U.S. DEPARTMENT OF ENERGY

DOE Hydrogen Program

Presented to the
Hydrogen and Fuel Cell
Technical Advisory Committee

October 2, 2006

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Presentation Outline

- Program Introduction
    - Goals/Challenges
    - Participants
    - Resources
- Program Planning
- Program Elements and Progress
- Milestones/Decision Points
- Evaluation and Coordination
- Next Steps

Program Goal/Challenges

Goal: Technology readiness to enable fuel cell vehicles and hydrogen fuel from diverse domestic resources

Challenges:

Critical Path Technology

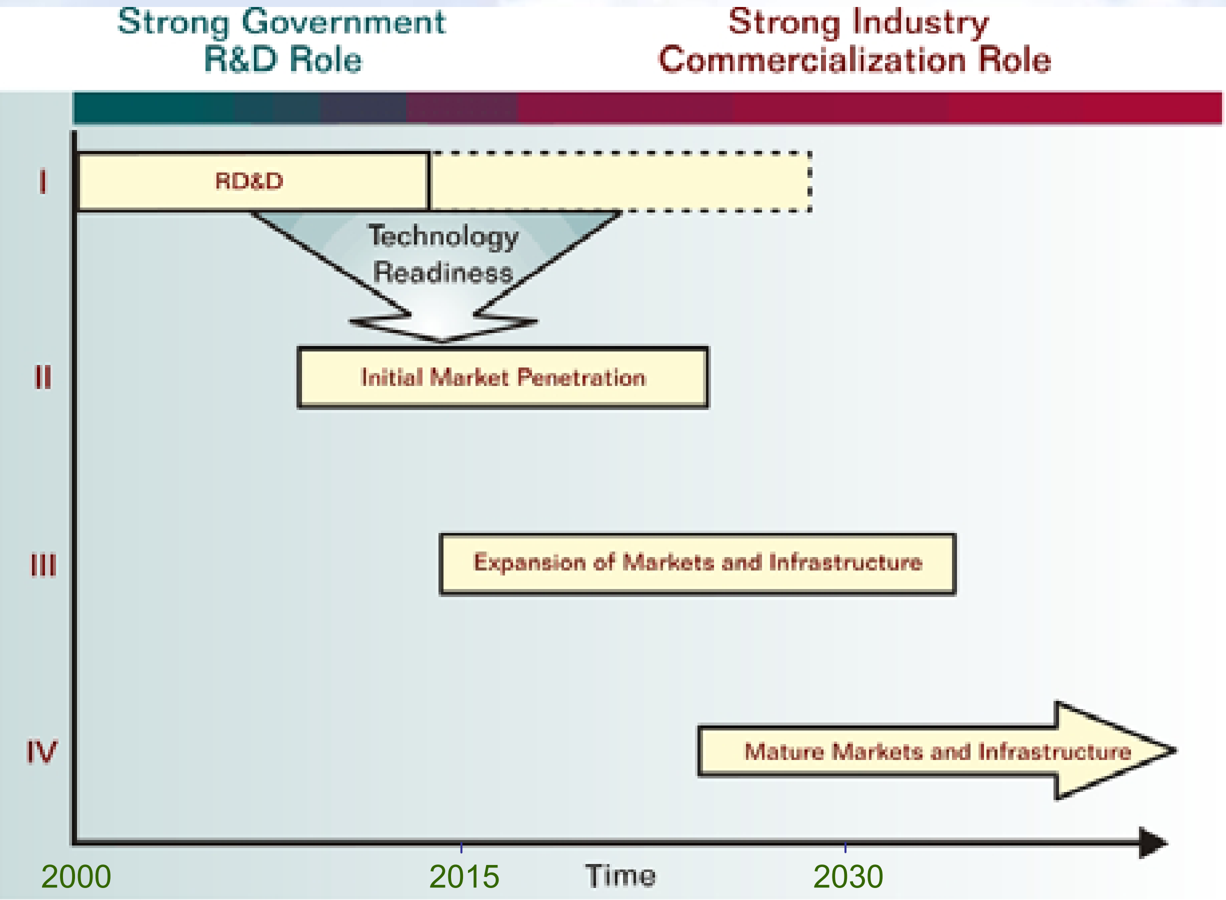
- ➔ Hydrogen Storage (target: >300-mile range)
- ➔ Fuel Cell Cost and Durability (targets: $30 per kW, 5000 hours)
- ➔ Hydrogen Cost (target: $2.00 - 3.00 per gallon gasoline equivalent*)

Economic/Institutional

- ➔ Codes and Standards (Safety, and Global Competitiveness)
- ➔ Hydrogen Delivery (Investment for new Distribution Infrastructure)
- ➔ Education (safety and code officials, local communities, state and local governments, students)

*One kilogram of hydrogen contains nearly the same energy as a gallon of gasoline.

Hydrogen Technology Development Timeline



I. Technology Development
Research to meet technology performance and cost targets and establish technology readiness

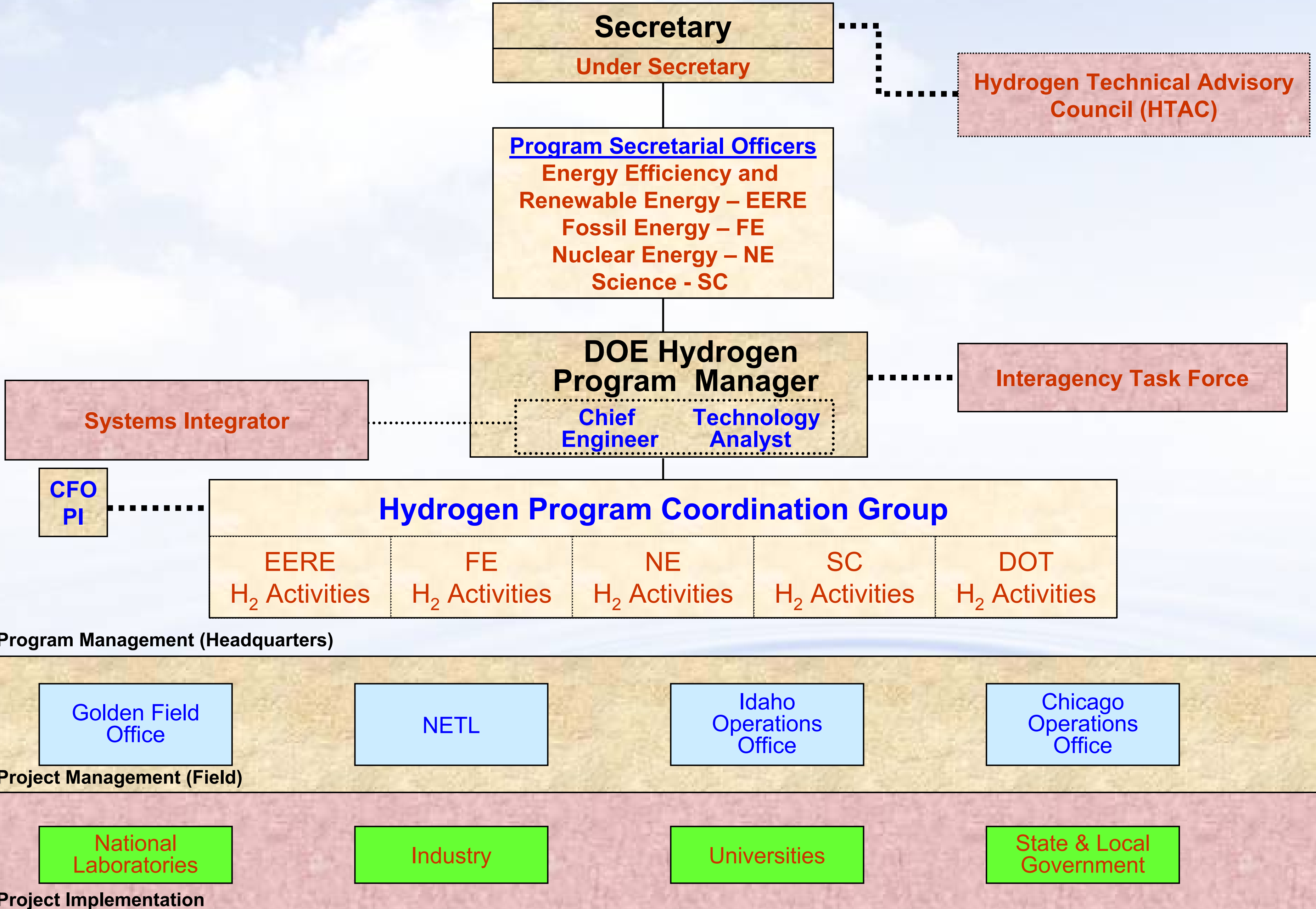
II. Initial Market Penetration
Portable power and stationary/transport systems are validated; infrastructure investment begins with governmental policies

