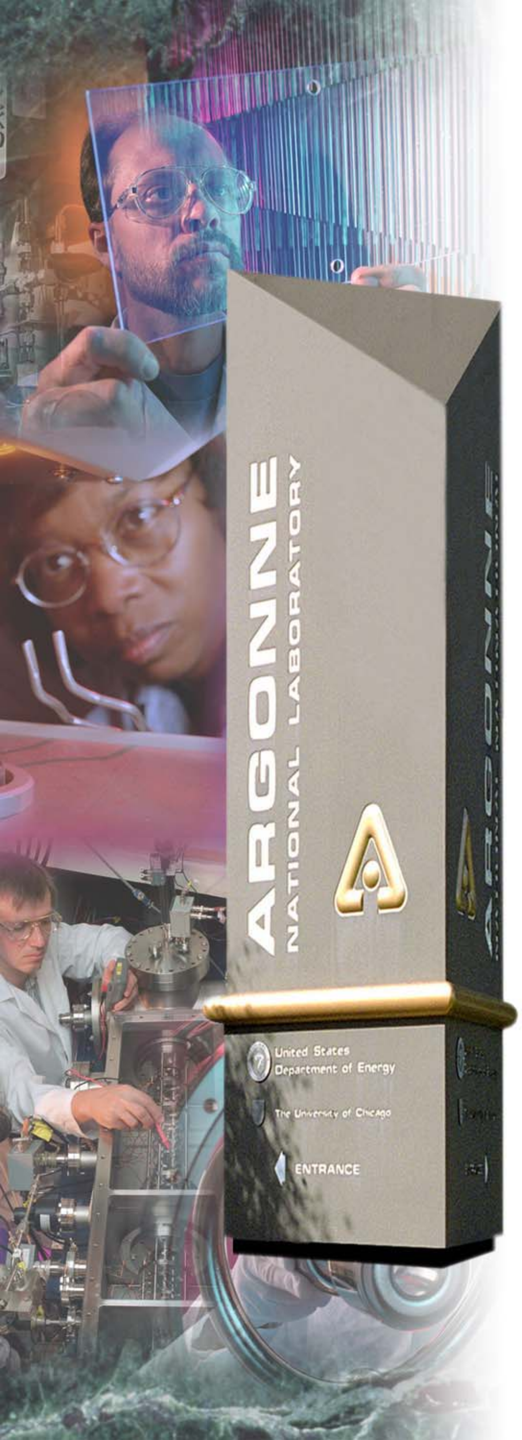


Basic Research Needs for the Hydrogen Economy

George Crabtree
Senior Scientist and Director
Materials Science Division

FMS Congressional Briefing
June 17, 2004

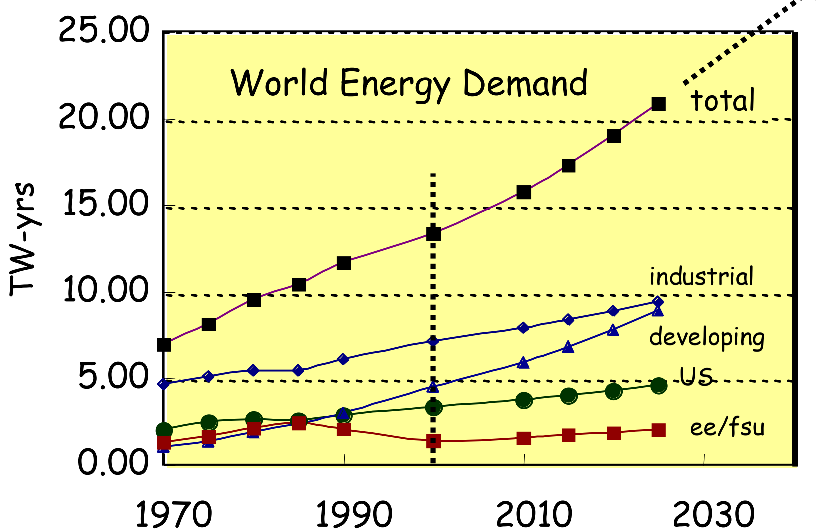
Argonne National Laboratory

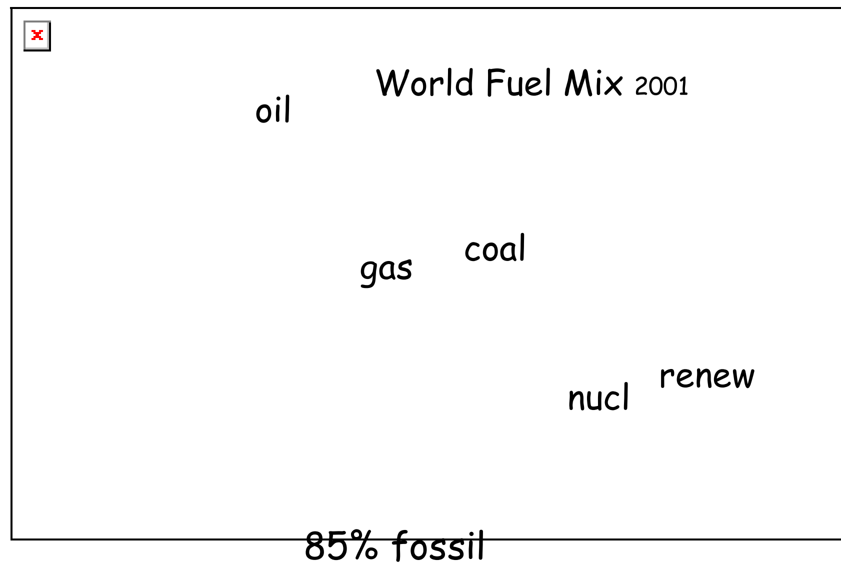
Office of Science
U.S. Department of Energy

