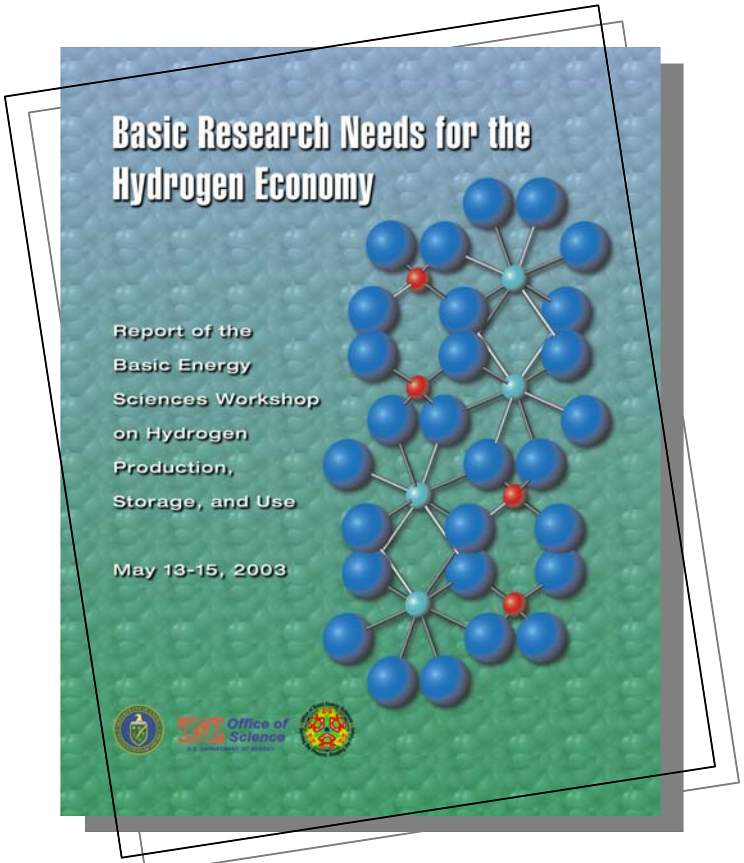
Basic Research Needs for the Hydrogen Economy



March 23, 2004
APS March Meeting
Montreal, Canada

Presented by:
Mildred Dresselhaus
Massachusetts Institute of Technology
millie@mgm.mit.edu
617-253-6864

Hydrogen: A National Initiative

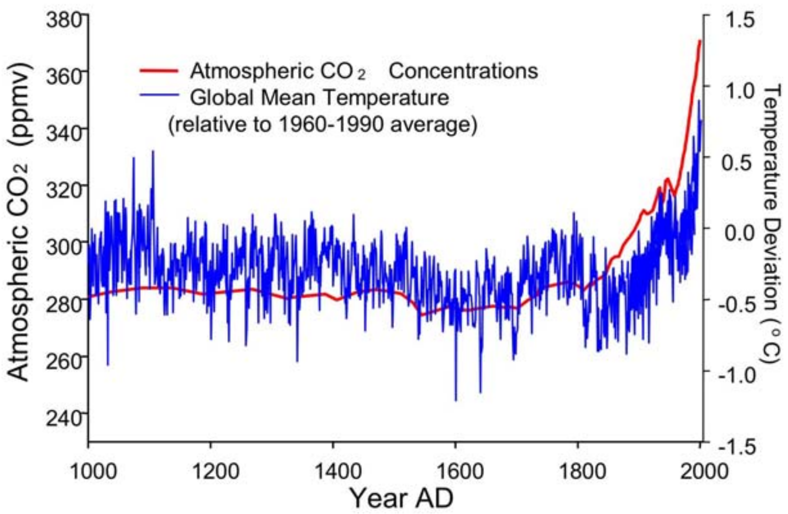
"Tonight I'm proposing $1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles… With a new national commitment, our scientists and engineers will overcome obstacles to taking these cars from laboratory to showroom, so that the first car driven by a child born today could be powered by hydrogen, and pollution-free."

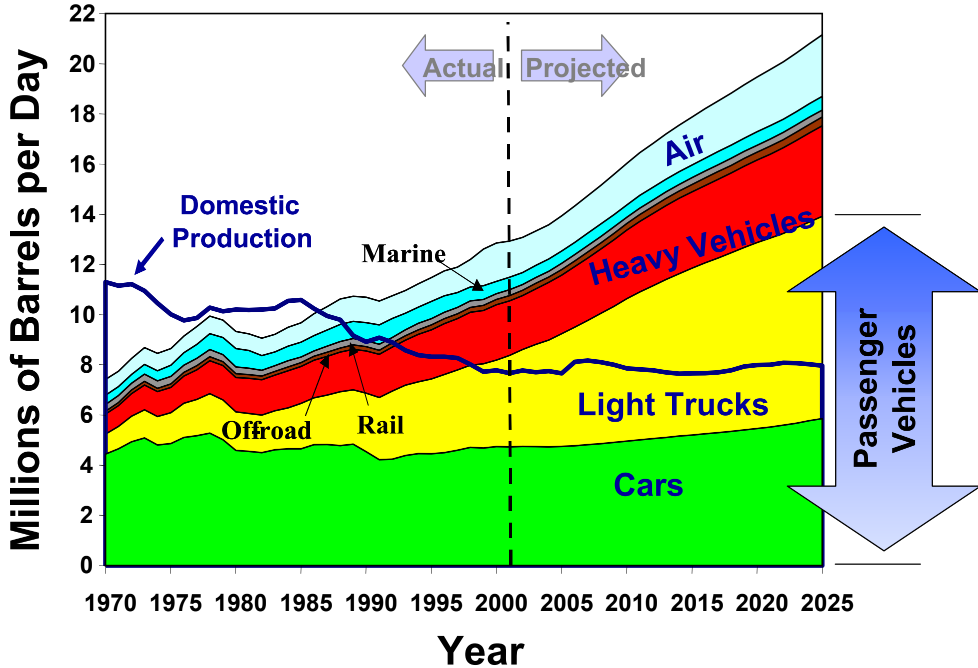
President Bush, State-of the-Union Address, January 28, 2003