III. Expansion of Markets and Infrastructure
H_2 power and transport systems commercially available infrastructure business case realized

IV. Fully Developed Markets and Infrastructure
H_2 power and transport systems commercially available in all regions; national infrastructure

By 2015: Enable industry to make decisions regarding commercialization of fuel cell vehicles and H_2 infrastructure

DOE Hydrogen Program Organization



Secretary

Under Secretary

Hydrogen Technical Advisory Council (HTAC)

Program Secretarial Officers

Energy Efficiency and Renewable Energy – EERE

Fossil Energy – FE

Nuclear Energy – NE

Science - SC

DOE Hydrogen Program Manager

Chief Engineer

Technology Analyst

Interagency Task Force

Systems Integrator

CFO PI

Hydrogen Program Coordination Group

EERE	FE	NE	SC	DOT
H_2 Activities	H_2 Activities	H_2 Activities	H_2 Activities	H_2 Activities

Program Management (Headquarters)

Golden Field Office

NETL

Idaho Operations Office

Chicago Operations Office

Project Management (Field)

National Laboratories

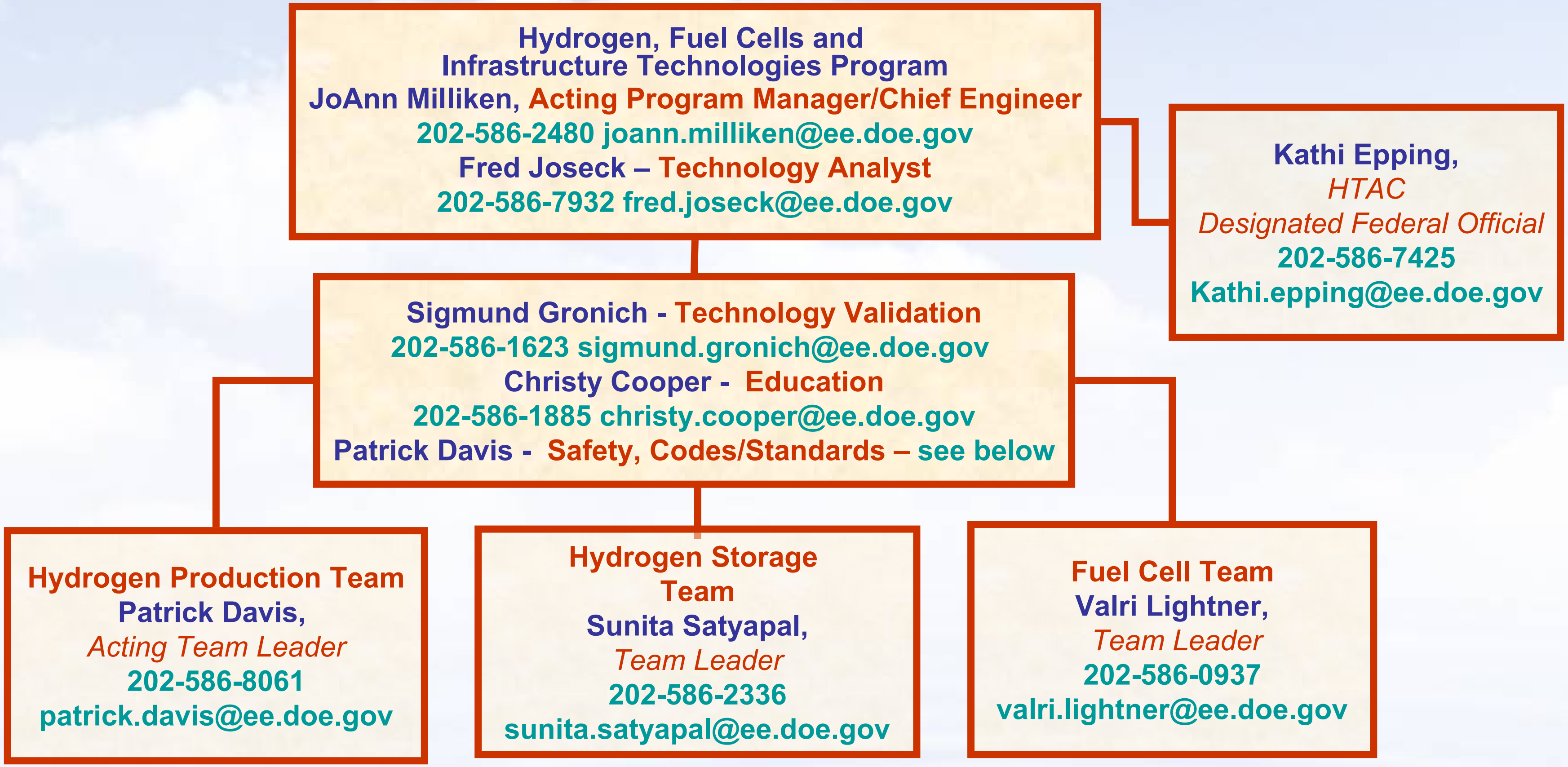
Industry

Universities

State & Local Government

Project Implementation

DOE Hydrogen Program Contact Information



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Hydrogen Coordination Group

- **Department of Energy**
    - Office of Energy Efficiency and Renewable Energy (EE)
    - Office of Fossil Energy (FE)
    - Office of Nuclear Energy (NE)
    - Office of Science (SC)
    - Office of Policy and International Affairs
    - Office of the Chief Financial Officer
- **Department of Transportation**
    - Research and Innovative Technology Administration

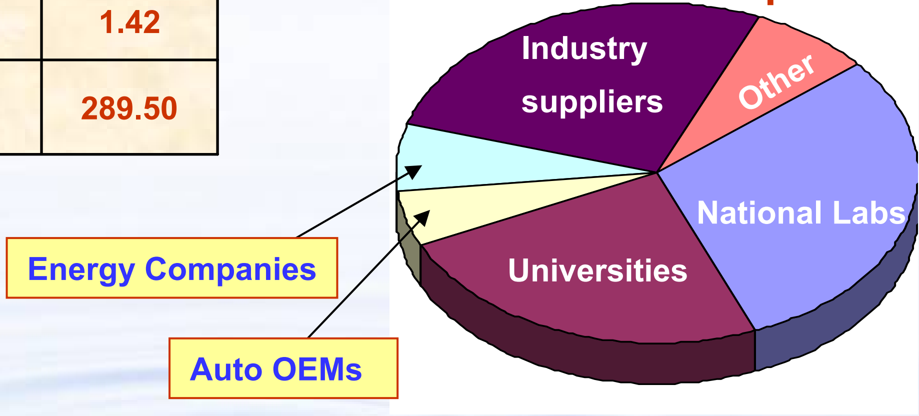
- **Developed Hydrogen Posture Plan**
- **Meets monthly to coordinate activities**
- **Shares information on both direct and related hydrogen and fuel cell activities**