A U.S. Department of Energy
Office of Science Laboratory
Operated by The University of Chicago

World Energy Use

2100: 46 TW
2050: 30 TW Hoffert et al Nature 395, 883,1998

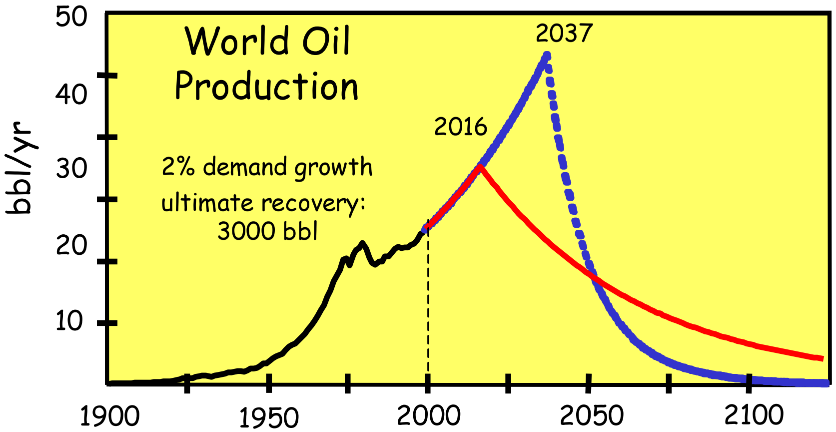




EIA Intl Energy Outlook 2004

Fossil Fuel Challenges

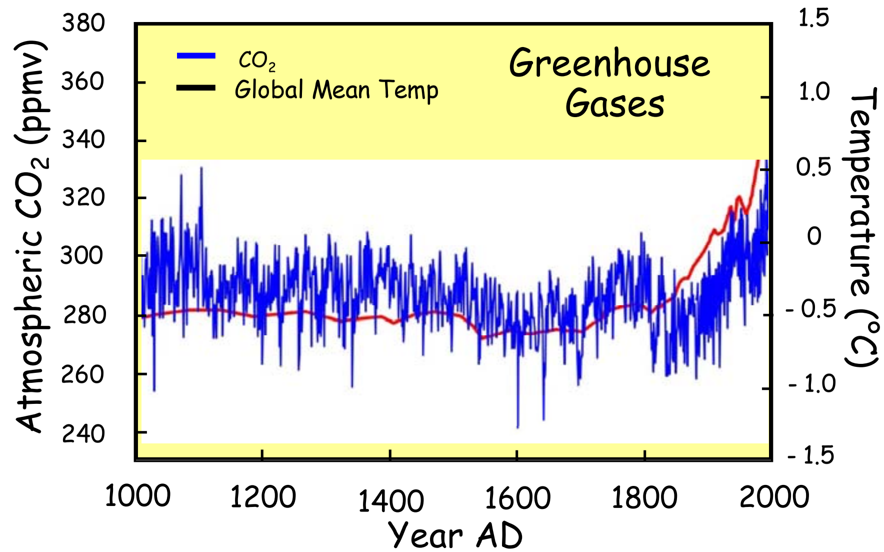
when will production peak?



