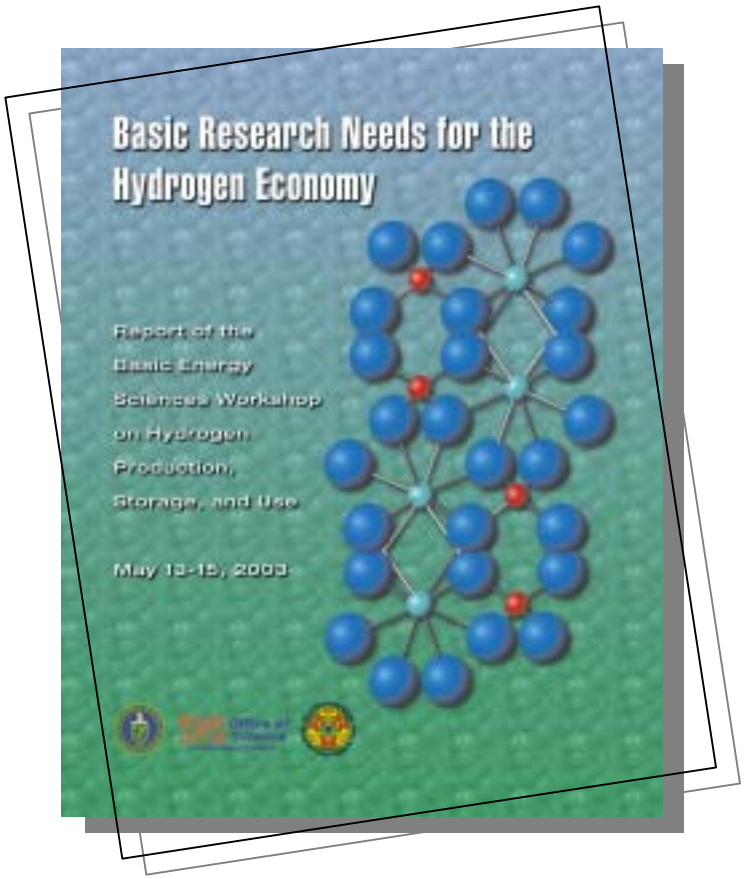
Basic Research Needs For the Hydrogen Economy



Presentation for
Annual DOE Hydrogen Program Review

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May 24, 2004

Fundamental Issues

The hydrogen economy is a compelling vision:

- It provides an abundant, clean, secure and flexible energy source
- Its elements have been demonstrated in the laboratory or in prototypes

However . . .

- It does not operate as an integrated network
- It is not yet competitive with the fossil fuel economy in cost, performance, or reliability
- It will take decades to realize the full potential of a hydrogen economy

Basic Research for Hydrogen Production, Storage and Use Workshop
May 13-15, 2003

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

Breakout Sessions and Chairs:

Hydrogen Production
Tom Mallouk, PSU & **Laurie Mets**, U. Chicago

Hydrogen Storage and Distribution
Kathy Taylor, GM (retired) & **Puru Jena,** VCU

Fuel Cells and Novel Fuel Cell Materials
Frank DiSalvo, Cornell & **Tom Zawodzinski**, CWRU

EERE Pre-Workshop Briefings:

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

Plenary Session Speakers:

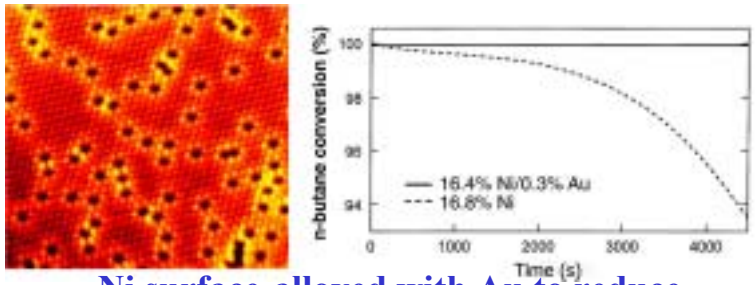
Steve Chalk (DOE-EERE) -- overview
George Thomas (SNL-CA) -- storage
Scott Jorgensen (GM) -- storage
Jae Edmonds (PNNL) -- environmental
Jay Keller (SNL-CA) – hydrogen safety

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.