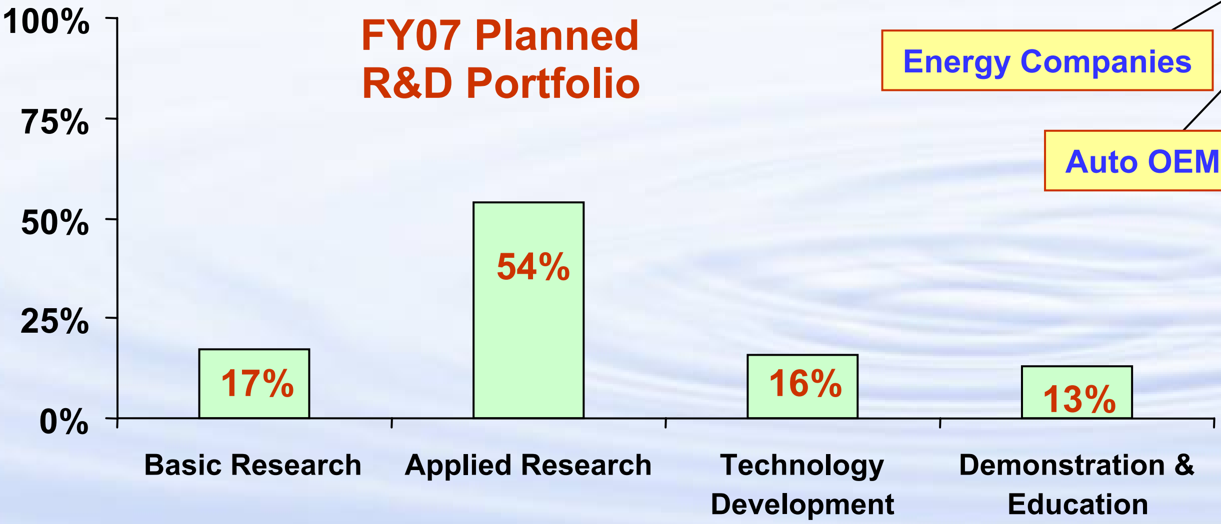
President's Hydrogen Fuel Initiative

Appropriation/Request (in $M)

Organization	FY 2004 Appropriation	FY 2005 Appropriation	FY 2006 Appropriation	FY 2007 Request
EERE	144.88	166.77	155.63	195.80
FE (Coal)	4.88	16.52	21.63	23.61
NE	6.20	8.68	24.75	18.67
BES	0	29.18	32.50	50.00
DOT	0.56	0.55	1.41	1.42
Total	156.52	221.7	235.92	289.50

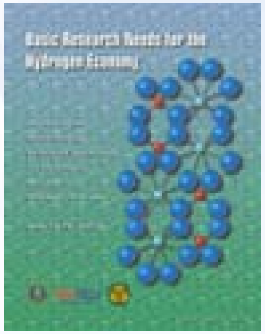
FY 2006 R & D Participants

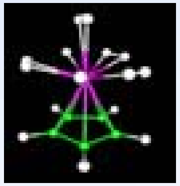


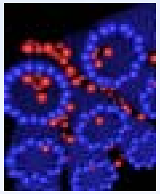

FY07 Planned R&D Portfolio

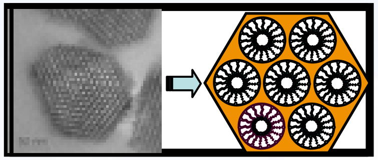
Fostering Synergy between Basic Science and Applied Research

Example: Hydrogen Storage







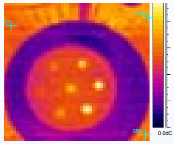


Basic Research

Develop and use theoretical models & fundamental experimentation to generate knowledge:

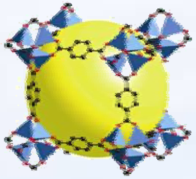
- Fundamental property & transport phenomena
- Novel material structures, characterization
- Theory, modeling, understand reaction mechanisms

Applied Research & Development



Apply theory & experimentation to design & develop novel, high-performance materials to meet specific performance targets:

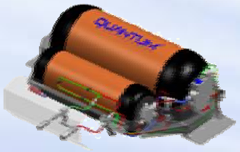
- Leverage knowledge from basic research, develop new materials
- Optimize materials and testing to improve performance
- Use engineering science to design, develop and demonstrate prototype systems to meet milestones.

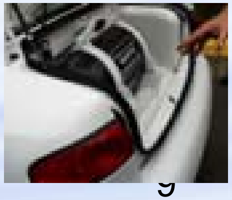


Technology Validation & Demonstration

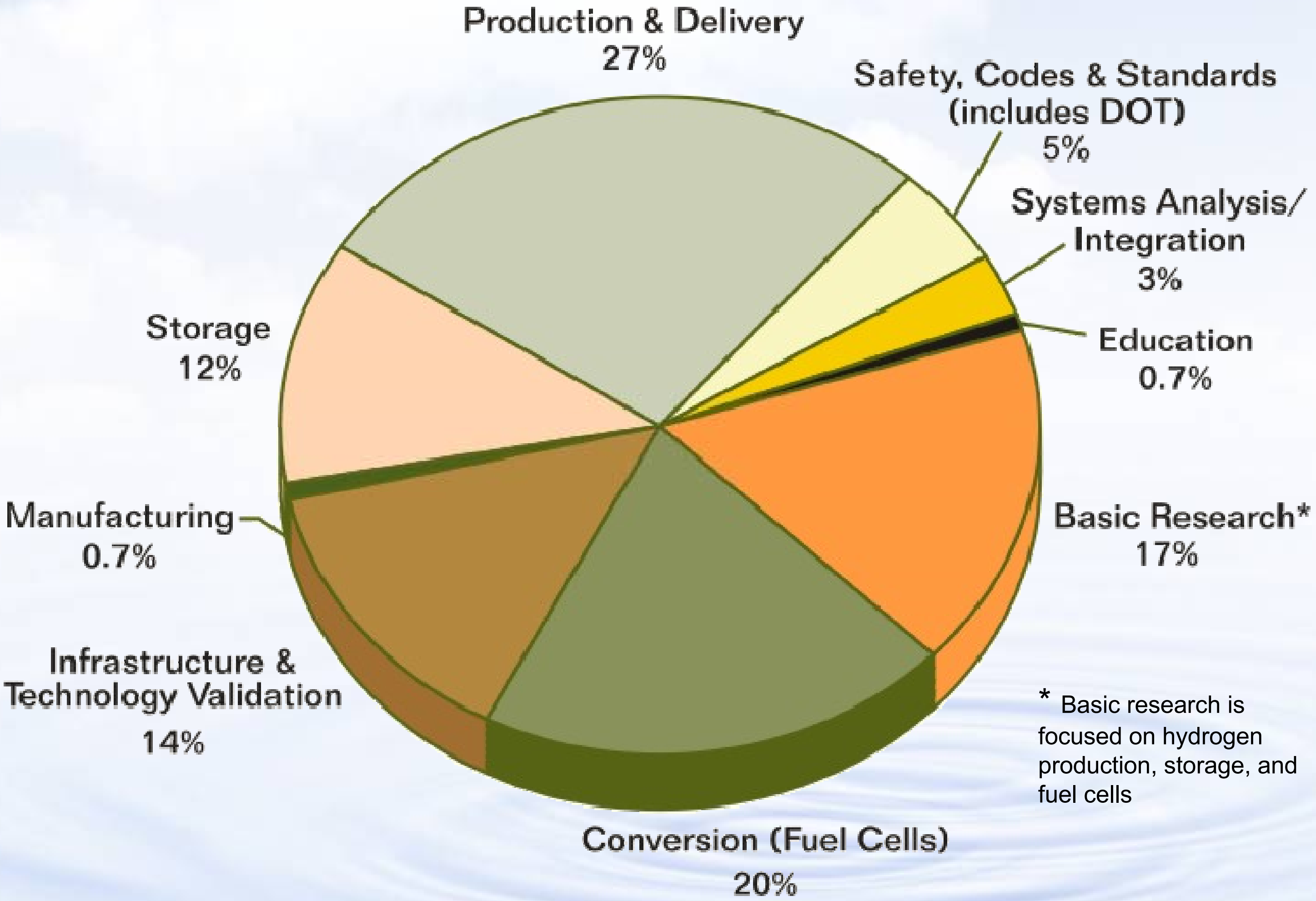
Test Systems under Real World Conditions

- Demonstrate and validate performance against targets
- Gain knowledge (e.g. fueling time, driving range, durability, cost, etc.) and apply lessons learned to R&D





FY2007 HFI Budget Request by Key Activity



* Basic research is focused on hydrogen production, storage, and fuel cells

TOTAL: $289.49 Million

Program Planning

Energy Policy Act of 2005 - SECTION 804. PLAN

Not later than 6 months after the date of enactment of this Act, the Secretary shall transmit to Congress a coordinated plan for the programs described in this title and any other programs of the Department that are directly related to fuel cells or hydrogen. The plan shall describe, at a minimum--