Drivers for the Hydrogen Economy:

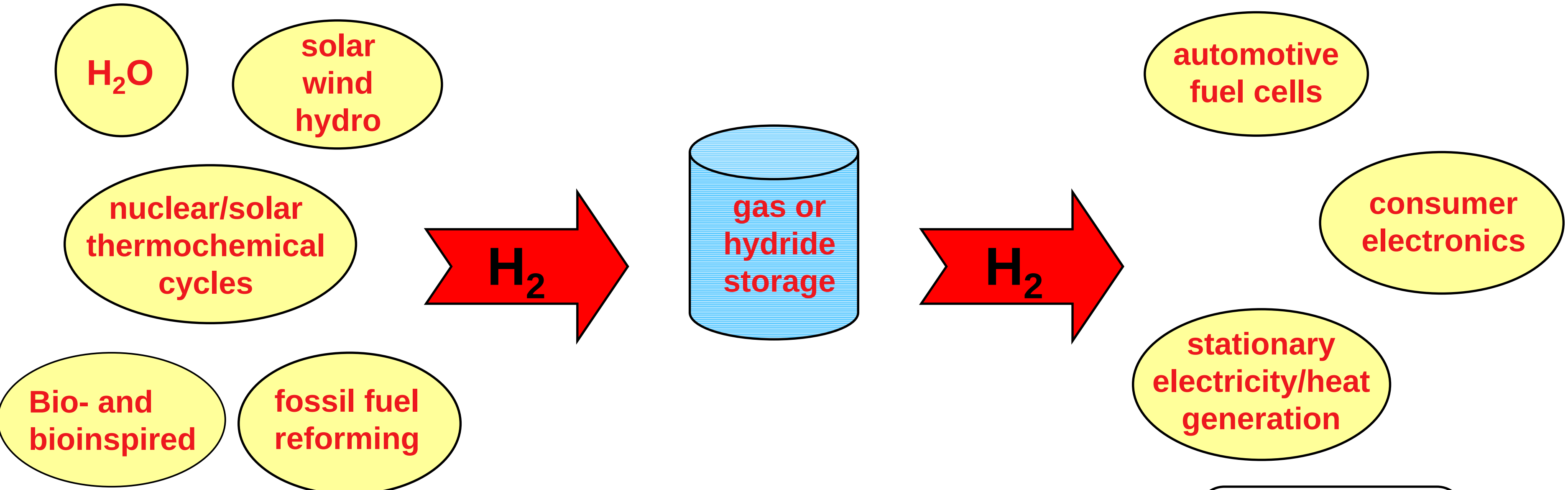
- Reduce Reliance on Fossil Fuels
- Reduce Accumulation of Greenhouse Gases

Energy Source	% of U.S. Electricity Supply	% of Total U.S. Energy Supply
Oil	3	39
Natural Gas	15	23
Coal	51	22
Nuclear	20	8
Hydroelectric	8	4
Biomass	1	3
Other Renewables	1	1





The Hydrogen Economy



production	storage	use in fuel cells
9M tons/yr	4.4 MJ/L (Gas, 10,000 psi) 8.4 MJ/L (LH2)	\$3000/kW
↓	↓	↓
40M tons/yr (Transportation only)	9.72 MJ/L (2015 FreedomCARTarget)	\$35/kW (Internal Combustion Engine)

Fundamental Issues

The hydrogen economy is a compelling vision:

- It potentially 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

Requirements of a Hydrogen Economy

- Safe, efficient, and economical means for
  - hydrogen production
  - storage/distribution
  - use
- In all these sectors, present knowledge and technology fall far short of US Department of Energy technical and cost requirements.
- An aggressive basic research program is needed, especially in gaining a fundamental understanding of the interaction between hydrogen and materials.

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.

Basic Research for Hydrogen Production, Storage and Use Workshop

125 Participants:

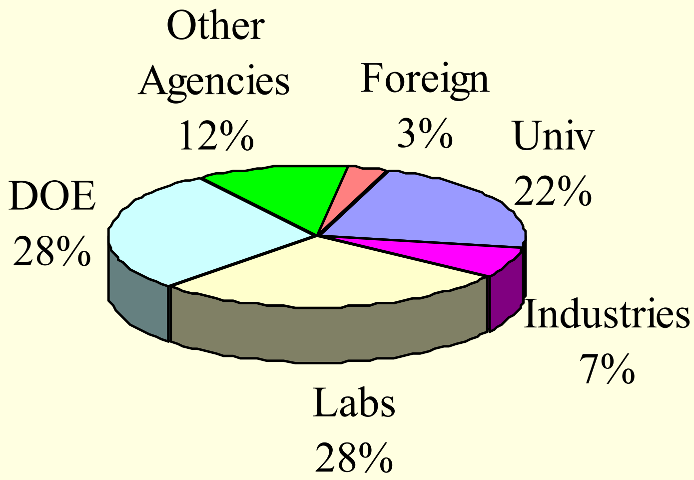
Universities

National Laboratories

Industries

DOE: SC and Technology Program Offices

Other Federal Agencies - including OMB, OSTP, NRL, NIST, NSF, NAS, USDA, and House Science Committee Staffer