Priority Research Areas in Hydrogen Production

Fossil Fuel Reforming

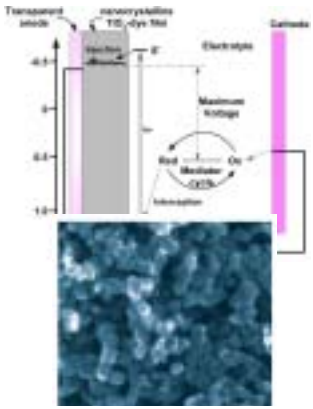
In the intermediate term, the reforming of coal will be the main source of hydrogen. A molecular level understanding of catalytic mechanisms, nanoscale catalyst design, and high temperature gas separation is needed.



Ni surface-alloyed with Au to reduce carbon poisoning

Solar Photoelectrochemistry/Photocatalysis

Long term, hydrogen will be produced using the sun as a renewable energy source. Research on light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis and photocatalysis, organic semiconductors, theory and modeling, and materials degradation are needed.



Dye-Sensitized Solar Cells

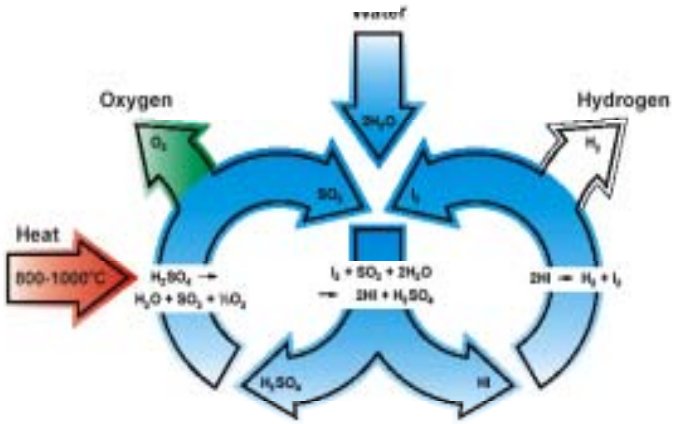
Synthetic Catalysts for H_2 Production

Bio- and Bio-inspired H_2 Production

Living systems produce hydrogen at room temperature with high efficiency. Research on microbes & component redox enzymes, nanostructured 2D & 3D hydrogen and oxygen catalysts, and energy transduction are needed to engineer robust biological and biomimetic H_2 production.

