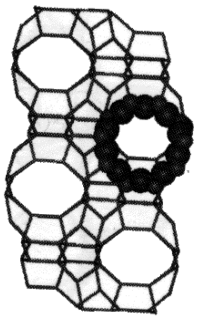
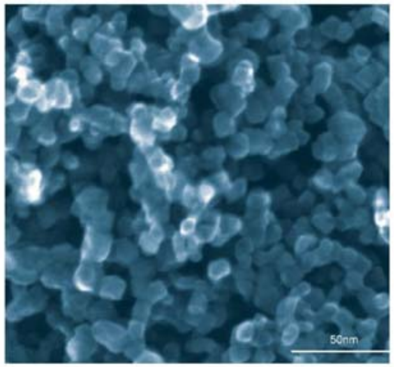
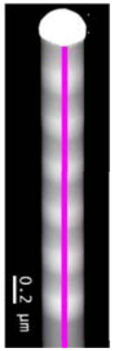
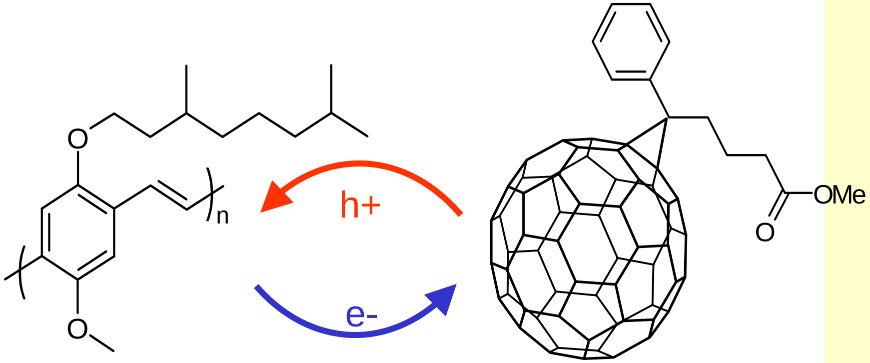
Basic Research Needs for Hydrogen Production