EIA: http://tonto.eia.doe.gov/FTPROOT/presentations/long_term_supply/index.htm

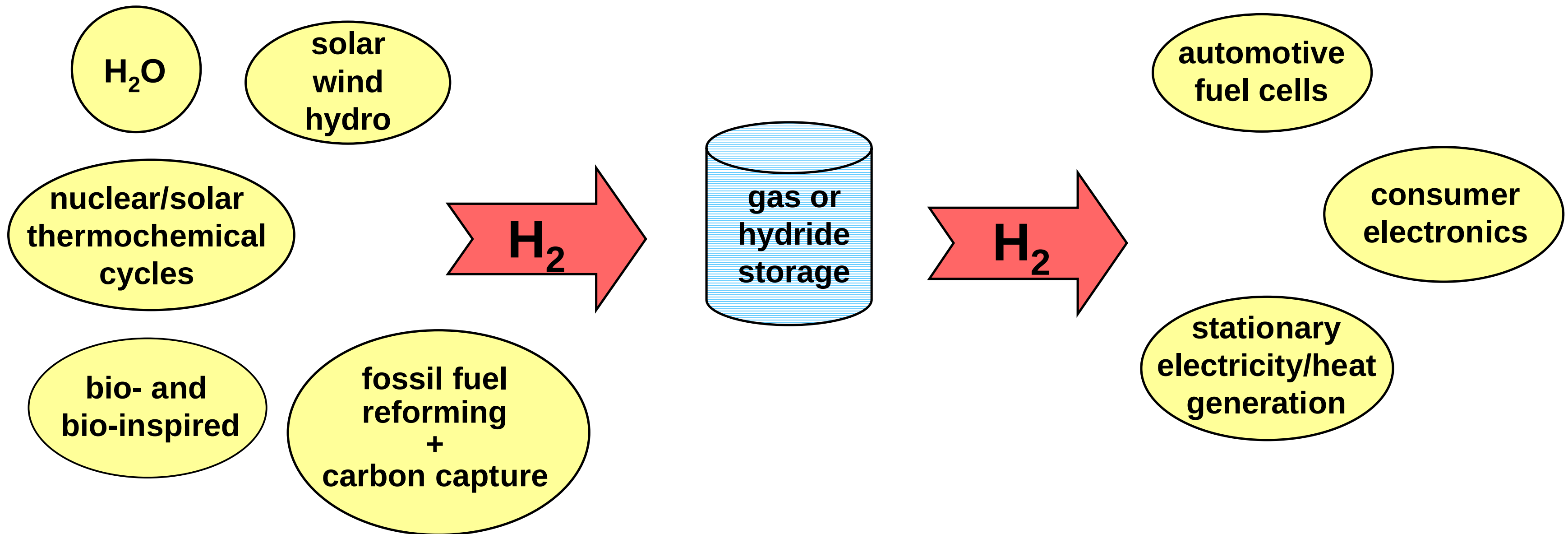
gas: beyond oil
coal: > 200 yrs

find alternate sources
nuclear
renewable



capture/store CO_2
cumulative effect
→ urgent problem
enables remaining
fossil fuel to be used

The Hydrogen Economy



production	*storage*	*use in fuel cells*
9M tons/yr ↓ 150 M tons/yr (light cars and trucks in 2040)	4.4 MJ/L (Gas, 10,000 psi) 8.4 MJ/L (LH2) ↓ 9.72 MJ/L (2015 FreedomCAR Target)	\$3000/kW ↓ \$35/kW (Internal Combustion Engine)

Fundamental Issues

The hydrogen economy is a compelling vision:

- It provides an abundant, clean, secure and flexible energy carrier
- 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
- The most optimistic estimates put the hydrogen economy decades away

Basic Research for Hydrogen Production, Storage and Use Workshop

May 13-15, 2003

Workshop Chair: **Millie Dresselhaus** (MIT)
Associate Chairs:N **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

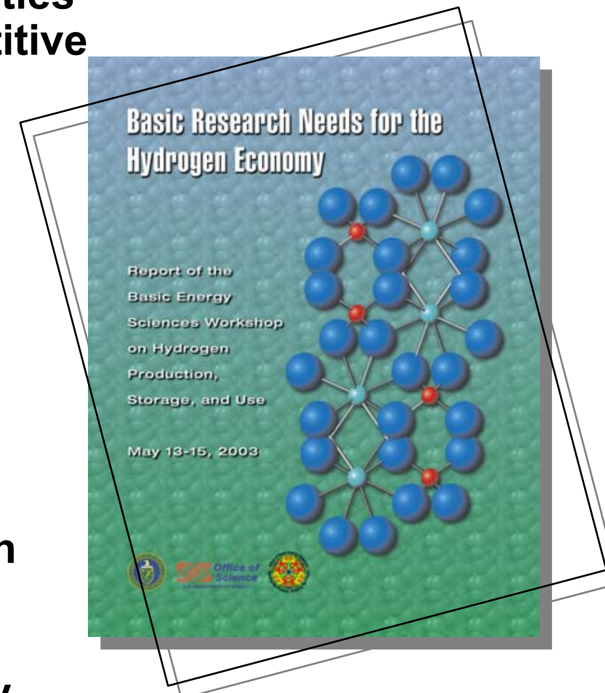
CHARGE

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.