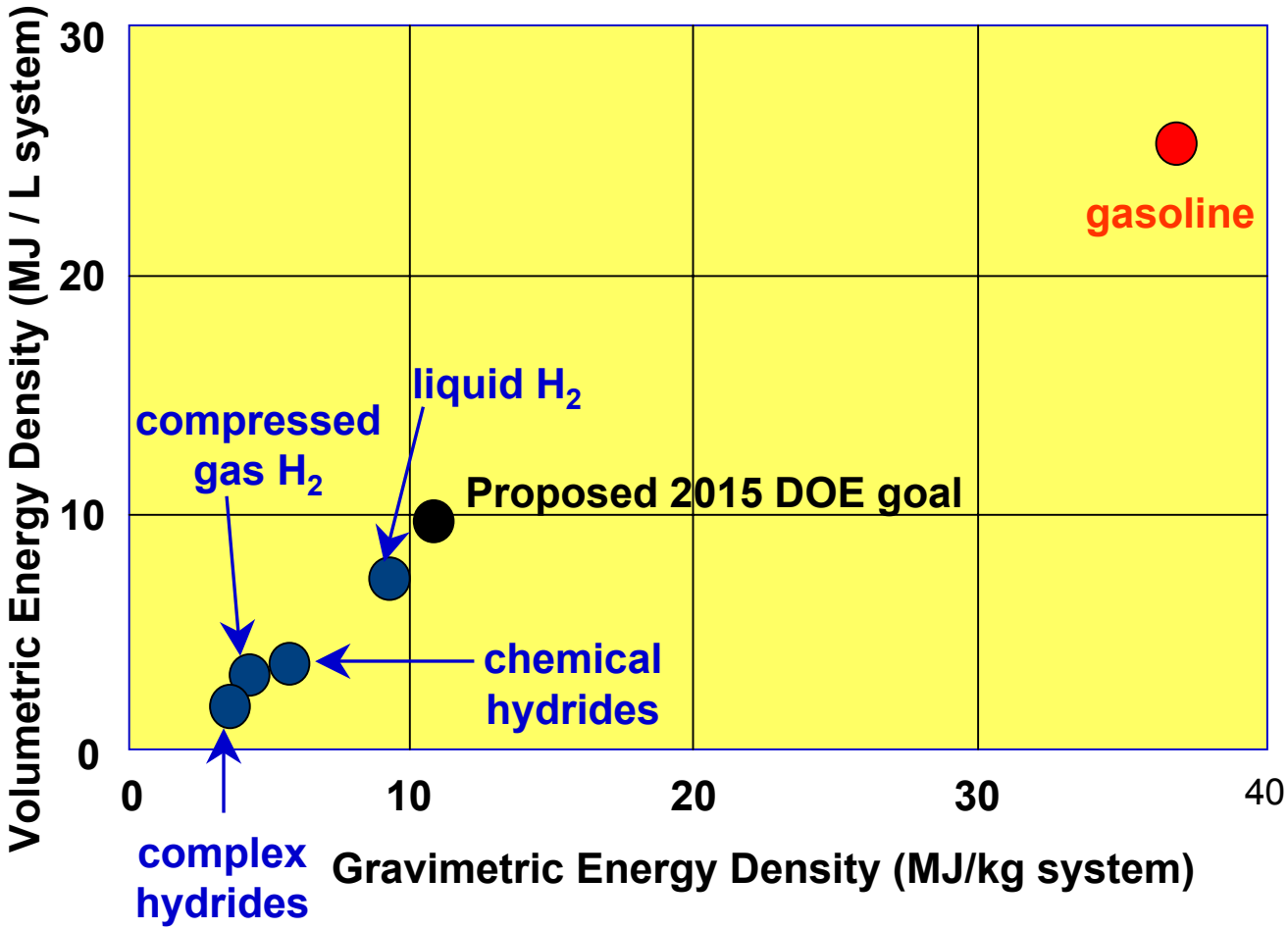
Nuclear and Solar Thermal Hydrogen

Research on thermodynamic data, modeling for thermochemical cycles (TC), high temperature materials and membranes, TC heat exchanger materials, and improved catalysts should benefit from this approach.