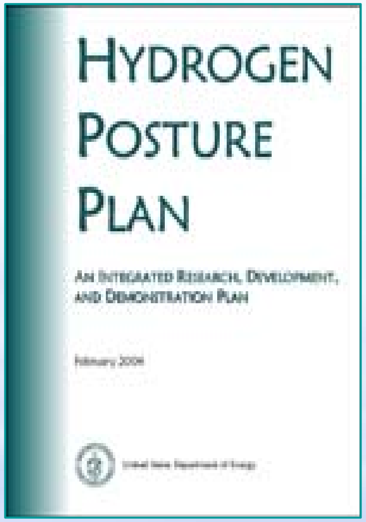
(1) the agenda for the next 5 years for the programs authorized under this title, including the agenda for each activity enumerated in section 805(e);

(2) the types of entities that will carry out the activities under this title and what role each entity is expected to play;

(3) the milestones that will be used to evaluate the programs for the next 5 years;

(4) the most significant technical and nontechnical hurdles that stand in the way of achieving the goals described in section 805, and how the programs will address those hurdles; and

(5) the policy assumptions that are implicit in the plan, including any assumptions that would affect the sources of hydrogen or the marketability of hydrogen-related products



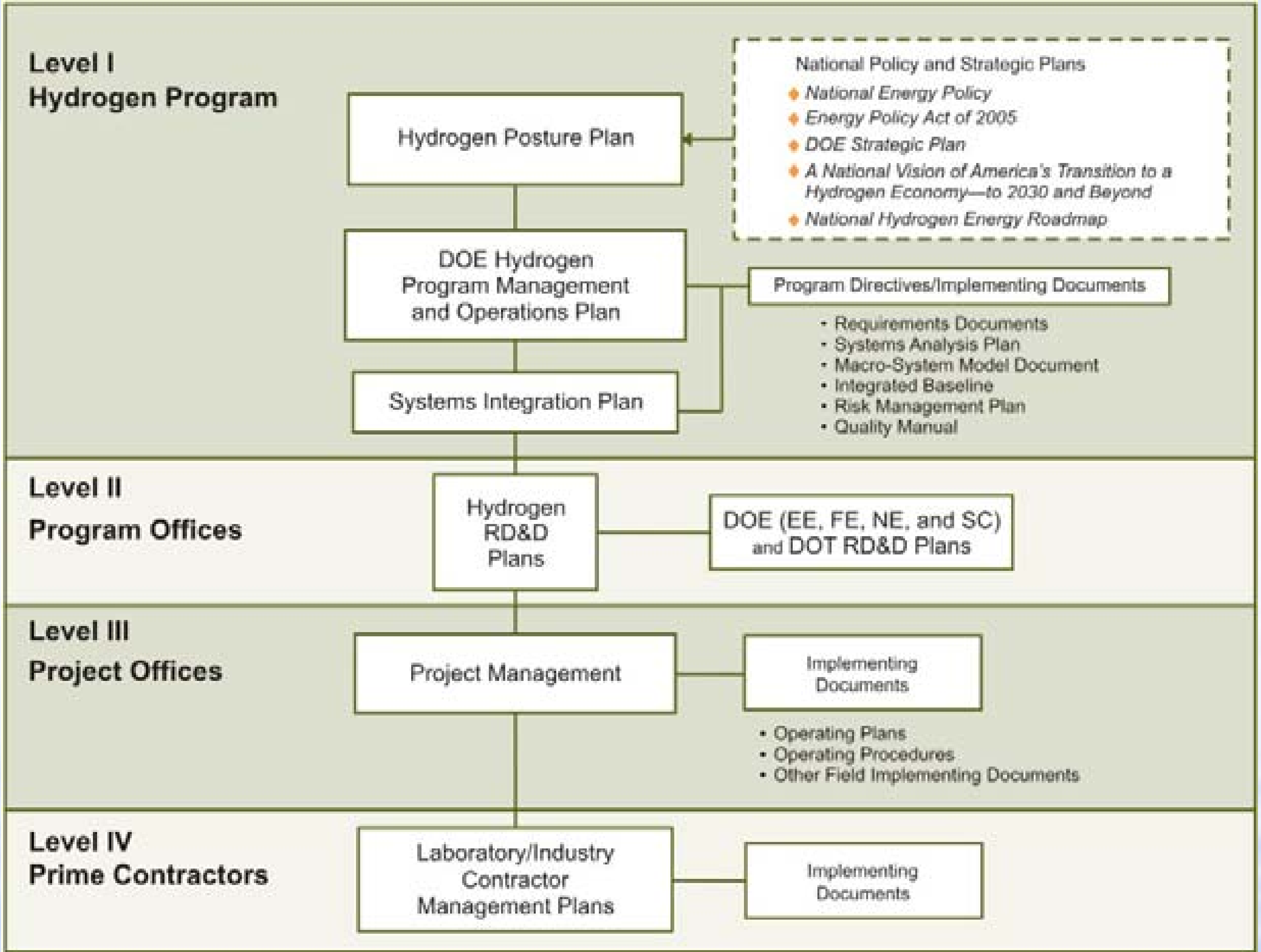
HYDROGEN
POSTURE
PLAN

AN INTEGRATED RESEARCH, DEVELOPMENT, AND DEMONSTRATION PLAN

February 2004

- **Posture Plan published February 2004**
- **Revised *Posture Plan* is key deliverable for program, mandated by Energy Policy Act of 2005, Section 804. Draft document is under DOE review**

HFI Program Planning and Operations Document Hierarchy



Level I
Hydrogen Program

Hydrogen Posture Plan

National Policy and Strategic Plans
- *National Energy Policy*
- *Energy Policy Act of 2005*
- *DOE Strategic Plan*
- *A National Vision of America's Transition to a Hydrogen Economy—to 2030 and Beyond*
- *National Hydrogen Energy Roadmap*

DOE Hydrogen Program Management and Operations Plan

Systems Integration Plan

Program Directives/Implementing Documents
- Requirements Documents
- Systems Analysis Plan
- Macro-System Model Document
- Integrated Baseline
- Risk Management Plan
- Quality Manual

Level II
Program Offices

Hydrogen RD&D Plans

DOE (EE, FE, NE, and SC) and DOT RD&D Plans

Level III
Project Offices

Project Management

Implementing Documents
- Operating Plans
- Operating Procedures
- Other Field Implementing Documents

