DOE-BES Sponsored Workshop on *Basic Research for Hydrogen Production, Storage and Use*

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Workshop dates: May 13-15, 2003

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

Workshop Charter

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.

Workshop Organizers

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

Pre-Workshop Briefing Presenters:

	JoAnn Milliken	(EERE)
	Nancy Garland	(EERE)
	Mark Paster	(EERE)

EERE: DOE Office of Energy Efficiency and Renewable Energy

Workshop Panel Chairs

Basic Research Challenges in Hydrogen Production

Session Chairs: Tom Mallouk (Penn State University)
Laurie Mets (University of Chicago)

Hydrogen Storage and Distribution

Session Chairs: Kathy Taylor (General Motors, Retired)
Puru Jena (Virginia Commonwealth University)

Fuel Cells and Novel Fuel Cell Materials

Session Chairs: Frank DiSalvo (Cornell University)
Tom Zawodzinski (Case Western Reserve Univ.)

Four Questions

- Where are we now?
- What do we already know?
- Where do we want to be?
- What do we need to do to get there?

Workshop Approaches

- Recognize the Great Challenge of Implementing the Hydrogen Economy
- Solicit Participation of Stakeholders
- Recognize Roles of Various DOE Programs: Technology Goals, Objectives, and Milestones
- Understand Time Scale of the Objectives
- Coordinate Basic Research with Technology Development

Workshop Goals

To identify:

- Research needs and opportunities to address long term "Grand Challenges" and to overcome "show-stoppers."
- Prioritized research directions with greatest promise for impact on reaching long-term goals for hydrogen production, storage and use.
- Issues cutting across the different research topics/panels that will need multi-directional approaches to ensure that they are properly addressed.
- Research needs that bridge basic science and applied technology:
  - So challenging that long term sustained effort is required
  - Opportunity driven by advances in science and technology
  - Technology needs driven- basic research with highest potential for impact

Plenary Session Presentations

President's Hydrogen Initiative
Steve Chalk (DOE EE/RE)

Hydrogen Storage: State of the Art
George Thomas (SNL-CA, Retired)

Onboard Hydrogen Storage, Who's Driving and Where Are We Going?
Scott Jorgensen (General Motors)

Hydrogen and Climate Change
Jae Edmonds (PNNL)

Science of Hydrogen Safety
Jay Keller (SNL-CA)

Hydrogen Production Session Team

Co-Chairs: Tom Mallouk (Penn State), Laurens Mets (U of Chicago)

Speakers

Allen Bard (UT, Austin)
  Solar Production

Charles Dismukes (Princeton)
  Biological and Biomimetic

Jennifer Holmgren (UOP)
  Fossil production

Ken Schultz (General Atomics)
  Nuclear Production

Lenny Tender (NRL)
  Bio/Inorganic interfaces

Panelists

Michael Adams (Univ of Georgia)
Les Dutton (Univ of Pennsylvania)
Charles Forsberg (ORNL)
Heinz Frei (LBL)
Tom Moore (Arizona State Univ)
Jens Nørskov (Technical Univ of Denmark)
Arthur J. Nozik (NREL)
K. Lee Peddicord (Texas A&M Univ)
Tom Rauchfuss (Univ of Illinois)
John A. Turner (NREL)
Luping Yu (Univ of Chicago)

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 South Florida)

James Ritter, Univ South Carolina)

Hannes Jonsson (Univ of Washington)

BjÖrgvin HjÖrvarsson (Uppsala Univ, Sweden)

George Thomas (SNL (Retired))

Vitalij Pecharsky (Ames Laboratory)

Fuel Cells and Novel Fuel Cell Materials Team

Co-Chairs: Frank DiSalvo (Cornell) and Tom Zawodzinski (CWSU)

Panelists

Fernando Garzon, LANL
Sossina Haile, Cal Tech
John Lannutti, OSU
Zachary Fisk, FSU

Speakers

Shimshon Gottesfeld, MTI Micro FCs
Jim McGrath,Virginia Tech
Levi Thompson, U/Michigan
Joel Christian, Osram/Sylvania
Adam Heller, U/Texas
Hubert Gasteiger, GM
Ray Gorte, Penn
Woods Halley, UMN

Additional Contributors

Andrew Gewirth, UI
Radoslav Adzic, BNL
Marvin Singer, DOE Office of Science
David Ginley, NREL
Giselle Sandi, ANL

Hydrogen Production Panel

Current Status, Challenges and Opportunities

Status: Steam-reforming of Oil and Natural Gas produces 9M tons H_2/yr; expandable to 40M tons/yr needed for transportation, given better catalysts. Requires CO_2 sequestration to meet fundamental goals of H_2 economy.

Alternative energy resources and conversion technologies:

Coal: cheap; lower H_2 yield/C; more contaminants; R&D needed for process development, gas separations, catalysis, impurity removal.

Solar: widely distributed; carbon-neutral; low energy density. PV/electrolysis current standard – 15% efficient - needs 0.03% of land area to serve transportation.

Nuclear: abundant; carbon-neutral; long development cycle.

Intermediate goals: better CATALYSTS and better materials for fossil and biomass conversion processes.

Long term goals: more efficient, cheaper, more durable solar conversion processes; Development of nuclear resources; reduce dependence on noble metal catalysis.