Thermochemical Water Splitting

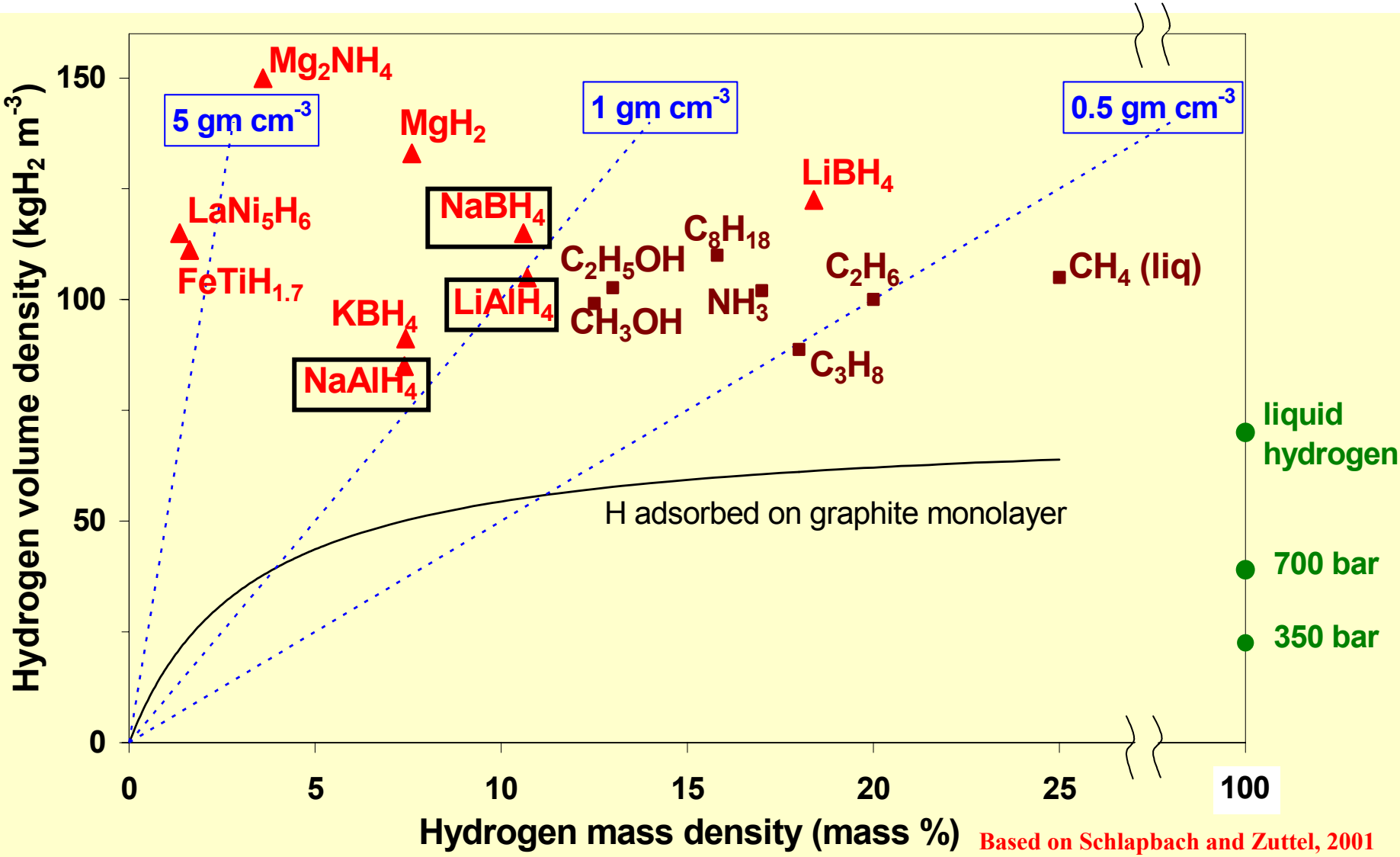
Energy Density of Fuels



Ideal Hydrogen Storage Material

- High gravimetric and volumetric density (10 wt %)
- Fast kinetics
- Favorable thermodynamics
- Reversible and recyclable
- Material integrity
- Minimal lattice expansion
- Absence of embrittlement
- Safe
- Cost effective