Remarks from News Reporters:

American Institute of Physics Bulletin of Science Policy News Number 71

"Dresselhaus remarked that there were some "very promising" ideas, and she was more optimistic after the workshop that some of the potential showstoppers may have solutions." "… solving the problems will need long-term support across several Administrations. Progress will require the cooperation of different offices within DOE, and also the involvement of scientists from other countries, …"

C&E News June 9, 2003

"MOVING TOWARD A HYDROGEN ECONOMY" DOE Workshop Brings Together Scientists to Prioritize Research Needs for Switching to Hydrogen Economy.

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

Hydrogen Production Panel

Panel Chairs: Tom Mallouk (Penn State), Laurie Mets (U of Chicago)

Current status:

- Steam-reforming of oil and natural gas produces 9M tons H_2/yr
- We will need 40M tons/yr for transportation
- Requires CO_2 sequestration.

Alternative sources and technologies:

Coal:

- Cheap, lower H_2 yield/C, more contaminants
- Research and Development needed for process development, gas separations, catalysis, impurity removal.

Solar:

- Widely distributed carbon-neutral; low energy density.
- Photovoltaic/electrolysis current standard – 15% efficient
- Requires 0.03% of land area to serve transportation.

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

DOE/EERE Production Goal and Objectives

Goal : Research and develop low cost, highly efficient hydrogen production technologies from diverse, domestic sources, including fossil, nuclear, and renewable sources.

Objectives for 2010

- By 2010: Reduce the cost of distributed production of hydrogen from natural gas and/or liquid fuels to $1.50/gallon gasoline equivalent (**$1.50/kg**) delivered, untaxed, at the pump [without carbon sequestration];
- By 2010: Develop and verify technology to supply purified hydrogen from biomass at **$2.60/kg** at the plant gate. The objective is to be **competitive** with gasoline by 2015.
- By 2010: Develop and verify renewable integrated hydrogen production with water electrolysis at a hydrogen cost of **$2.50/kg** with electrolyser capital of $300/kWe for 250 kg/day and 73% system efficiency.

Mark Paster, DOE/EERE

DOE/EERE Production Goal and Objectives

- Develop advanced renewable photolytic hydrogen generation technologies.
  - By 2015: Demonstrate direct photoelectrochemical water splitting with a plant-gate hydrogen production cost of **$5/kg**
  - By 2015: Demonstrate an engineering-scale photobiological system which produces hydrogen at a plant-gate cost of **$10/kg**.

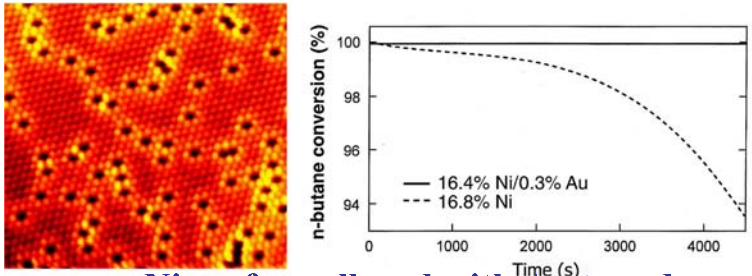
  The long term objective for these production routes is to be **competitive** with gasoline.

- By 2015: Research and develop high and ultra-high temperature thermochemical water splitting processes to convert hydrogen from high temperature heat sources (nuclear,solar, other) with a projected cost **competitive** with gasoline.

Priority Research Areas in Hydrogen Production

Fossil Fuel Reforming

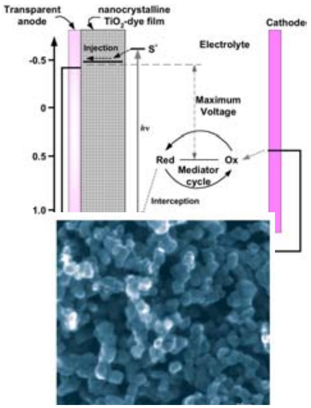
Molecular level understanding of catalytic mechanisms, nanoscale catalyst design, high temperature gas separation