Basic Research Needs for the Hydrogen Economy

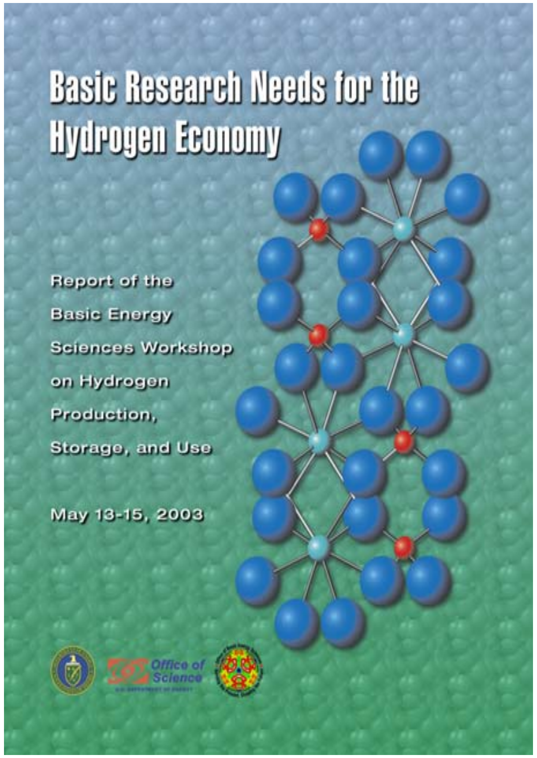
BES Report July 2003/Feb 2004

- Enormous 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 ⇒ 150M tons (vehicles)
  - storage: 4.4 MJ/L (10K psi gas) ⇒ 9.72 MJ/L
  - fuel cells: \$3000/kW ⇒ \$35/kW (gasoline engine)
- Enormous R&D efforts will be required
  - Simple improvements of today's technologies will not meet requirements
  - Technical barriers can be overcome only with high risk/high payoff basic research
- 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

Hydrogen Studies



Basic Energy Sciences
Department of Energy
July 2003/February 2004

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

THE HYDROGEN ECONOMY: OPPORTUNITIES, COSTS, BARRIERS AND R&D NEEDS

Committee on Alternatives and Strategies for Future Hydrogen Production and Use

Board on Energy and Environmental Systems
Division on Engineering and Physical Sciences

NATIONAL RESEARCH COUNCIL

NATIONAL ACADEMY OF ENGINEERING OF THE NATIONAL ACADEMIES

THE NATIONAL ACADEMIES PRESS
Washington, D.C.
www.nap.edu

National Research Council
National Academy of Sciences
February 2004

http://www.nap.edu/catalog/10922.html

APS PANEL ON PUBLIC AFFAIRS

March 2004

THE HYDROGEN INITIATIVE

Current technology is promising but not competitive. More emphasis needed on solving fundamental science problems.

Issue

President Bush has proposed a $1.2 billion Hydrogen Initiative that has a goal of developing a hydrogen-fueled car and supporting infrastructure by the year 2020.

Recommendations

Major scientific breakthroughs are required for the Hydrogen Initiative to succeed. Basic science must have greater emphasis both in planning and in the research program. The Hydrogen Technical Advisory Committee should include members who are deeply familiar with the core basic science problems. "Bridge" technologies should be given greater attention. And, the Hydrogen Initiative should not displace research into promising energy efficiency and renewable energy areas.

Detailed Recommendations: p11, 14

The APS

The American Physical Society is the nation's primary organization of research physicists with 43,000 members in industry, universities, and national laboratories.

APS Discussion Paper

The APS occasionally produces discussion papers on topics currently debated in Congress in order to inform the debate with the perspectives of physicists working in the relevant issue areas. The papers are overseen by the APS Panel on Public Affairs but have not been endorsed by the APS Council.

Executive Summary

In 2003, President Bush announced a multi-year $1.2 billion Hydrogen Initiative intended to reduce the nation's dependence on foreign oil through the production of hydrogen fuel and a hydrogen-fueled car. The Initiative has envisioned the competitive use of hydrogen in commercial transportation by the year 2020.

Currently, the US hydrogen industry produces 9,000,000 tons of hydrogen per year. Several hydrogen-fueling stations are scheduled to open this year. And, several models of hydrogen-fueled cars have been demonstrated.

However, none of the current technologies are competitive options for the consumer. The most promising hydrogen-engine technologies require factors of 10 to 100 improvements in cost or performance in order to be competitive. Further, hydrogen cannot simply be extracted from the air, ground or water – it must be produced. Yet, as the Secretary of Energy has stated, current hydrogen production methods are four times more expensive than gasoline. Finally, no material exists to construct a hydrogen fuel tank that meets the consumer benchmarks. A new material must be developed.

These are enormous performance gaps. Incremental improvements to existing technologies are not sufficient to close all the gaps. For the Hydrogen Initiative to succeed, major scientific breakthroughs are needed.

Basic science must have greater emphasis both in planning and in the research program. The Hydrogen Technical Advisory Committee should include members of the basic research community who are familiar with the relevant science problems. Further, given the multidisciplinary nature of the scientific problems involved, principal-investigator funded research should be complemented with the creation of several peer-reviewed, competitively bid, Research Centers that focus on the relevant research problems in hydrogen production, storage and use.

In the event that the timeline for hydrogen vehicles slips beyond 2020, there will be greater need for technologies that serve as a so-called "bridge" between the current fossil-fuel economy and any future hydrogen economy. Increasing the focus on basic science and engineering that advances such technologies would serve as a sensible hedge and at the same time maintain the development of technologies that show clear short-term promise. Similarly, the Hydrogen Initiative must not displace research into promising energy efficiency and renewable energy areas.