High Gravimetric H Density Candidates

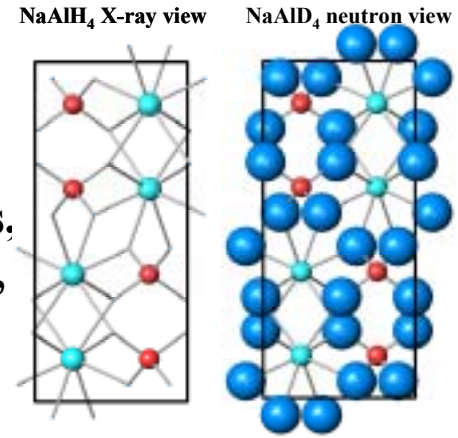


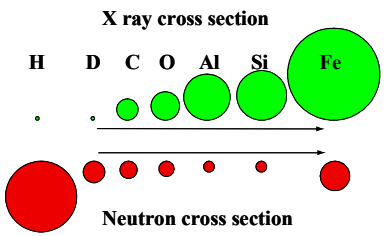
Based on Schlapbach and Zuttel, 2001

Priority Research Areas in Hydrogen Storage

Metal Hydrides and Complex Hydrides

Research is needed on high gravimetric and volumetric capacity materials, nanocatalysts for improving H_2 uptake and release kinetics, degradation and embrittlement mechanisms, effect of surfaces and dopants for hydrogen storage and release.

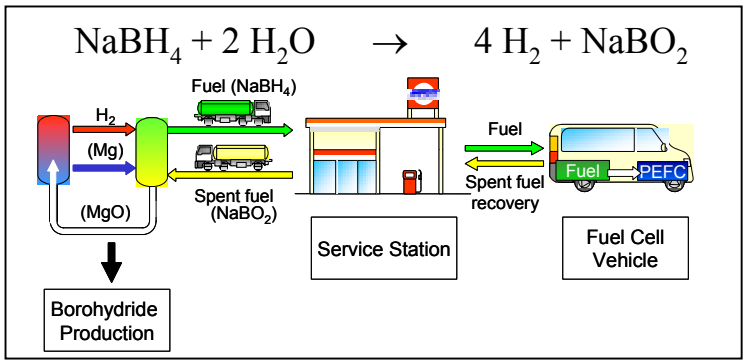




Neutron Imaging of Hydrogen

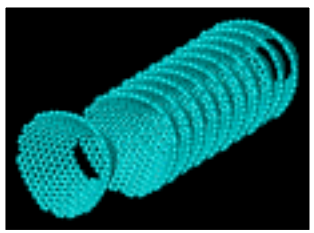
Nanoscale/Novel Materials

Research is needed on finite size, shape, and curvature effects on electronic states, catalytic activity, thermodynamics, bonding, and degradation mechanisms.

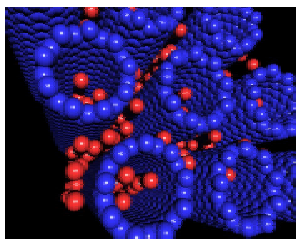


Theory and Modeling

Theory, simulation and first principles methods are needed for studying hydrogen bonding over a wide range of length and time scales. Hydrogen storage and release may be the most challenging problems of the hydrogen economy.



Cup-Stacked Carbon Nanofiber

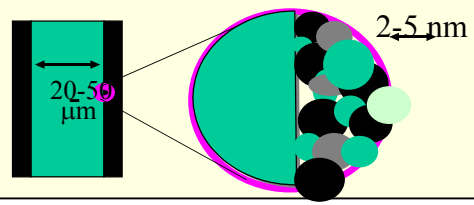


H Adsorption in Nanotube Array

Priority Research Areas in Fuel Cells

Electrocatalysts and Membranes

Develop catalysts to reduce overpotential, minimize rare metal usage and improve design of triple percolation electrodes.

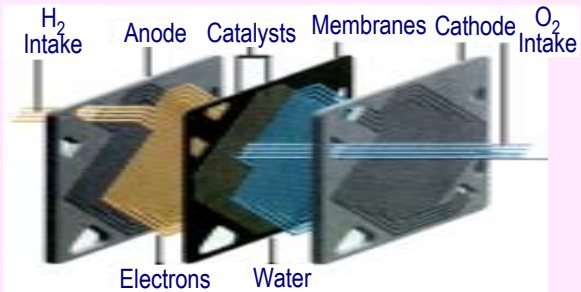


Controlled design of triple percolation nanoscale networks: ions, electrons, and porosity for gases

Low Temperature Fuel Cells

Develop 'Higher' temperature proton conducting membranes, study degradation mechanisms, and develop functionalized materials with tailored nano-structures for enhanced efficiency.