Ni surface-alloyed with Au to reduce carbon poisoning

Solar Photoelectrochemistry/Photocatalysis

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



Dye-Sensitized Solar Cells

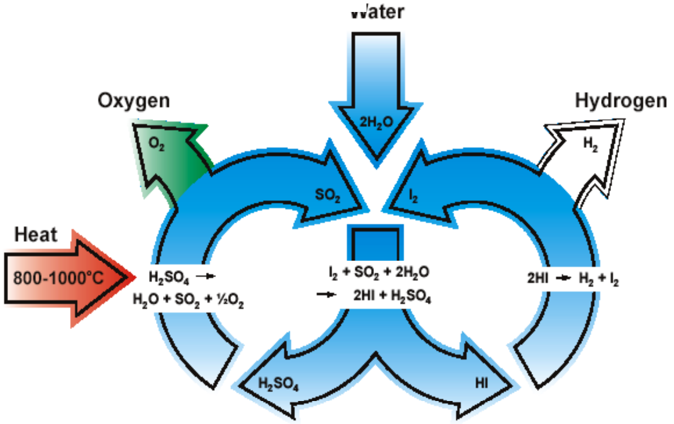
Bio- and Bio-inspired H_2 Production

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

Synthetic Catalysts for H_2 Production

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



Thermochemical Water Splitting

Hydrogen Storage Panel

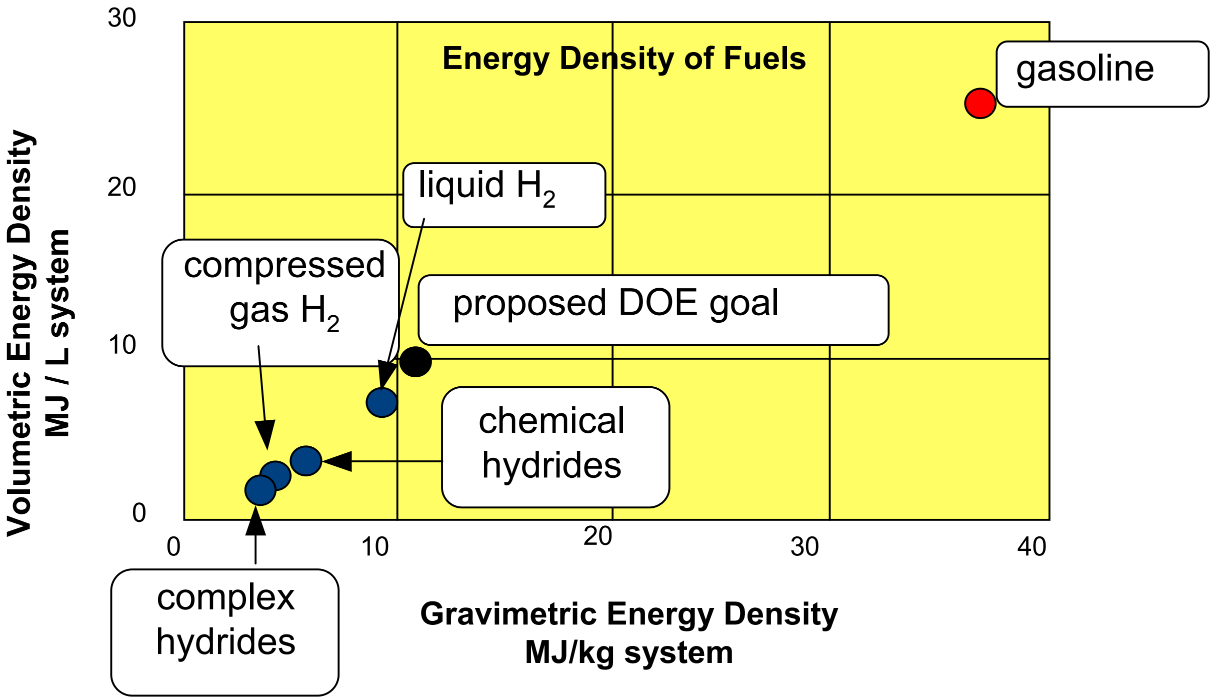
Panel Chairs: Kathy Taylor (GM, Retired) and Puru Jena (Virginia Commonwealth U)

Current Technology for automotive applications

- Tanks for gaseous or liquid hydrogen storage.
- Progress demonstrated in solid state storage materials.