March 23, 2005
DOE Hydrogen Program Review Meeting
Arlington, VA

Presented by:
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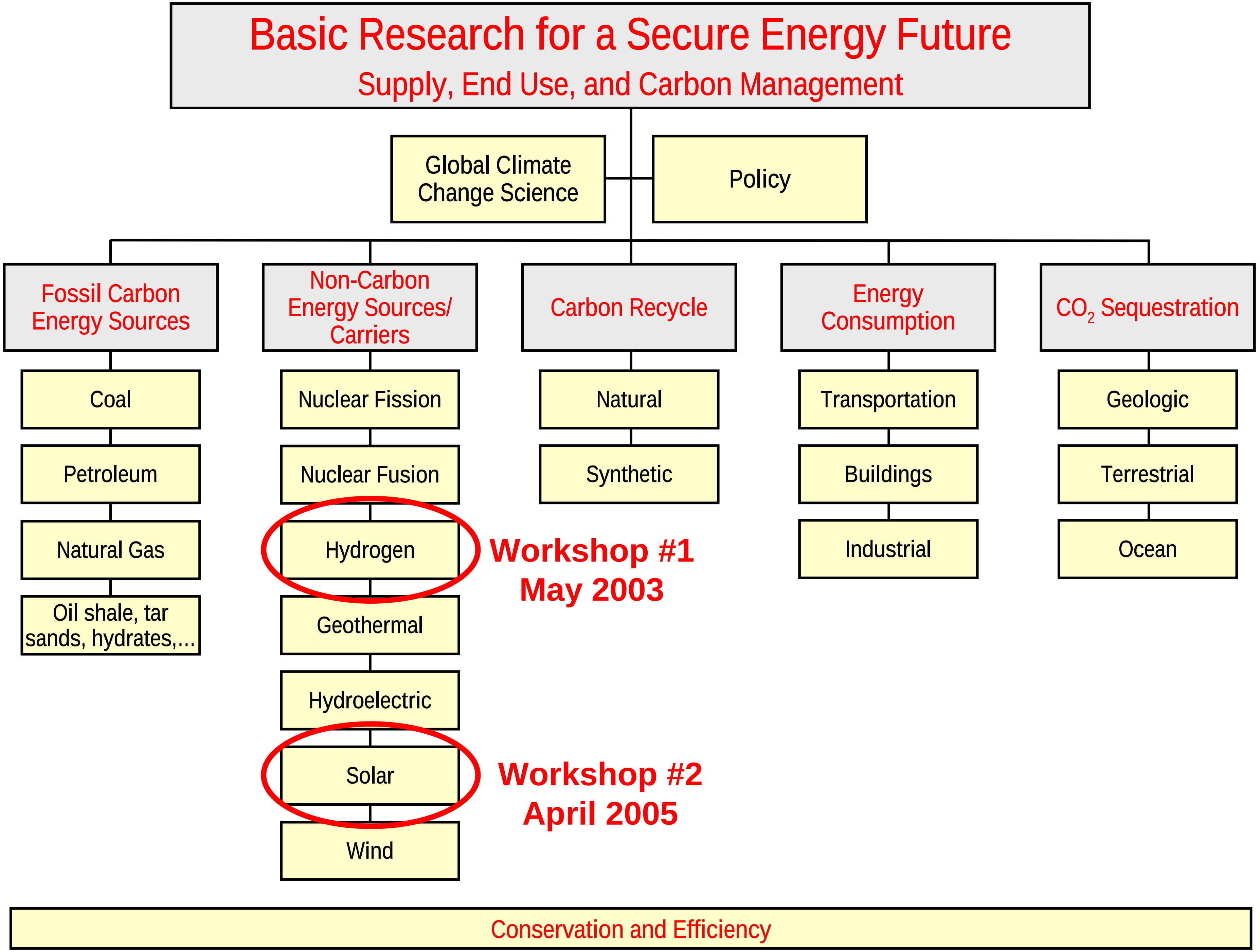
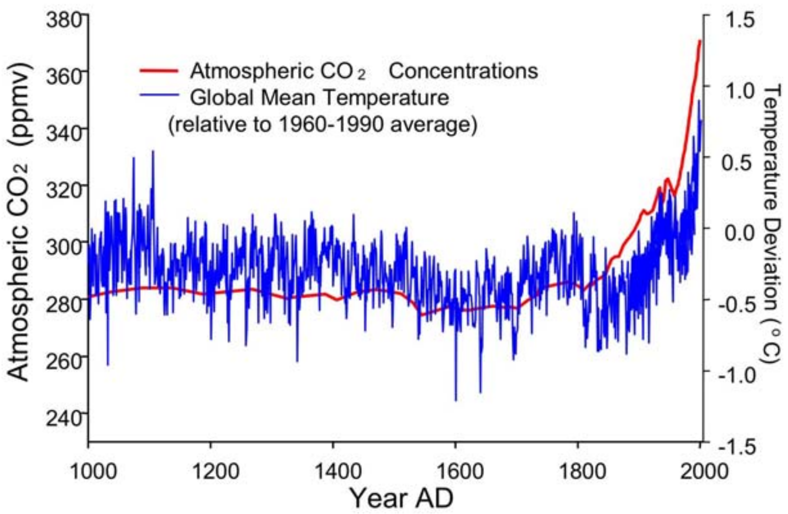
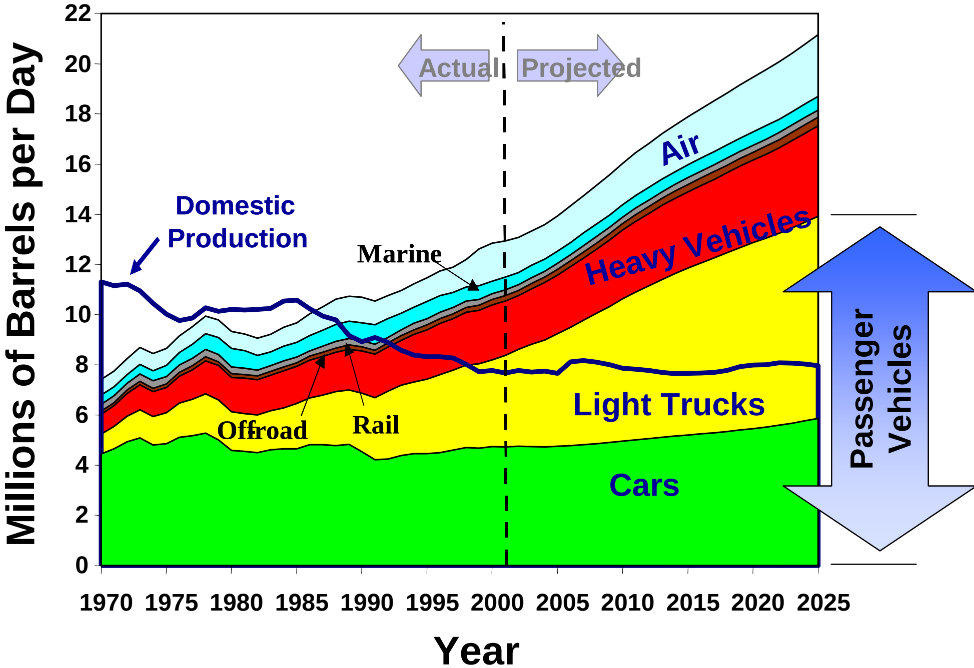