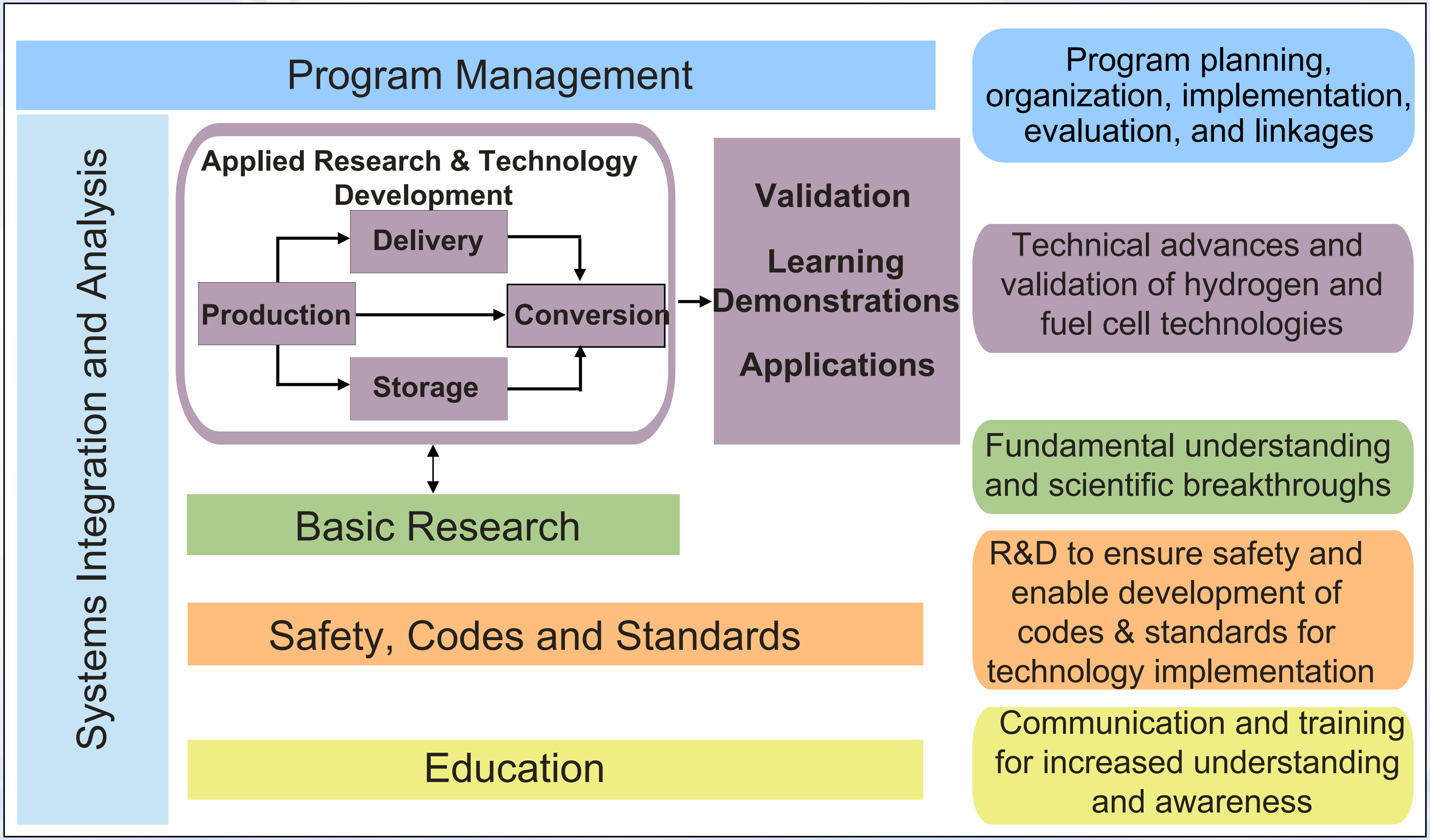
Level IV
Prime Contractors

Laboratory/Industry Contractor Management Plans

Implementing Documents

Program Elements
and
Progress

Program Elements



Program Management

Systems Integration and Analysis

Applied Research & Technology Development

Delivery

Production

Conversion

Storage

Validation

Learning Demonstrations

Applications

Basic Research

Safety, Codes and Standards

Education

Program planning, organization, implementation, evaluation, and linkages

Technical advances and validation of hydrogen and fuel cell technologies

Fundamental understanding and scientific breakthroughs

R&D to ensure safety and enable development of codes & standards for technology implementation

Communication and training for increased understanding and awareness

Producing Hydrogen

Goal: Hydrogen produced domestically, reducing our dependence on foreign energy sources and providing clean, carbon-free fuel.

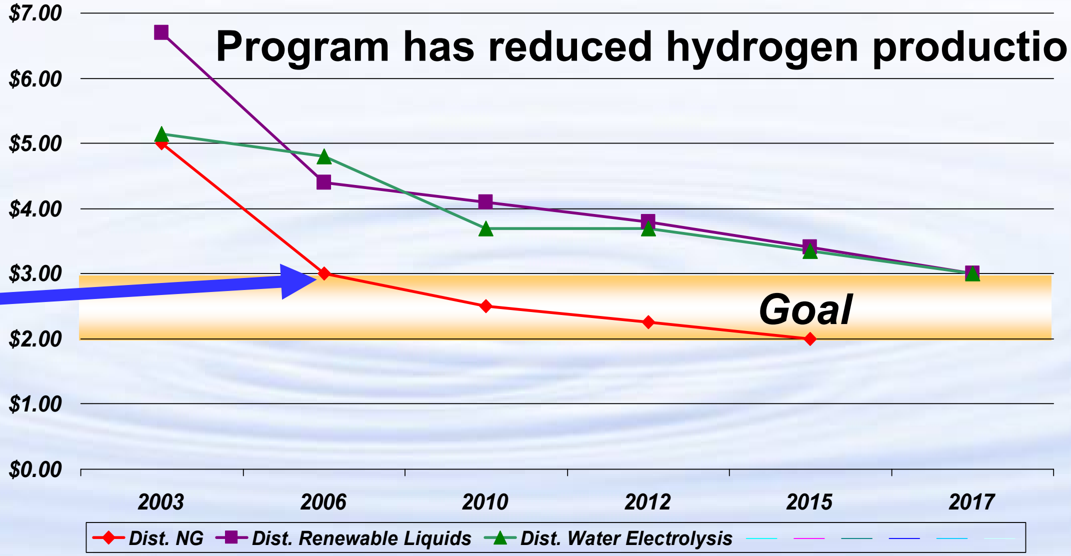
Production Pathways: Hydrogen can be produced from renewable, nuclear, and fossil energy resources using a variety of process technologies, including:

- Renewable electrolysis (using wind, solar, or geothermal energy)
- Biomass and renewable liquids
- High temperature thermochemical
    - ➔ Nuclear energy
    - ➔ High temperature solar
- Biological and photoelectrochemical technologies
- Coal (with carbon sequestration)
- Natural gas

Quick Fact:
The U.S. hydrogen industry currently produces ~9 million tons of hydrogen a year – that's enough to power about 34 million vehicles.

Major Accomplishment:

Achieved $3/gge for Natural Gas to Hydrogen



Program has reduced hydrogen production cost

Delivering Hydrogen

Hydrogen produced centrally or semi-centrally must be delivered to the point-of-use. Delivery also includes the operations of compression, storage, and dispensing at refueling stations.

Hydrogen can be delivered as a gas, cryogenic liquid, or as hydrogen stored in liquid or solid carriers.

Hydrogen can be transported by pipeline, high pressure tube trailers, cryogenic liquid trucks, or carriers.

Program is focused on:
- **Low cost, off-board storage**
- **Reliable compression technology**
- **Pipelines: solve embrittlement issues**
- **Dramatic reductions in liquefaction cost and energy use**
- **Novel carriers**

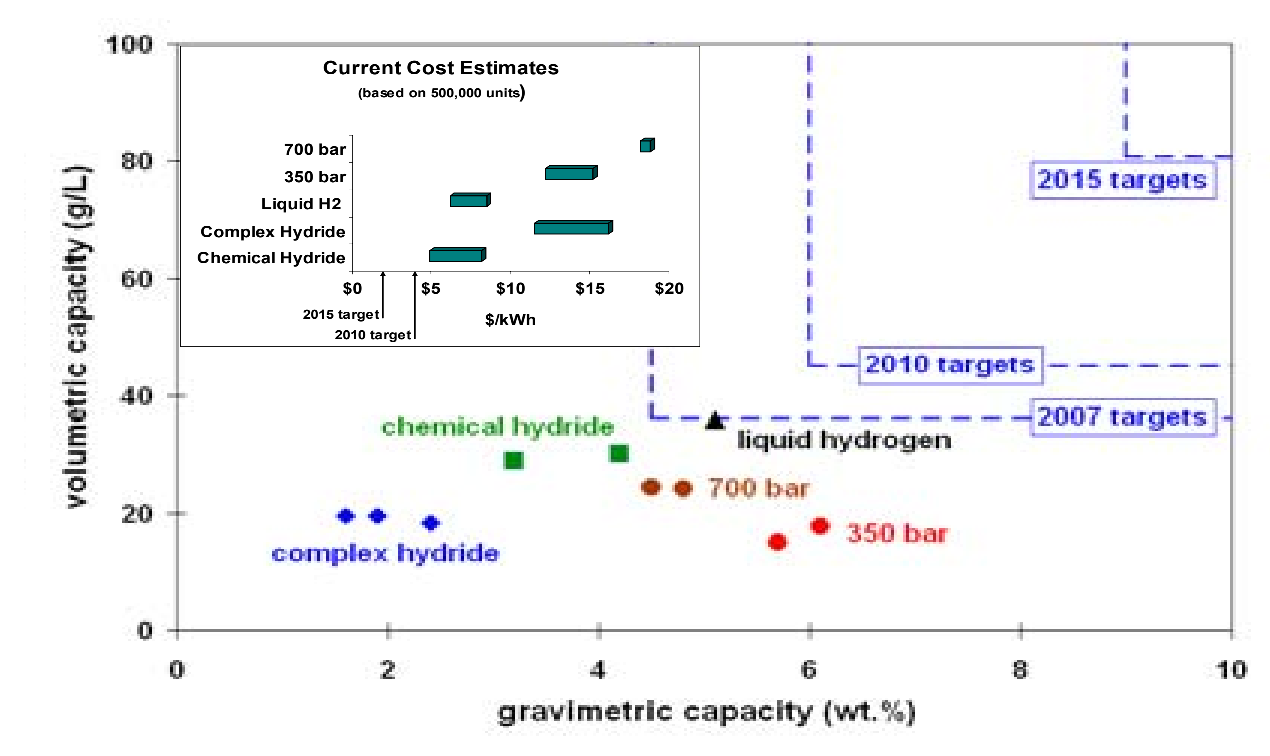
Quick Facts:

- **Today there are about 700 miles of hydrogen pipelines in the U. S. (compared to more than 1 million miles of natural gas pipelines).**
- **Current delivery costs are estimated to be about \$3.50/gge; the long term target for hydrogen delivery, including refueling station operations, is <\$1.00/gge.**

On-Board Hydrogen Storage

Consumers demand more than 300-mile driving range while meeting vehicle packaging, cost, safety, and performance requirements.