System Requirements

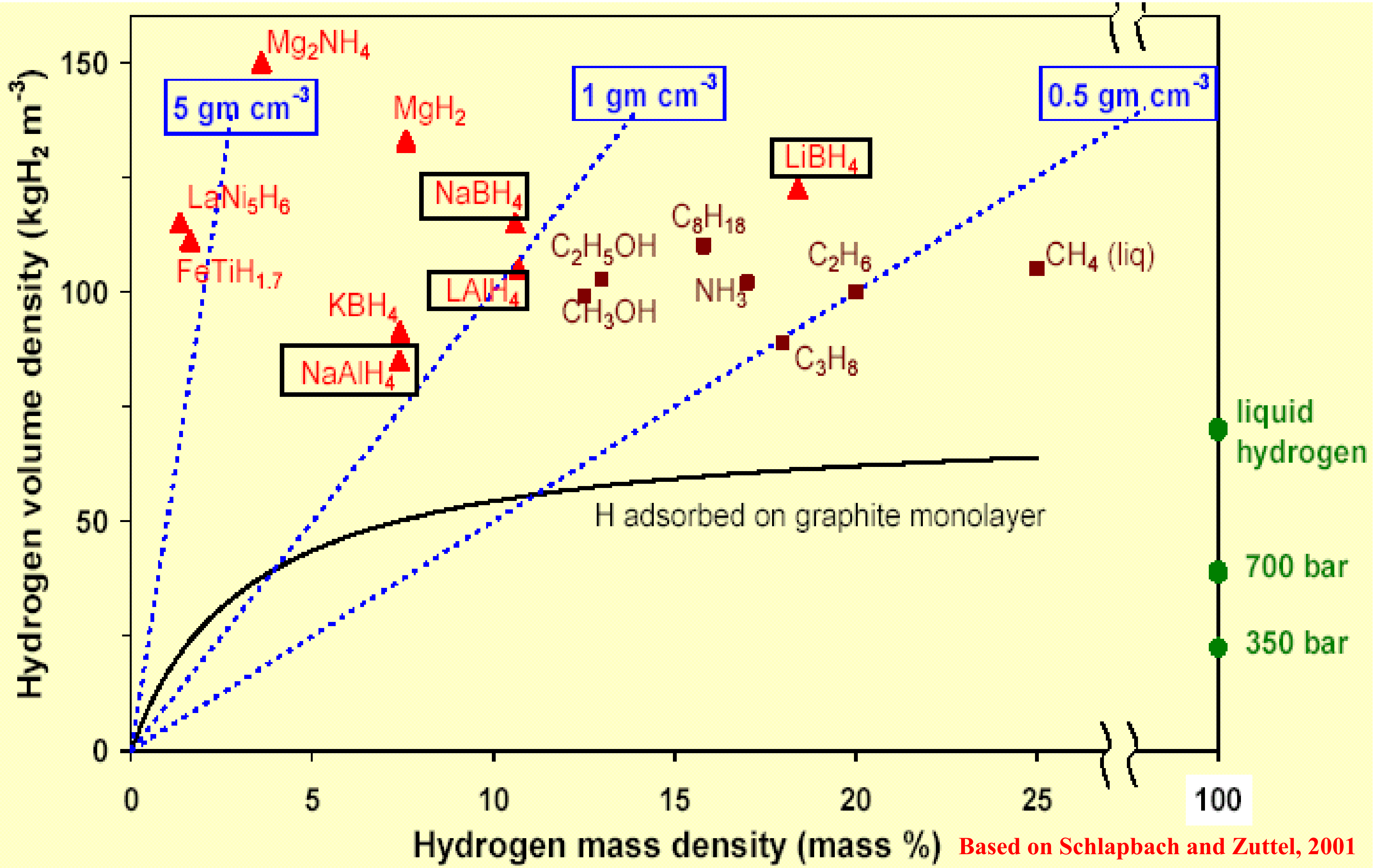
- Compact, light-weight, affordable storage.
- System requirements set for FreedomCAR: 4.5 wt% hydrogen for 2005, 9 wt% hydrogen for 2015.
- No current storage system or material meets all targets.



Ideal Solid State Storage Material

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

High Gravimetric H Density Candidates



Based on Schlapbach and Zuttel, 2001

FreedomCAR Hydrogen Storage System Targets

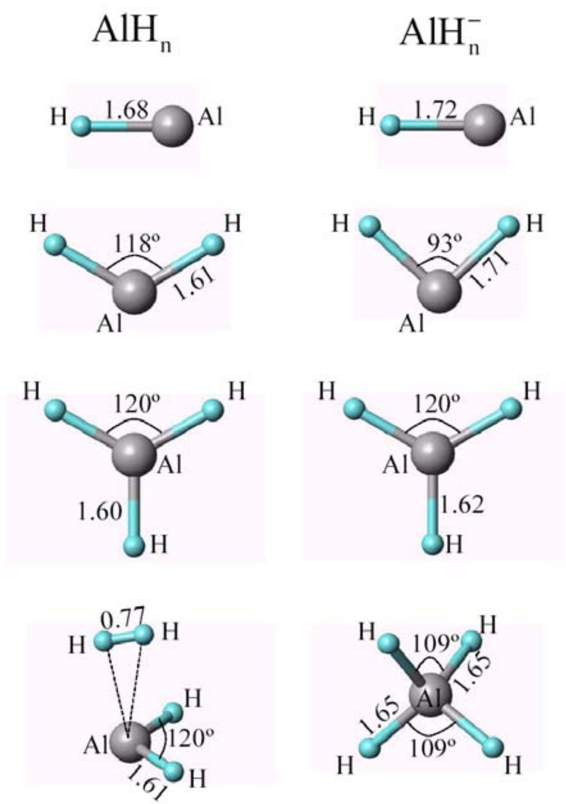
	2005	2010	2015
• specific energy (MJ/kg)	5.4	7.2	10.8
weight percent hydrogen	4.5%	6.0%	9.0%
• energy density (MJ/liter)	4.3	5.4	9.72
• system cost (\$/kg H_2)	200	133	67
• operating temperature (°C)	-20/50	-30/50	-40/60
• cycle life (cycles)	500	1000	1500
• flow rate (g/sec)	3	4	5
• Max delivery pressure (Atm)	100	100	100
• transient response (sec)	1.75	0.75	0.5
• refueling rate (kg H2/min)	0.5	1.5	2.0

- loss, permeation, leakage, toxicity, safety

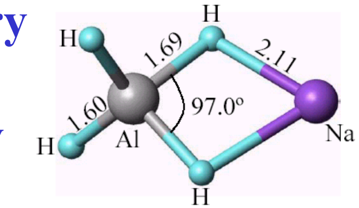
JoAnn Milliken, DOE/EERE

Theory and Modeling

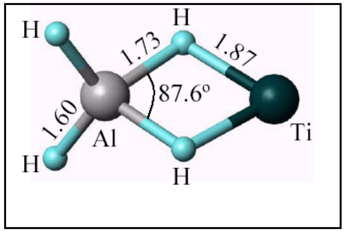
Model systems for benchmarking against calculations at all length scales, integrating disparate time and length scales, first principles methods applicable to condensed phases

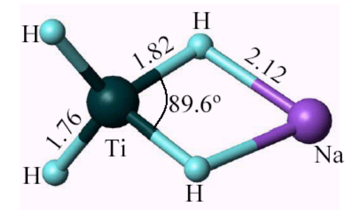


First principles density functional theory shows that neutral AlH_4 dissociates into $AlH_2 + H_2$ but that ionized AlH_4^- tightly binds 4 hydrogens.