Basic Research for a Secure Energy Future
Supply, End Use, and Carbon Management
Global Climate Change Science
Policy
Fossil Carbon Energy Sources
Non-Carbon Energy Sources/ Carriers
Carbon Recycle
Energy Consumption
CO_2 Sequestration
Coal
Petroleum
Natural Gas
Oil shale, tar sands, hydrates,...
Nuclear Fission
Nuclear Fusion
Hydrogen
Geothermal
Hydroelectric
Solar
Wind
Natural
Synthetic
Transportation
Buildings
Industrial
Geologic
Terrestrial
Ocean
Workshop #1
May 2003
Workshop #2
April 2005
Conservation and Efficiency

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

H_2O

solar
wind
hydro

nuclear/solar
thermochemical
cycles

Bio- and
bioinspired

fossil fuel
reforming

H_2

gas or
hydride
storage

H_2

automotive
fuel cells

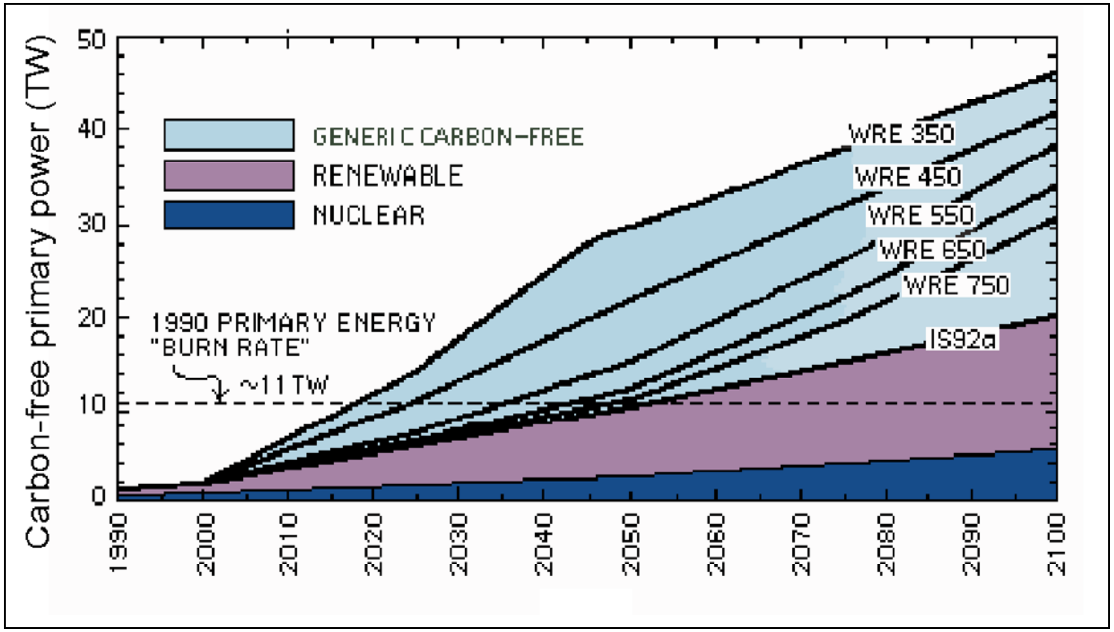
consumer
electronics

stationary
electricity/heat
generation

production	***storage***	***use in fuel cells***
9M tons/yr	**4.4 MJ/L (Gas, 10,000 psi)** **8.4 MJ/L (LH2)**	**$200-3000/kW**
↓	↓	↓
40M tons/yr **(Transportation only)**	**9.72 MJ/L** **(2015 FreedomCARTarget)**	**$35/kW** **(Internal Combustion Engine)**

Hydrogen Production Needs

The need for **carbon-free** power will grow steadily in the 21st century:



M. I. Hoffert, *et al.*, *Nature*, **1998**, *395*, 881.

Need for economic, sustainable, safe, environmentally benign hydrogen production (+40 M tons/yr for transportation)

Near- to midterm goals: Increased efficiency of fossil fuel conversion (with carbon sequestration), biomass utilization

Long term: Higher capacity, sustainable resources: renewable (**solar**, wind, geothermal) and nuclear hydrogen

Hydrogen Production Technology

Current status:

- Steam-reforming of oil and natural gas produces 9M tons H_2/yr
- We will need 40M tons/yr for transportation by 2015
- 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.
- Cost per peak watt is ~10 times too high for transportation use.

Nuclear: Abundant; carbon-neutral; long development cycle. May be limited in long term by fuel supply, siting, security.

Reforming of fixed carbon resources
Natural gas, petroleum, coal, biomass

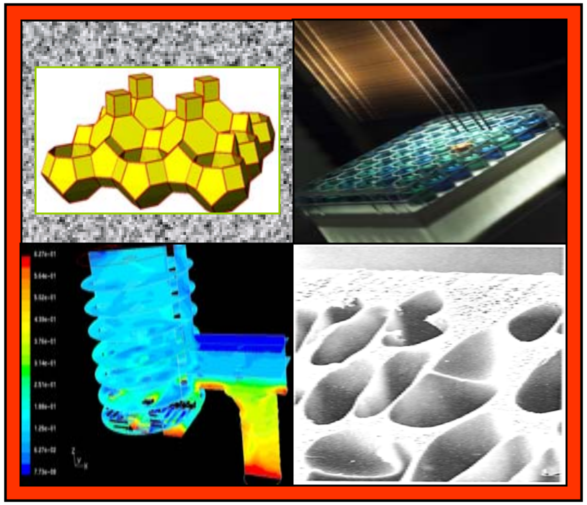
Goals

- Improved **efficiency** of H_2 production in distributed generation (>60%)
- **Low- or non-noble metal**, durable catalysts Improved **purity** of the H_2 product (<20 ppm CO for PEM fuel cells, no S)
- Efficient, cost-effective CO_2 **sequestration**