► Contact: Francis Slakey, Associate Director of Public Affairs, American Physical Society (202) 662-8700 ◄

American Physical Society
Panel on Public Affairs
March 2004

http://www.aps.org/public_affairs/index.cfm

Hydrogen Studies

universal finding:

the hydrogen economy requires
breakthrough basic research to find new materials and processes

incremental advances in the present state of the art
will not meet the challenge

Priority Research Areas in Hydrogen Production

Fossil Fuel Reforming

Molecular level understanding of catalytic mechanisms, nanoscale catalyst design, high temperature gas separation

Solar Photoelectrochemistry/Photocatalysis

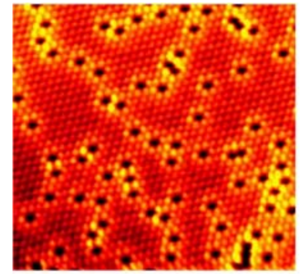
Light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis and photocatalysis, organic semiconductors, theory and modeling, and stability

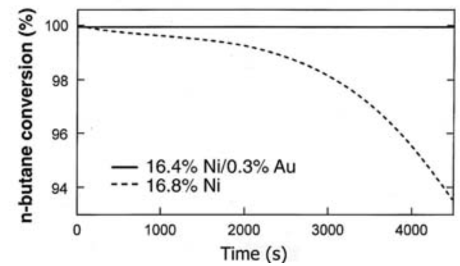
Bio- and Bio-inspired H_2 Production

Microbes & component redox enzymes, nanostructured 2D & 3D hydrogen/oxygen catalysis, sensing, and energy transduction, engineer robust biological and biomimetic H_2 production systems

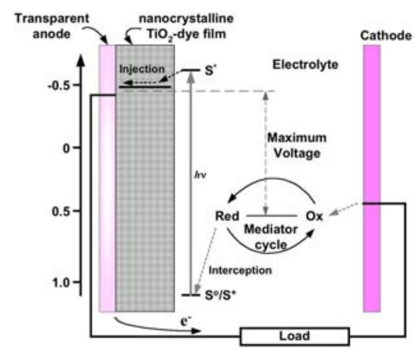
Nuclear and Solar Thermal Hydrogen

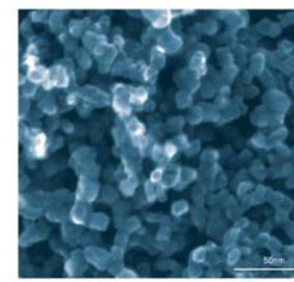
Thermodynamic data and modeling for thermochemical cycle (TC), high temperature materials: membranes, TC heat exchanger materials, gas separation, improved catalysts



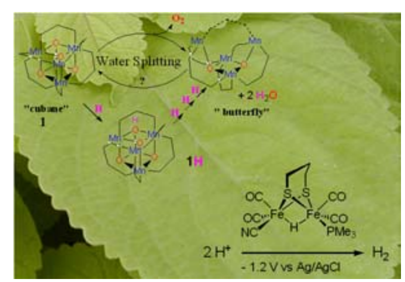


Ni surface-alloyed with Au to reduce carbon poisoning





Dye-Sensitized Solar Cells



Synthetic Catalysts for Water Oxidation and Hydrogen Activation

Priority Research Areas in Hydrogen Storage

Metal Hydrides and Complex Hydrides

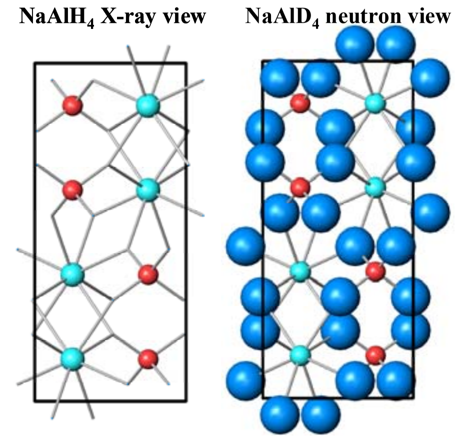
Degradation, thermophysical properties, effects of surfaces, processing, dopants, and catalysts in improving kinetics, nanostructured composites

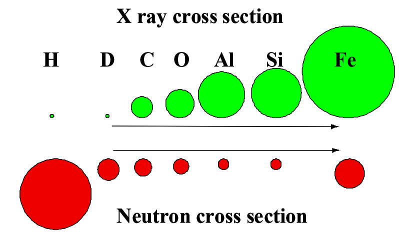
Nanoscale/Novel Materials

Finite size, shape, and curvature effects on electronic states, thermodynamics, and bonding, heterogeneous compositions and structures, catalyzed dissociation and interior storage phase