Calculations further show that Ti substitutes for Na in $NaAlH_4$ and weakens the Al-H ionic bond, thus making it possible to lower the temperature of H_2 desorption from 200°C to 120°C.





(unpublished calculations of P. Jena, co-chair of Hydrogen Storage Panel).

Priority Research Areas in Hydrogen Storage

Metal Hydrides and Complex Hydrides

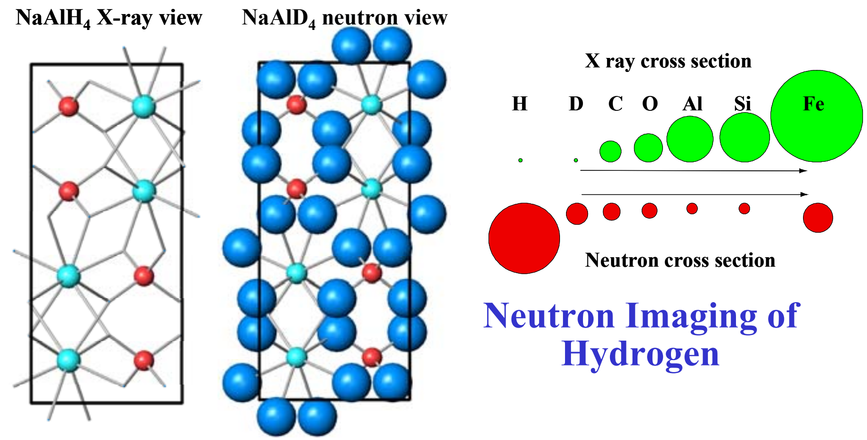
Degradation, thermophysical properties, effects of surfaces, processing, dopants, and catalysts in improving kinetics, nanostructured composites

Nanoscale/Novel Materials

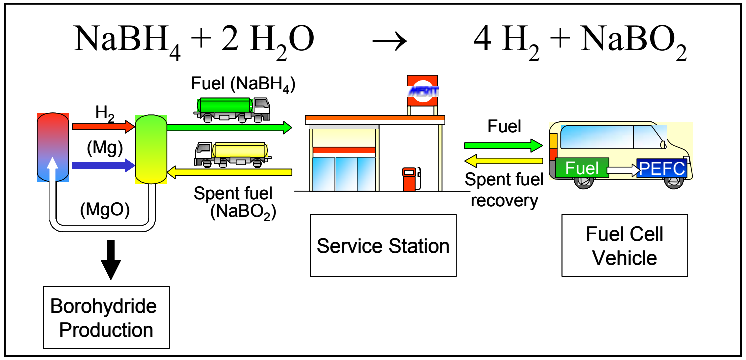
Finite size, shape, and curvature effects on electronic states, thermodynamics, and bonding, heterogeneous compositions and structures, catalyzed dissociation and interior storage phase

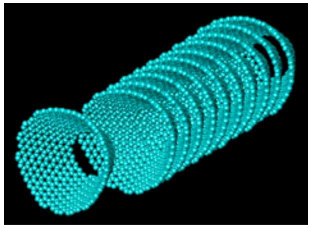
Theory and Modeling

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

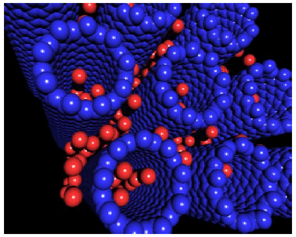


Neutron Imaging of Hydrogen





Cup-Stacked Carbon Nanofiber



H Adsorption in Nanotube Array

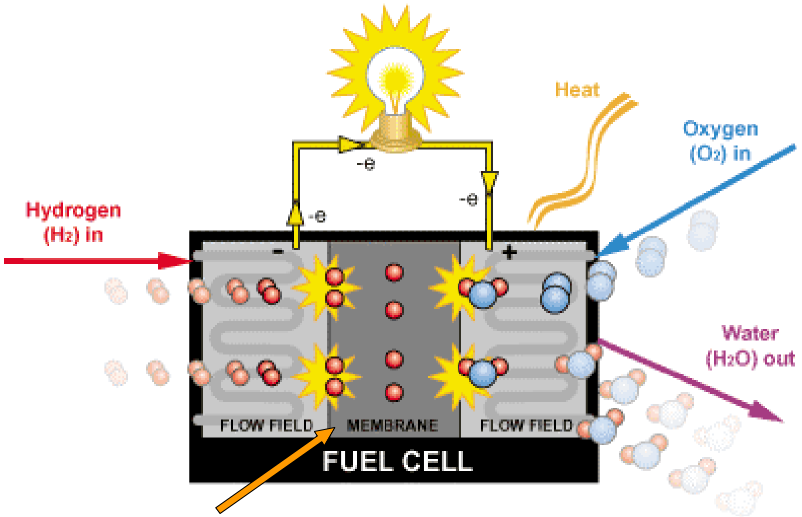
Fuel Cells and Novel Fuel Cell Materials Panel

Panel Chairs: Frank DiSalvo (Cornell), Tom Zawodzinski (Case Western Reserve)

$2H_2 + O_2 \rightarrow 2H_2O$ + electrical power + heat

Current status:

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



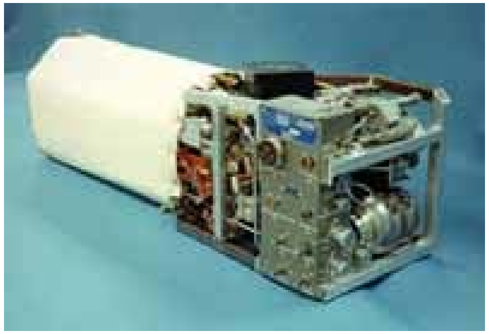
Membrane conducts protons from anode to cathode
proton exchange membrane (PEM)

Challenges:

- Membranes
  - Operation in lower humidity, strength and durability.
  - Higher ionic conductivity.
- Cathodes
  - Materials with lower overpotential and resistance to impurities.
  - Low temperature operation needs cheaper (non- Pt) materials.
  - Tolerance to impurities: CO, S, hydrocarbons.
- Reformers
  - Need low temperature and inexpensive reformer catalysts.

Types of Fuel Cells

Phosphoric Acid FC
(PAFC), 250 kW
United Technologies



Alkaline Fuel Cell
(AFC), Space Shuttle
12 kW
United Technologies

Low-Temp

High Temp

Proton Exchange
Membrane (PEM)
50 kW, Ballard

Solid Oxide FC
(SOFC) 100 kW
Siemens-
Westinghouse

Molten Carbonate FC
(MCFC) 250 kW
FuelCell Energy,

Technical targets: 50 kWe (net) integrated fuel cell power systems operating on direct hydrogen[a]

All targets must be achieved simultaneously and are consistent with those of FreedomCAR

Nancy Garland, DOE/EERE

	Units	Status	2005	2010
Energy efficiency @ rated power	%	50	50	50
Power density				
excluding H_2 storage	W/L	400	500	650
including H_2 storage	W/L	TBD	150	220
Specific power				
excluding H_2 storage	W/kg	400	500	650
including H_2 storage	W/kg	TBD	250	325
Cost[c] (including H_2 storage)	**$/kW**	**200**	**125**	**45**
Transient response (10% to 90% of rated power)	s	3	2	1
Cold start-up time to maximum power				
@ –20°C ambient temperature	s	120	60	30
@+20°C ambient temperature	s	60	30	15
Emissions		Zero	Zero	Zero
Durability[d]	**hours**	**1000**	**2000[e]**	**5000[f]**
Survivability[g]	°C	–20	–30	–40

[a]Targets are based on hydrogen storage targets in an aerodynamic 2500-lb vehicle.
[b]Ratio of DC output energy to the lower heating value of the input fuel (hydrogen).
[c]Includes projected cost advantage of high-volume production (500,000 units per year).
[d]Performance targets must be achieved at the end of the durability time period.
[e]Includes thermal cycling.
[f]Includes thermal and realistic drive cycles.
[g]Achieve performance targets at 8-hour cold-soak at temperature.

The Challenge – ≤ $45/kW for 50-kW Gasoline-Fueled PEMFC Integrated System

Subsystem	2005 Target[a]	2010 Target[a]	2003 Status[a,b]
Fuel Cell	$100	$35	$200
Fuel Processor	$25	$10	$65
BOP/ Assembly	(c)	(c)	$35
Total[d]	$125	$45	$300

a. HFCIT MYPP Draft March 2003
b. Based on TIAX and Directed Technologies cost studies
c. BOP/Assembly in fuel cell & fuel processor
d. High-volume projections

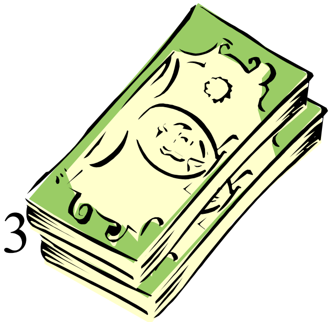
Show Me The Money

$ MEA and bipolar plate materials and fabrication techniques
20-30 %

$ Increased stack power density by operation at lower voltage, higher current (also lowers system efficiency)
20-25 %

$Reduce Platinum Group Metals in stack and fuel processor
15-20 %

Non-PGM Electrocatalyst Workshop March 21-22, 2003

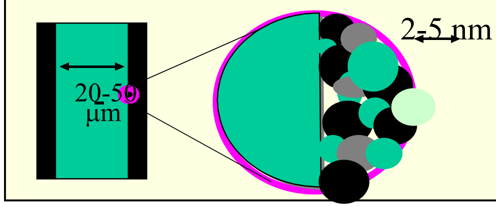


Nancy Garland, DOE/EERE

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

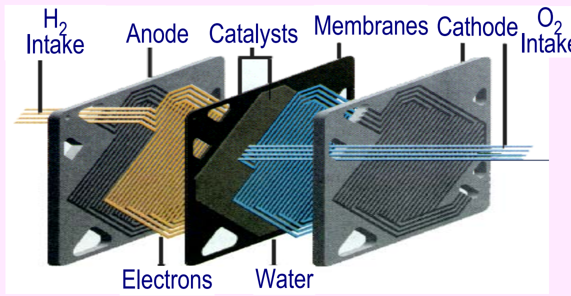


Controlled design of triple percolation nanoscale networks: ions, electrons, and porosity for gases