Opportunities

- Recent advances in **high throughput methods** and **rational design** enable understanding and discovery of nano-scale structures and catalytic reaction mechanisms
- Synergistic loop between experiment and **predictive modeling** promises dramatic advances in catalysis

Materials Combi



Modeling Separations

Solar PV/photoelectrochemistry/photocatalysis

Current Status

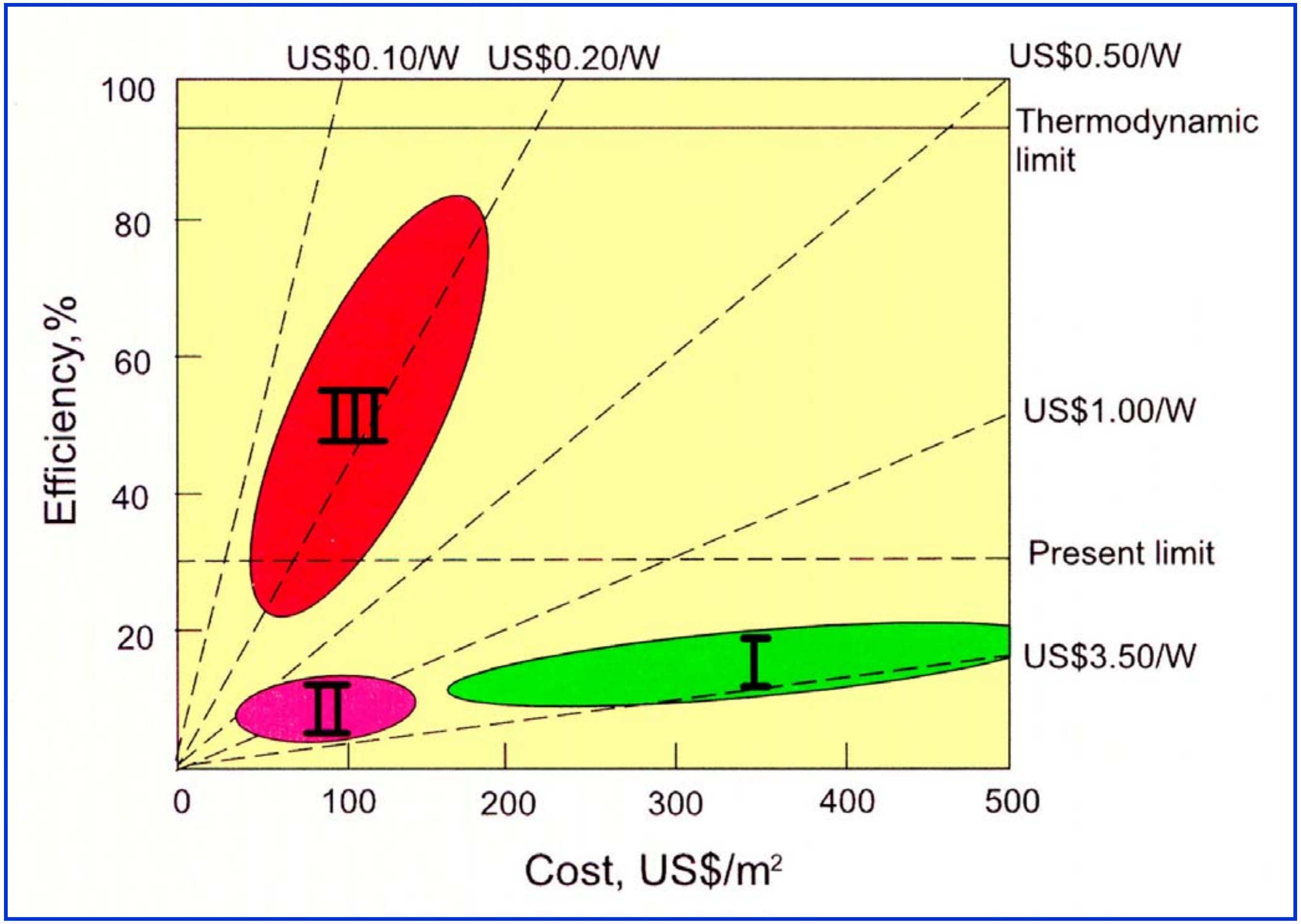
- **Si and thin film PV** – Efficient (η = 10-25%) but too expensive
- **Emerging technologies** – Dye sensitized cells, organic PV (η = 2-10%)
- **Nanomaterials** – Could lead to low cost novel devices