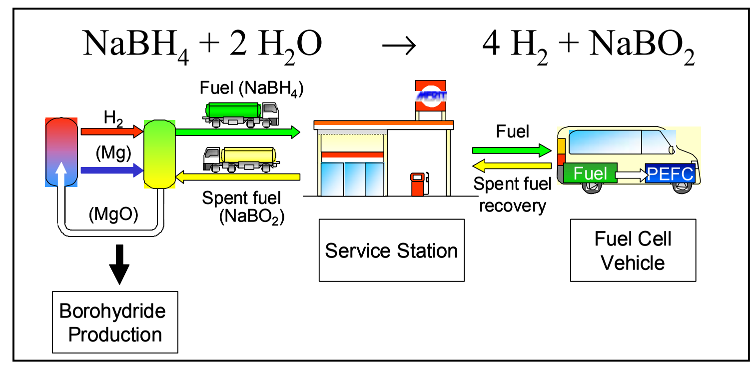
Theory and Modeling

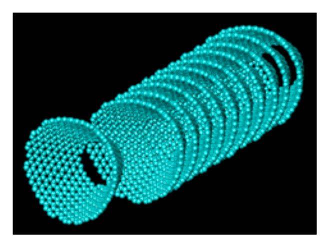
Model systems for benchmarking against calculations at all length scales, integrating disparate time & length scales, first principles methods applicable to condensed phases