- Compressed hydrogen tanks in the near term
- DOE focus is high-risk, high-payoff R&D on materials
- National Hydrogen Storage Project includes
    - ➔ 3 Centers of Excellence
    - ➔ 40 universities, 15 companies, 10 federal labs
    - ➔ Coordinated basic & applied R&D



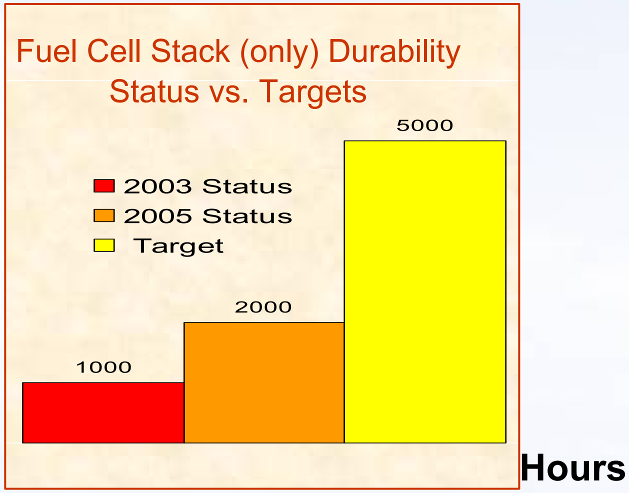
Significant progress in identifying several new high-capacity materials with potential to meet 2010 targets

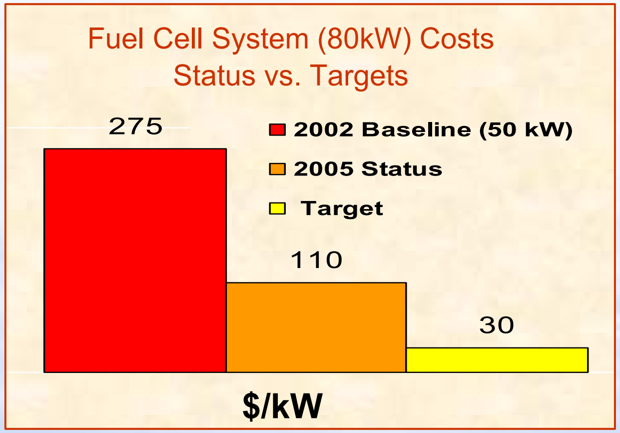
Automotive Fuel Cell Targets & Progress: Reduced Cost and Increased Durability

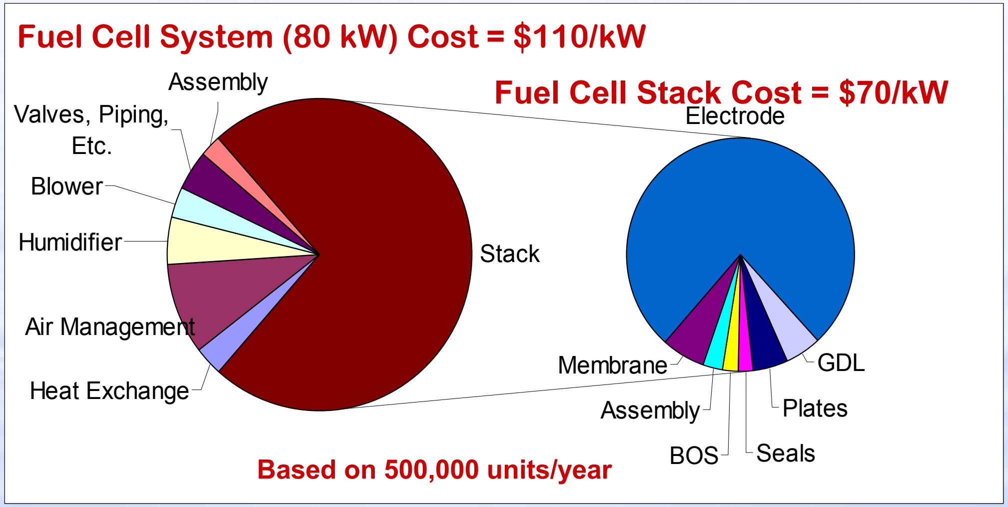
- Primary focus is transportation fuel cell applications.
- Secondary focus is on stationary and other early market fuel cells.

DOE sponsoring component R&D rather than systems R&D

- ➔ Membranes
- ➔ Electrodes
- ➔ Membrane Electrode Assemblies
- ➔ Catalysts
- ➔ Bipolar Plates


Fuel Cell Stack (only) Durability Status vs. Targets


Fuel Cell System (80kW) Costs Status vs. Targets


Fuel Cell System (80 kW) Cost = $110/kW

Fuel Cell Stack Cost = $70/kW

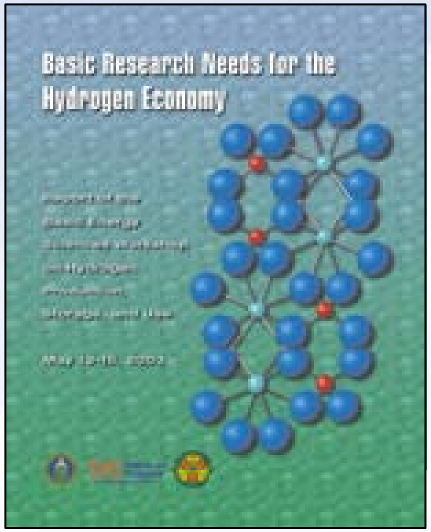
Based on 500,000 units/year

Technology Validation

- Obtain detailed component data under real-world conditions to provide feedback to Department’s hydrogen and fuel cell component and materials research
- Validate the technology against time-phased performance-based targets, by 2009
  - ➔ ***2,000 hour fuel cell durability***
  - ➔ ***$3.00 per gge (high capacity facility, volume manufacturing)***
  - ➔ ***250 mile range***

- Four auto/energy company teams: Chevron/Hyundai-Kia, DaimlerChrysler/BP, Ford/BP, and GM/Shell
- Nine hydrogen fueling stations in 2006; a total of 18 planned by 2009
- In 2006, 63 hydrogen FCVs; an additional 68 planned for 2007-08 with 50,000-mile fuel cell systems.
- Fuel cell system has achieved 53-58% efficiency and vehicles have demonstrated range of 103-190 miles.