Hydrogen Production Panel

Fossil Fuel Reforming

Scientific Challenges

- Improved **catalysts** (e.g. lower T water-gas shift reaction; desulfurization catalysts)
  - more **active**, more **specific**, more **stable**, less susceptible to poisoning/fouling
- Improved gas **separations** (e.g. membranes – more robust and selective)

Opportunities

- **Combinatorial synthesis, analysis of catalysts**
- **Integrated experimental and computational approaches to understand/control**
  - active sites at atomic level
  - catalytic mechanisms
  - catalyst design on the nano-scale

Hydrogen Production Panel

Nuclear and solar thermal hydrogen

Scientific Challenges and Opportunities

- **Cost/efficiency (duty cycle) for solar thermochemical (TC)**
- **Separations and materials performance**
- **H_2 from direct thermolysis (>2500°C) and radiolysis are interesting but speculative**

Priority Research Areas

- **Thermodynamic data and modeling for TC**
- **High temperature materials in oxidizing environments at ~900°C**
  - Solid oxide materials and membranes
  - TC heat exchanger materials
- **High temperature gas separation**
- **Improved catalysts**

Hydrogen Production Panel

Solar PV/PEC/photocatalysis

Scientific Challenges and Opportunities

- **Integrate light harvesting, charge separation and transport, charge transfer (fuel formation) and stability into working systems**
- **Design and assembly of 2-D and 3-D systems**

Priority Research Areas

- **Light harvesting - absorption of full solar spectrum, efficiency**
- **Charge transport - effect of structure, energy loss mechanisms, charge separation**
- **Composite assemblies**
  - Organic/inorganic/polymer hybrid chemical systems
  - Effects of nanostructure and surface area

Hydrogen Production Panel

Bio- and bio-inspired H2 production

Findings: Scientific Challenges and Opportunities

- Identify microbes & component redox enzymes, proteins, cofactors, regulatory pathways for producing/metabolizing H_2 and other fuels (CO, CH_4,…)
- Efficiently interface biomimetic redox catalysts into complex 2D, 3D structures for hydrogen/oxygen catalysis, sensing, and energy transduction

Findings: Priority Research Areas

- Biomimetic catalysts for hydrogen "processing"
- Exploiting biodiversity for novel biocatalysts and determining mechanisms of assembly
- Coupling electrode materials to light-driven catalytic water oxidation, hydrogen production components
- Biomimetic nanostructures to organize catalytic functions of water oxidation and hydrogen production

Hydrogen Storage and Distribution Panel

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.

Hydrogen Storage and Distribution Panel

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

Fuel Cells Panel

Current Status, Technology Goals and Scientific Challenges

Status: Engineering investments have been a success. Limits to performance are materials, which have not changed much in 15 years.

- **Membranes**
  - Operation in lower humidity, strength and durability.
  - Higher ionic conductivity.
- **Anodes**
- **Cathodes**
  - Materials with lower overpotential and resistance to impurities.
  - Low temp operation needs cheaper (non- Pt) materials.
  - Tolerance to impurities: CO, S, hydrocarbons.
  - Low T operation needs cheaper (less Pt, or non- Pt) materials.
- **Reformers**
  - If H_2 storage is not solved, and perhaps in transition period, the H will be derived from hydrocarbons by reforming.
  - Need low temperature and inexpensive reformer catalysts.

Electrocatalysts

Scientific Challenges and Opportunities

- **New Materials**
  - Many classes of materials, previously ignored, have recently shown promise.
  - Need rapid synthesis, analysis and evaluation.

Priority Research Areas

- **Improved cathodes (low overpotential, durable, impurity tolerant)**
- **Materials that minimize rare metal usage in cathodes and anodes**
- **Synthesis and processing of designed triple percolation electrodes**

Fuel Cells Panel

Low Temperature Materials

Scientific Challenges and Opportunities

- Basic understanding of materials/structure/transport relationships
- Proton conduction in low- or zero-water environment at elevated temperature
- Understanding factors controlling durability
- New methodologies for materials discovery
- Complementary experimental and theoretical approaches

Priority Research Areas

- ‘High’ Temperature proton conductors
- Fundamental understanding of degradation mechanisms
- Functionalizing Materials with Tailored Nano-structures
- Interfaces and Adhesion

Fuel Cells Panel

Solid Oxide Fuel Cells

Scientific Challenges and Opportunities

- New materials and synthetic approaches
  - Electrolytes, anodes, cathodes
    - Higher conductivity, chemical stability, improved mechanical properties, exploratory materials synthesis
    - Ceramic proton conductors
    - Improved electrokinetics, nanostructured architecture, functionally graded interfaces
  - Interconnects with 'metallic conductivity, ceramic stability'
  - High strength, thermally shock resistant, chemically compatible materials for seals
- Modeling ionic and electronic transport processes in bulk, at surfaces and across interfaces
- New techniques for characterization of electrochemical processes
- Innovative fuel cell architectures

Fuel Cells Panel

Solid Oxide Fuel Cells

Priority Research Areas

- Theory, modeling and simulation, validated by experiment, for electrochemical materials and processes
- New materials – all components!
- Novel synthesis routes for optimized architectures
- Advanced in-situ analytical tools

Crosscut Issues

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

Proposed Workshop Report Outline

Executive Summary

I. Introduction and Overview

II. Panel Reports (three reports)

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

IV. Conclusions

Appendices

Research Direction Write-Ups