory, Modeling, and Simulation
- Safety

Proposed Workshop Report Outline

Executive Summary

I. Introduction and Overview

II. Panel Reports

- **Hydrogen Production**
- **Hydrogen Storage and Distribution**
- **Fuel Cells and Novel Fuel Cell Materials**

III. Integration of Major Findings, Cross-Cutting Issues, and Research Directions

IV. Conclusions

Appendices

- **Research Direction Write-Ups**

Workshop Report to be posted on BES website in August, 2003
http://www.sc.doe.gov/bes/bes.html