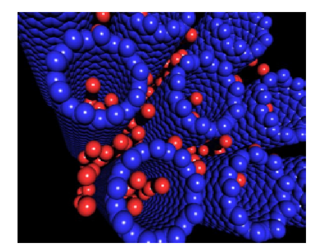


Neutron Imaging of Hydrogen



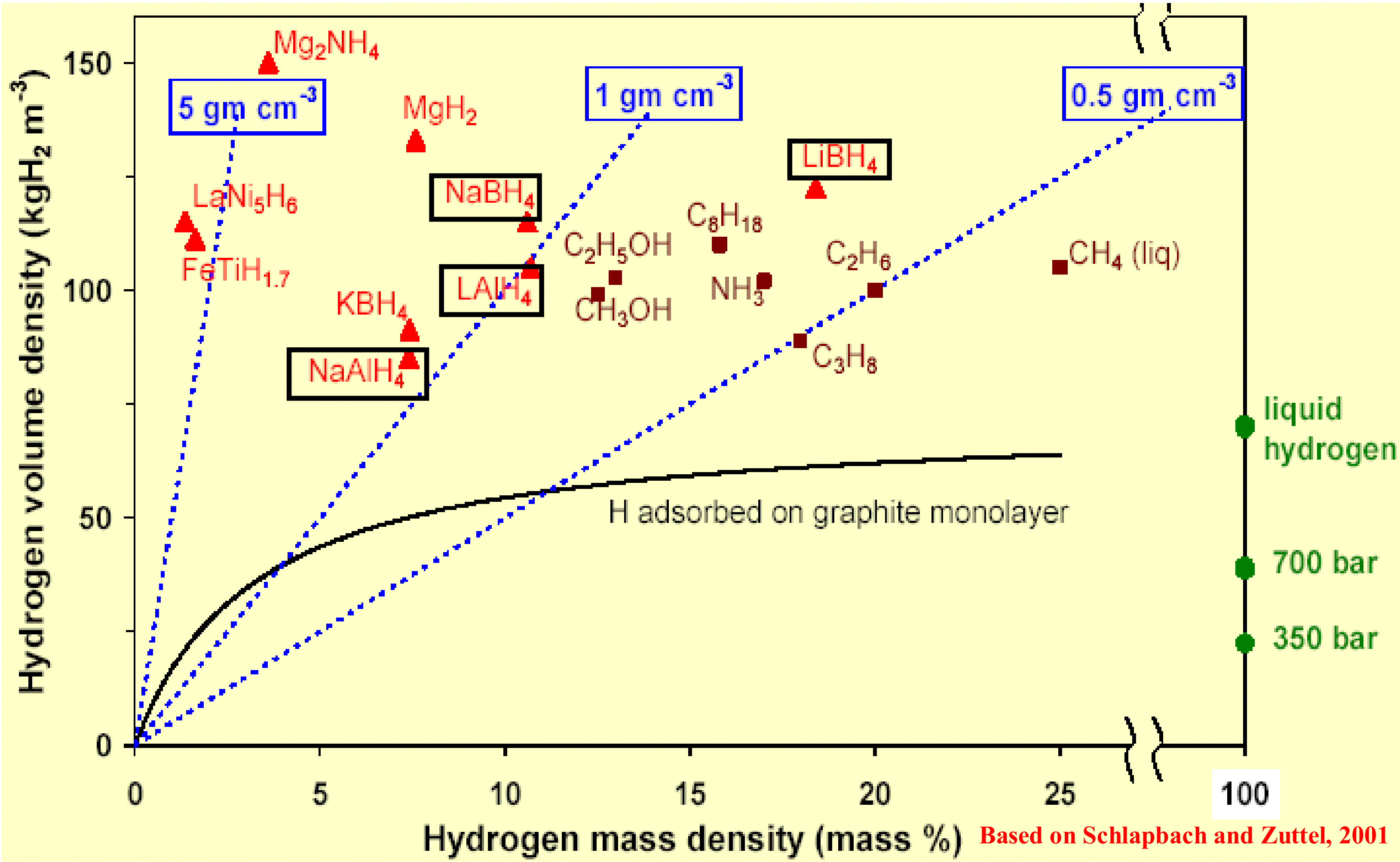


Cup-Stacked Carbon Nanofiber



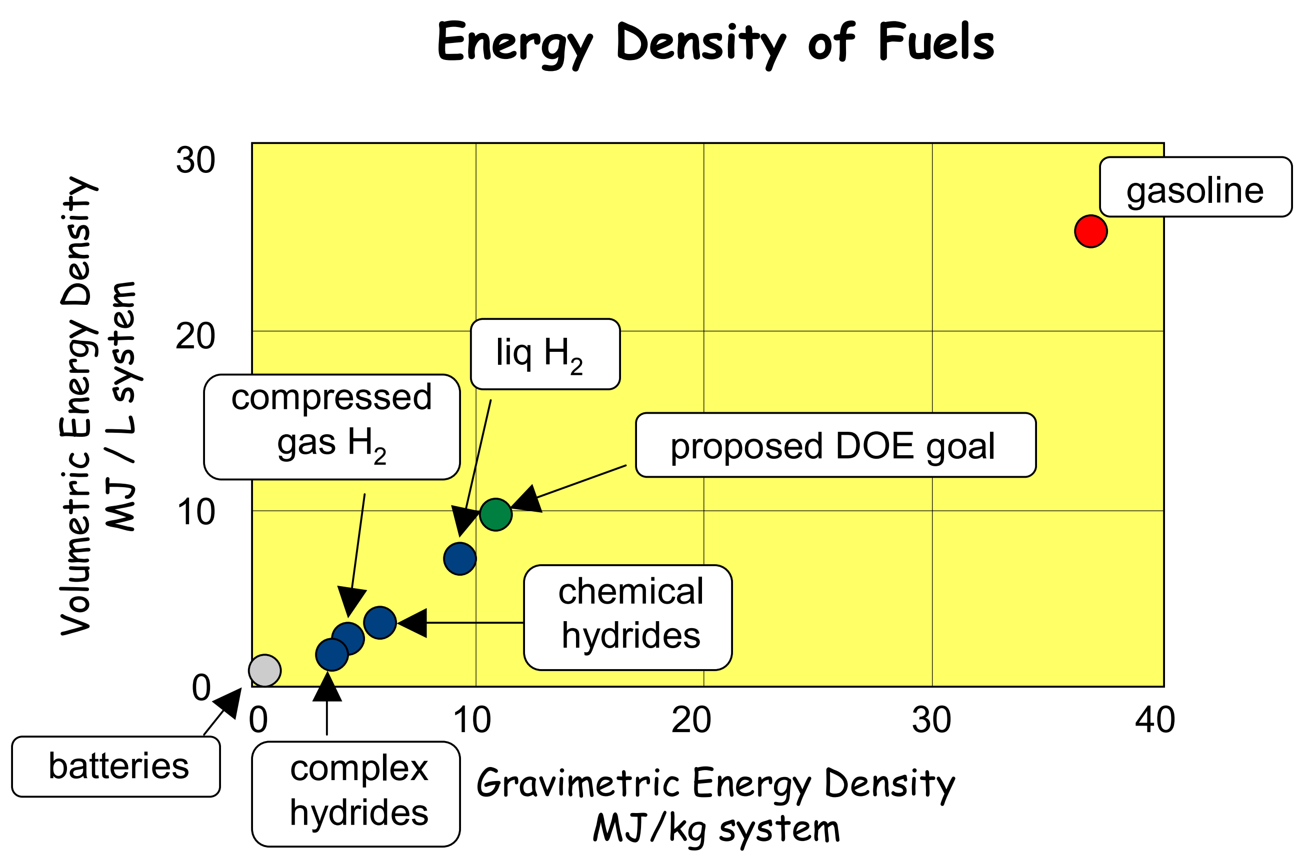
H Adsorption in Nanotube Array

High Hydrogen Density Materials



Based on Schlapbach and Zuttel, 2001

Energy Storage: the Fossil Fuel Challenge



Priority Research Areas in Fuel Cells

Electrocatalysts and Membranes

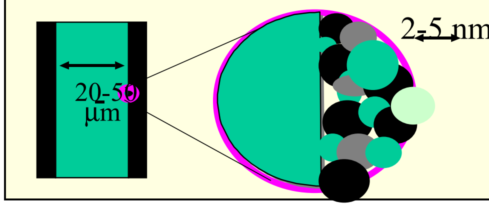
Oxygen reduction cathodes, minimize rare metal usage in cathodes and anodes, synthesis and processing of designed triple percolation electrodes

Low Temperature Fuel Cells

'Higher' temperature proton conducting membranes, degradation mechanisms, functionalizing materials with tailored nano-structures