Internal view of a PEM fuel cell (proton exchange membrane)

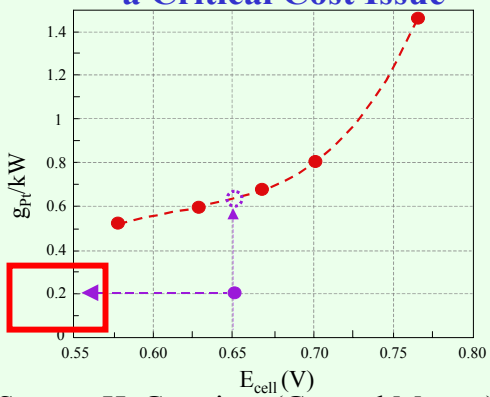


Source: T. Zawodzinski (CWRU)

Solid Oxide Fuel Cells

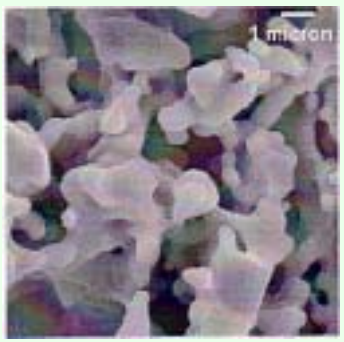
Use theory, modeling and simulation, validated by experiment, to develop electrochemical materials and processes, advanced in-situ analytical tools, new materials and novel synthesis routes for optimizing device architectures.

Mass of Pt Used in the Fuel Cell — a Critical Cost Issue



Source: H. Gasteiger (General Motors)

YSZ Electrolyte for SOFCs

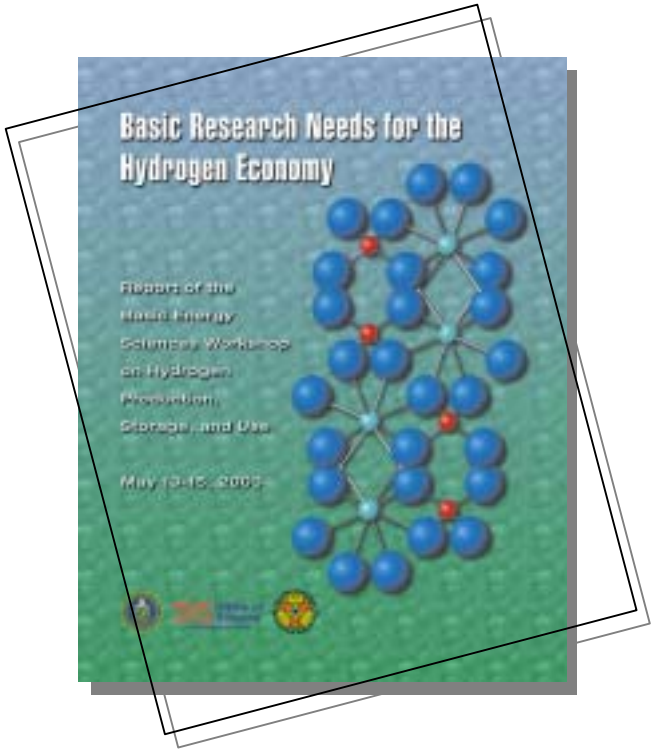


Porosity can be tailored

Source: R. Gorte (U. Penn)