Priority Research Areas

- **Light harvesting** - Use of full solar spectrum, up/down-conversion
- **Photoprocesses** - Understand effects of structure, energy loss mechanisms, charge separation, carrier thermalization
- **Chemical assembly** - Develop flexible processes for controlling composite material structure on the nanometer length scale
- **Components** - New semiconductors, quantum dots, sensitizers, redox mediators, electron/hole conducting polymers, transparent conductors, liquid crystals, photonic materials…
- **Catalysis** and photocatalysis - Low free energy losses, low cost
- **Theory** and modeling - Understand/predict the dynamic behavior of molecules, complex photosystems, and photoelectrochemical cells
- **Characterization** tools - for interfaces and for photoredox processes in polymers

Photovoltaic (PV) Cell Costs per Peak Watt

The Critical Need for High Efficiency



- **Type I (single crystal Si) and type II (thin film PV) ride on same cost curves**
- **Need high efficiency (η > 15%) at very low cost**

Same analysis applies to solar H_2 production

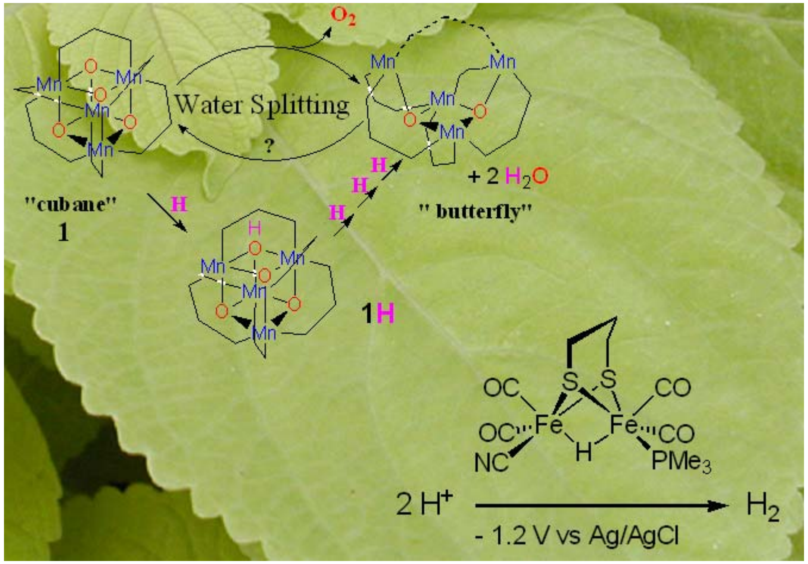
Bio- and bio-inspired H_2 production

Current Status

- Nature makes high purity H_2 from self-repairing, non-noble metal catalysts
- Biomass - fundamental limits to efficiency (< 5%)