Basic Research Highlights


Basic Research Needs for the Hydrogen Economy

FY05 solicitation based on the five priority research areas identified by the workshop report:

- 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

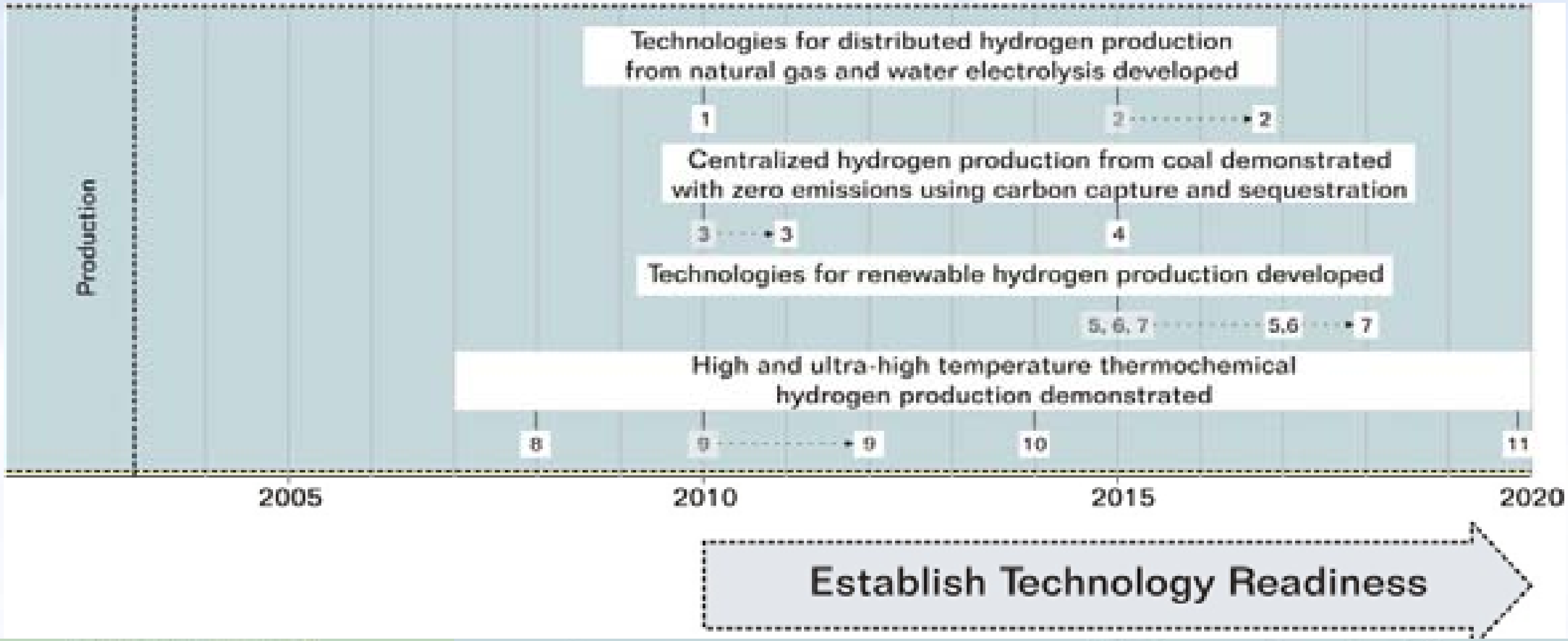
Examples of Activities:

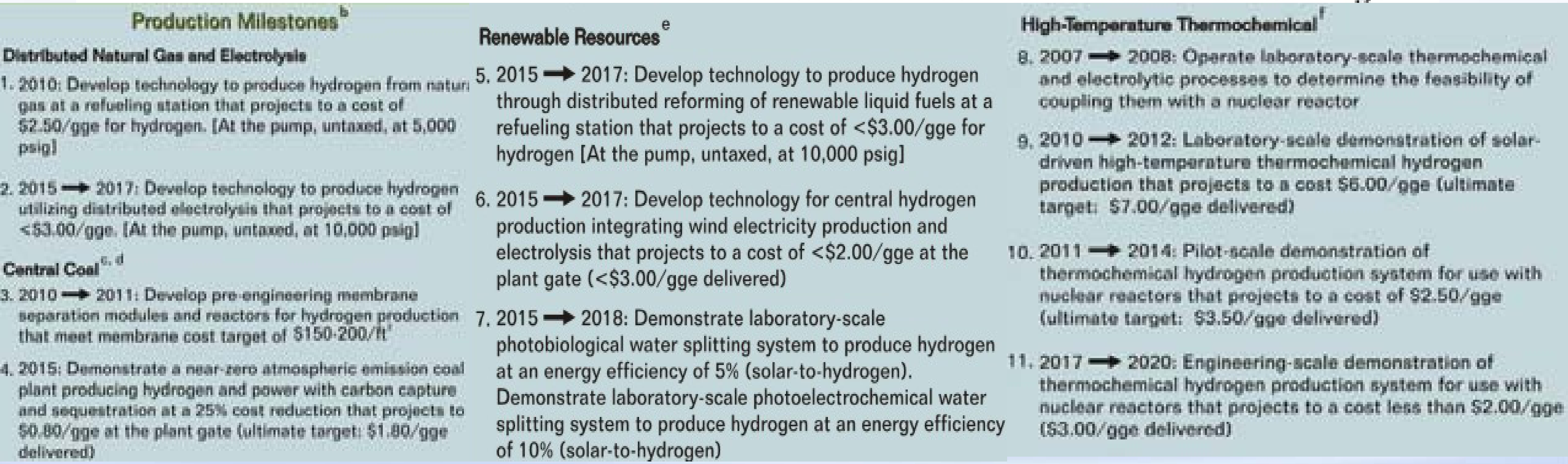
- **Hydrogen Storage:** Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides
- **Membranes:** Micro- and Nano-Patterning Boost Power Output & Miniaturization of Fuel Cells
- **Catalysts:** Predicting Catalysts for Hydrogen Production, Storage or Fuel-Cell Utilization
- **Solar Hydrogen Production:** Searching for the Ideal Mixed-Metal Oxide Photoelectrode
- **Bio-inspired Processes:** Effects of structure truncation on Oxygen Tolerance of Hydrogenase

FY07 solicitation focuses on:
- Novel materials for hydrogen storage
- Functional membranes
- Nanoscale catalysts

Milestones
and
Decision Points

Production Milestones and Decision Points





Production Milestones[b]

Distributed Natural Gas and Electrolysis

1. 2010: Develop technology to produce hydrogen from natur gas at a refueling station that projects to a cost of $2.50/gge for hydrogen. [At the pump, untaxed, at 5,000 psig]

2. 2015 → 2017: Develop technology to produce hydrogen utilizing distributed electrolysis that projects to a cost of <$3.00/gge. [At the pump, untaxed, at 10,000 psig]

Central Coal[c, d]

3. 2010 → 2011: Develop pre-engineering membrane separation modules and reactors for hydrogen production that meet membrane cost target of $150-200/ft^2

4. 2015: Demonstrate a near-zero atmospheric emission coal plant producing hydrogen and power with carbon capture and sequestration at a 25% cost reduction that projects to $0.80/gge at the plant gate (ultimate target: $1.80/gge delivered)

Renewable Resources[e]

5. 2015 → 2017: Develop technology to produce hydrogen through distributed reforming of renewable liquid fuels at a refueling station that projects to a cost of <$3.00/gge for hydrogen [At the pump, untaxed, at 10,000 psig]

6. 2015 → 2017: Develop technology for central hydrogen production integrating wind electricity production and electrolysis that projects to a cost of <$2.00/gge at the plant gate (<$3.00/gge delivered)

7. 2015 → 2018: Demonstrate laboratory-scale photobiological water splitting system to produce hydrogen at an energy efficiency of 5% (solar-to-hydrogen). Demonstrate laboratory-scale photoelectrochemical water splitting system to produce hydrogen at an energy efficiency of 10% (solar-to-hydrogen)

High-Temperature Thermochemical[f]

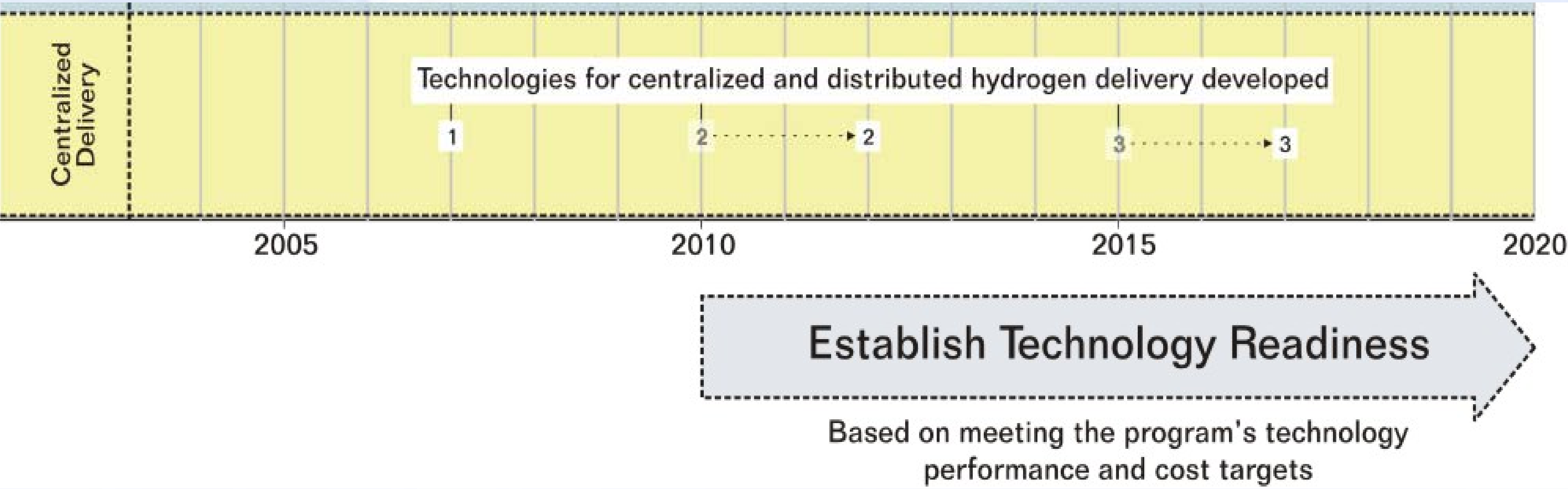
8. 2007 → 2008: Operate laboratory-scale thermochemical and electrolytic processes to determine the feasibility of coupling them with a nuclear reactor