Messages

- Significant gap between present state-of-the-art capabilities and requirements that will allow hydrogen to be competitive with today's energy technologies
  - production: 9M tons/yr ⇒ 40M tons/yr (150 million vehicles; ~75% of US fleet)
  - storage: 4.4 MJ/L (10K psi gas) ⇒ 9.7 MJ/L
  - fuel cells: $300/kW ⇒ $30/kW (gasoline engine high volume cost)
- Enormous R&D efforts will be required
  - Simple improvements of today's technologies will not meet requirements
  - High risk/high payoff basic research should be a critical component of the Hydrogen Fuel Initiative to overcome the technical barriers
- Research is highly interdisciplinary, requiring chemistry, materials science, physics, biology, engineering, nanoscience, computational science
- Basic and applied research should couple seamlessly



http://www.sc.doe.gov/bes/hydrogen.pdf

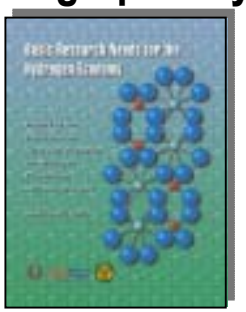
Planned BES Solicitation for Basic Research in Support of the President's Hydrogen Fuel Initiative

- Approximately $21.5 million will be awarded in FY 2005, pending appropriations.

- Separate solicitations for universities and FFRDCs are planned to be issued in May 2004. *Preapplications are required*. Tentative timeline:
  - July 15, 2004 — Preapplications due
  - September 1, 2004 — Decisions on preapplications sent to PIs
  - January 1, 2005 — Full proposals due
  - June - July 2005 — Awards made

- The solicitation will request preapplications for innovative basic research proposals to establish the scientific basis that underpins the physical, chemical, and biological processes governing the interaction of hydrogen with materials.

- Five high-priority research directions will be the focus of the solicitations:



  - Novel Materials for Hydrogen Storage
  - Membranes for Separation, Purification, and Ion Transport
  - Design of Catalysts at the Nanoscale
  - Solar Hydrogen Production
  - Bio-Inspired Materials and Processes

- The distribution of funds between universities and FFRDCs awards and among the five focus areas will depend on the outcomes of the merit review process (http://www.sc.doe.gov/bes/peerreview.html).

Intra- and Inter-Agency Coordination

DOE

- Hydrogen Posture Plan- EERE, FE, NE, SC
- Assisted in EERE Hydrogen Storage Grand Challenge Solicitation and Proposal Review
- Assisted in EERE Hydrogen Production Solicitation and Proposal Review
- Will Coordinate with EERE, NE, FE on BES Hydrogen Solicitation and Proposal Review

OSTP Hydrogen R & D Task Force Group

- Participated by DOC, DOD, DOE, DOT, DOS, CIA, EPA, NASA, NIST, NSF, USDA
- Developed Taxonomy of Research Directions to Facilitate Inter-Agency Coordination
- Lead "Fundamental Research" Subgroup to develop 10-Year Inter Agency Coordination Plans

International Hydrogen Activities

- Participated in multi-lateral and bi-lateral Hydrogen Meetings- IPHE, US/European Commission, US/Canada, US/India, US/United Kingdom, IEA Hydrogen Coordination Group
- Topics of Discussion: Hydrogen Production, Carbon Sequestration, Storage, Delivery, Fuel Cells, Codes and Standards, Economic/Cost Modeling

Outreach

OMB/OSTP Briefing / SC Briefing

American Physical Society March Meeting (March 22-26, 2004)

- Basic Research for the Hydrogen Economy Symposium

American Chemical Society National Meeting (March 28 – April 1, 2004)

- Hydrogen Symposium

Materials Research Society Spring Meeting (April 12-16, 2004)

- Federal Funding Workshop- Hydrogen R&D Needs and Opportunities

Council for Chemical Research (April 17-20, 2004)

- Hydrogen Forum

Materials Research Society Fall Meeting (Nov. 29 - Dec. 3, 2004)

- Hydrogen Storage Symposium

Physics Today- article by Dresselhaus, Buchanan, Crabtree

IUMRS Facets- article by Dresselhaus, Buchanan, Crabtree

Nova special program on Hydrogen- consultants are Nate Lewis, Millie Dresselhaus

Interviews by Jim Lehrer Newshour

Interviews by Brazil Major TV Talk Show / Newspaper

Interview by National Public Radio