Priority Research Areas

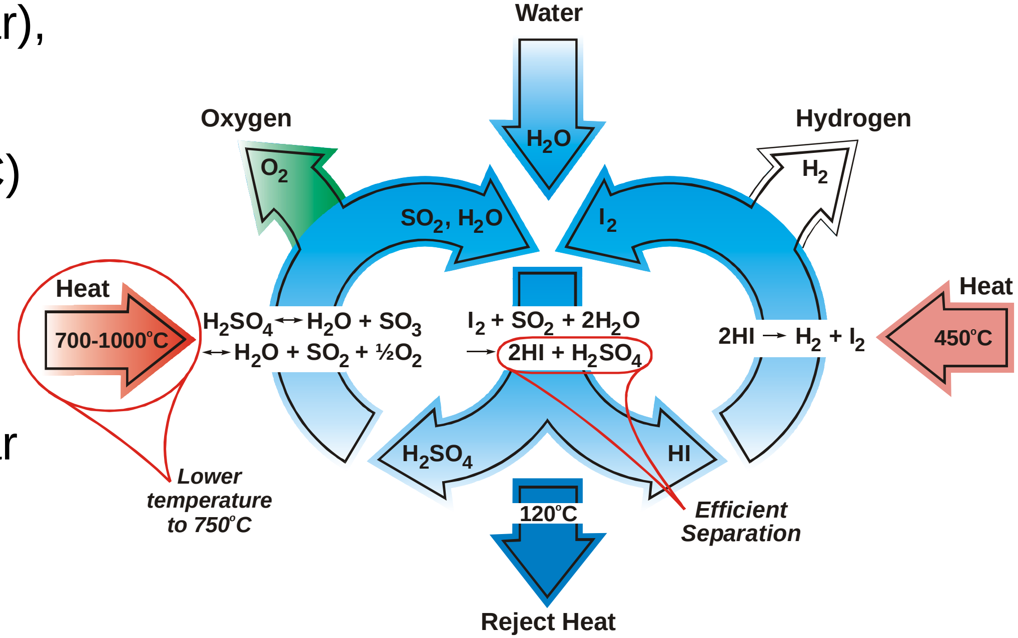
- Biomimetic catalysts for hydrogen "processing"
- Exploiting biodiversity for novel biocatalysts and determining mechanisms of assembly
- Coupling electrode materials to light-driven catalytic water oxidation, hydrogen production components
- Biomimetic nanostructures to organize catalytic functions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



Nuclear and solar thermal hydrogen

Current Status

- Low T electrolysis, proven technology, limited net efficiency (~26% nuclear heat to H_2), production cost \$4-5/kg H_2 (nuclear), \$15/kg (solar thermal)
- High T electrolysis (HTE), thermochemical water splitting (TC) in early development phase



Scientific Challenges

- **Materials** and processes (**separations**) for solar and nuclear TC - durable performance in extremely aggressive chemical environment
- **Materials**, high T cycles for solar thermal H_2

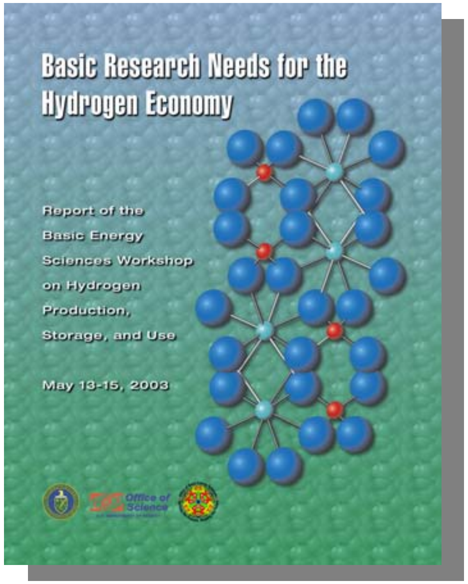
Hydrogen Production Summary

Challenges and Goals

- Carbon-neutral, sustainable, cost-effective production of hydrogen
- Low- and non-precious metal catalysis for low temperature water oxidation-reduction reactions
- Develop components and processes for highly efficient, low cost solar cells
- Understanding biological catalysis: hydrogen processing and allied enzymes

Priority Research Areas

- Nanoscale materials and nanostructured assemblies
- Catalysis
- Theory, modeling, and simulations
- Characterization and measurement techniques
- High temperature materials and separations



2003 Report - http://www.sc.doe.gov/bes/hydrogen.pdf