Low Temperature Fuel Cells

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

Internal view of a PEM fuel cell

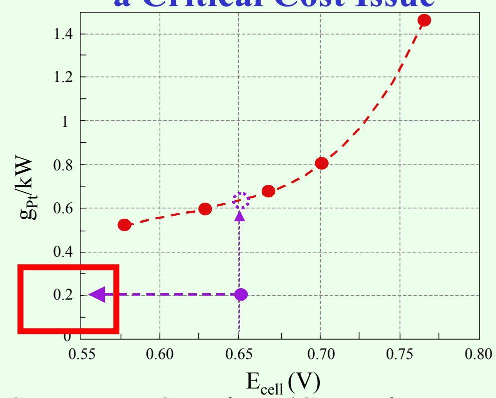


Source: T. Zawodzinski (CWRU)

Solid Oxide Fuel Cells

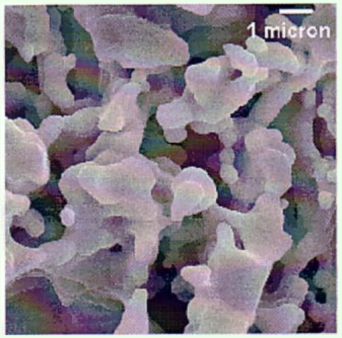
Theory, modeling and simulation, validated by experiment, for electrochemical materials and processes, new materials-all components, novel synthesis routes for optimized architectures, advanced in-situ analytical tools

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)

High Priority Research Directions for Hydrogen Economy

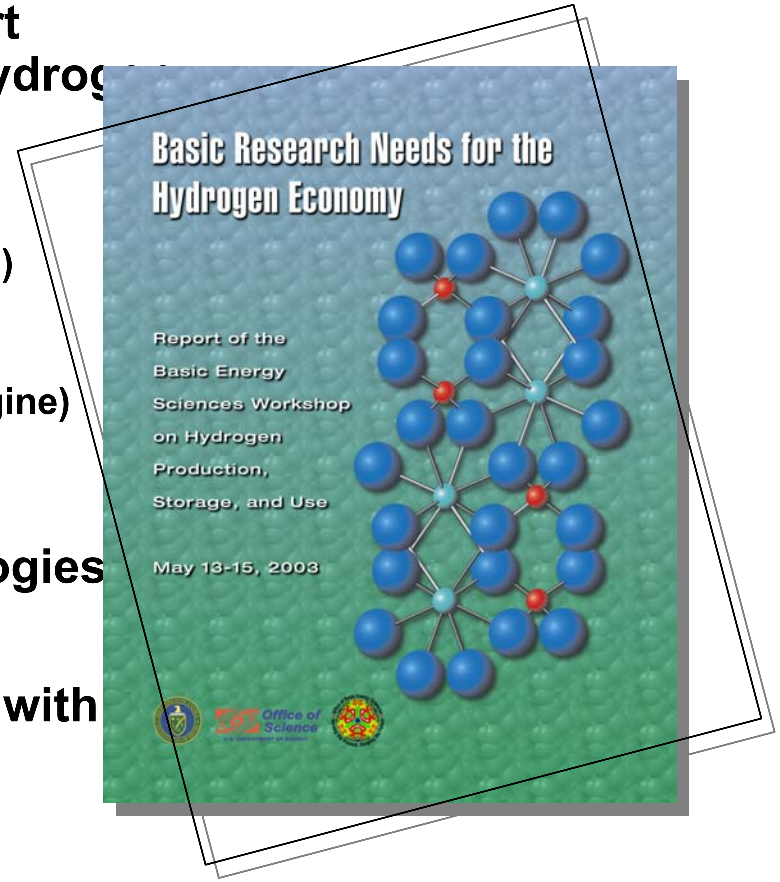
- Low-cost and efficient solar energy production of hydrogen
- Nanoscale catalyst design
- Biological, biomimetic, and bio-inspired materials and processes
- Complex hydride materials for hydrogen storage
- Nanostructured / novel hydrogen storage materials
- Low-cost, highly active, durable cathodes for low-temperature fuel cells
- Membranes and separations processes for hydrogen production and fuel cells

Cross-Cutting Research Directions

- **Catalysis**
  - hydrocarbon reforming
  - hydrogen storage kinetics
  - fuel cell and electrolysis electrochemistry
- **Membranes and Separation**
- **Nanoscale Materials and Nanostructured Assemblies**
- **Characterization and Measurement Techniques**
- **Theory, Modeling and Simulations**
- **Safety and Environment**

Messages

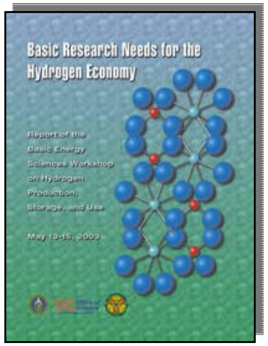
- Enormous gap between present state-of-the-art capabilities and requirements that will allow hydrogen to be competitive with today's energy technologies
  - production: 9M tons $\Rightarrow$ 40M tons (vehicles)
  - storage: 4.4 MJ/L (10K psi gas) $\Rightarrow$ 9.72 MJ/L
  - fuel cells: \$3000/kW $\Rightarrow$ \$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

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

- Approximately <u>$21.5 million</u> will be awarded in FY 2005, <u>pending appropriations</u>.
- Separate solicitations for universities and FERDCs are planned to be issued in May 2004. <u>Preapplications are required</u>. 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
- 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

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

- The distribution of funds between universities and FERDCs 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).