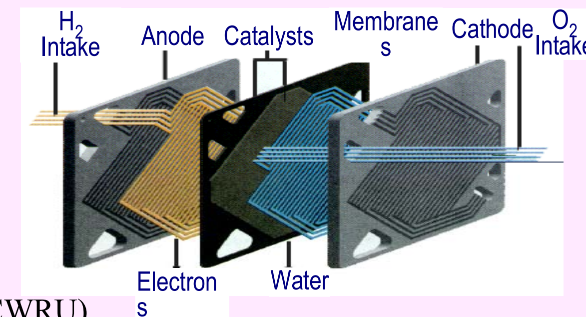
Solid Oxide Fuel Cells

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



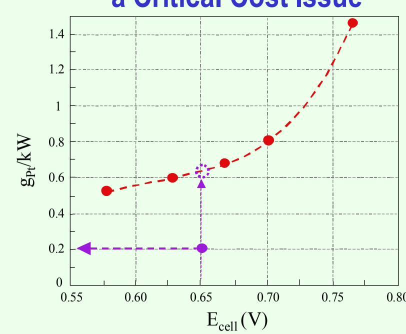
Controlled design of triple percolation nanoscale networks: ions, electrons, and porosity for gases

Internal view of a PEM fuel cell



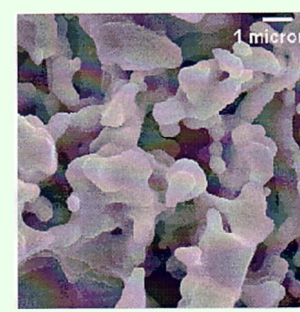
Source: T. Zawodzinski (CWRU)

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



Source: H. Gasteiger (General Motors)

YSZ Electrolyte for SOFCs

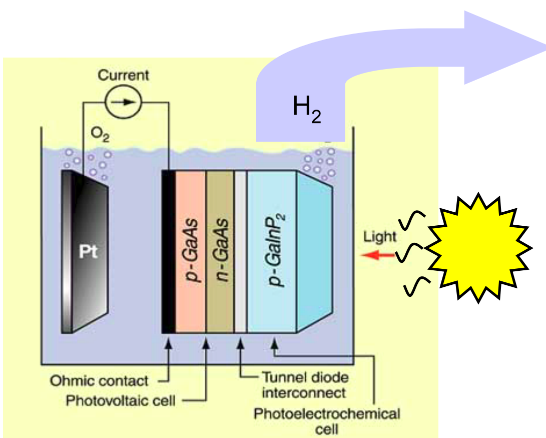


Porosity can be tailored

Source: R. Gorte (U. Penn)

Materials: the Cross-cutting Issue

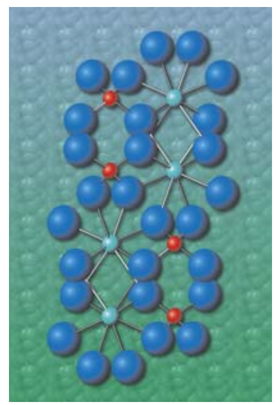
the challenge: understand and control the interaction of hydrogen with materials



John Turner, NREL

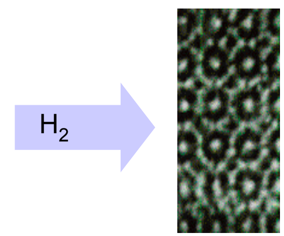
sunlight + $H_2O \rightarrow H_2 + O_2$

transparent semiconductor layers
nanoscale catalysts
nanostructured interfaces



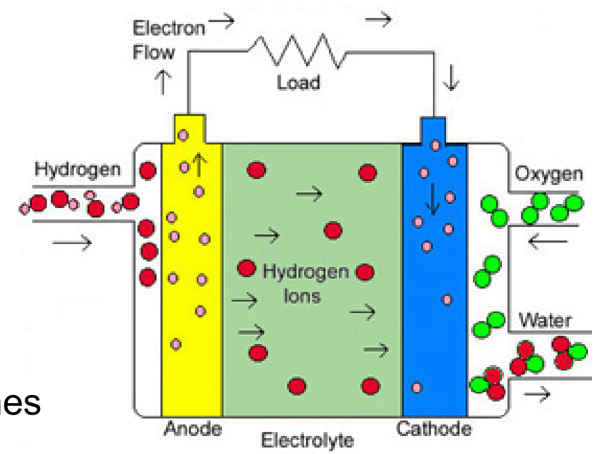
$H_2 \rightarrow NaAlH_4$

new H storage materials
catalytic reactions
nanoscale architecture



membranes

molecular separation of
H_2, O_2, CO, H_2O, CO_2



$H_2 + O_2 \rightarrow H_2O$

fuel cell catalysts
ionic membranes
nanoscale architecture

catalysts, nanoscale composites, membranes needed throughout

Useful References

International Energy Outlook 2004 (Energy Information Administration)
http://www.eia.doe.gov/oiaf/ieo/index.html

Basic Research Needs for the Hydrogen Economy, 2004 (DOE/BES)
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National Hydrogen Energy Roadmap (DOE/EERE)
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