9. 2010 → 2012: Laboratory-scale demonstration of solar-driven high-temperature thermochemical hydrogen production that projects to a cost $6.00/gge (ultimate target: $7.00/gge delivered)

10. 2011 → 2014: Pilot-scale demonstration of thermochemical hydrogen production system for use with nuclear reactors that projects to a cost of $2.50/gge (ultimate target: $3.50/gge delivered)

11. 2017 → 2020: Engineering-scale demonstration of thermochemical hydrogen production system for use with nuclear reactors that projects to a cost less than $2.00/gge ($3.00/gge delivered)

Delivery Milestones and Decision Points



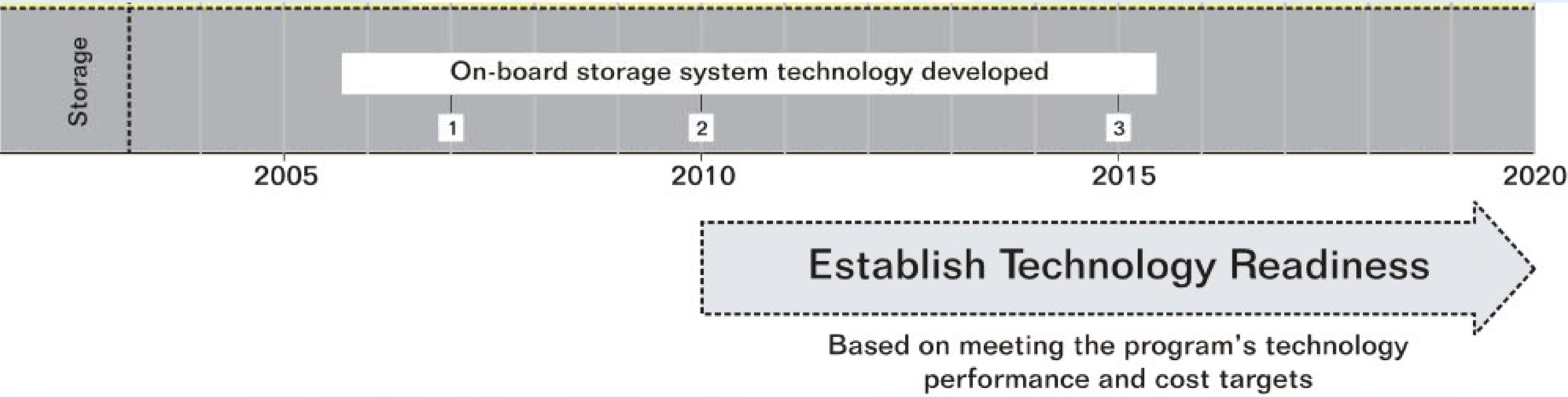
Centralized Delivery Milestones[e]

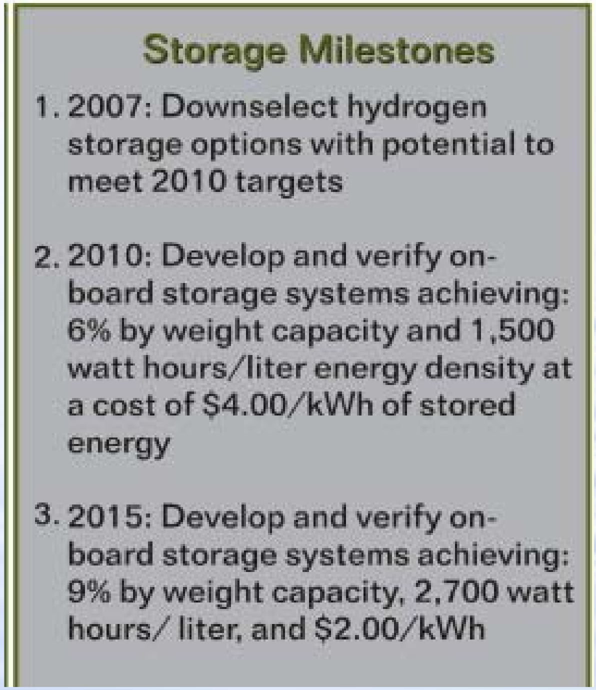
1. 2007: Define the criteria for a cost-effective hydrogen fuel delivery infrastructure for supporting the introduction and long-term use of hydrogen for transportation and stationary power

2. 2010 ➞ 2012: Develop technologies to reduce the cost of hydrogen fuel delivery from the point of production to the point of use in vehicles or stationary power units to <$1.70/gge of hydrogen

3. 2015 ➞ 2017: Develop technologies to reduce the cost of hydrogen fuel delivery from the point of production to the point of use in vehicles or stationary power units to <$1.00/gge of hydrogen

Storage Milestones and Decision Points

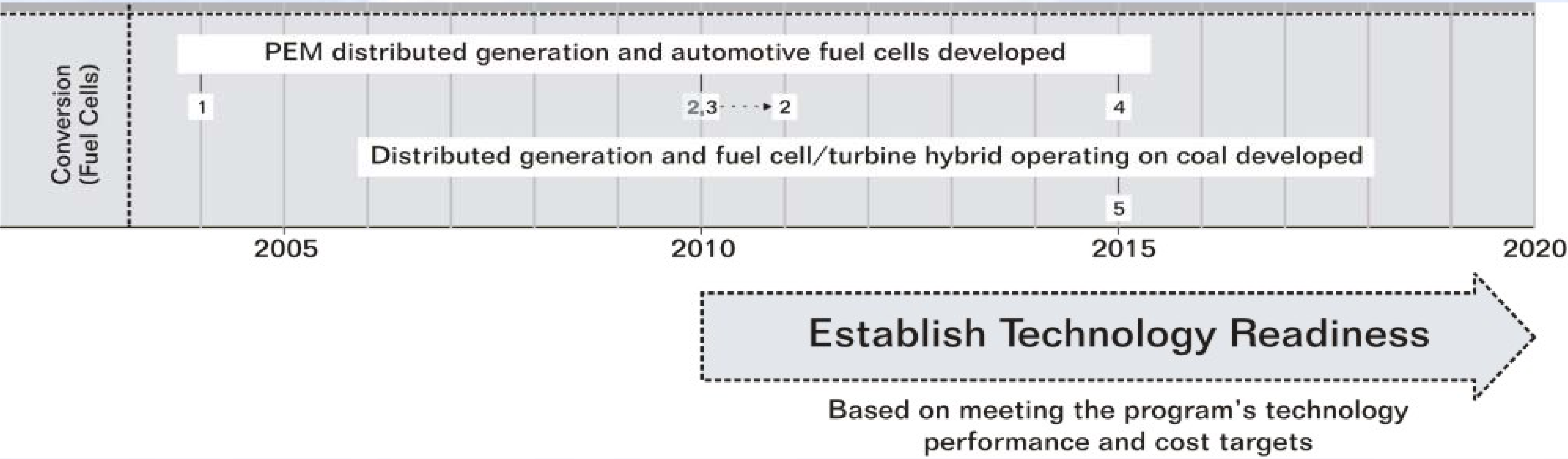


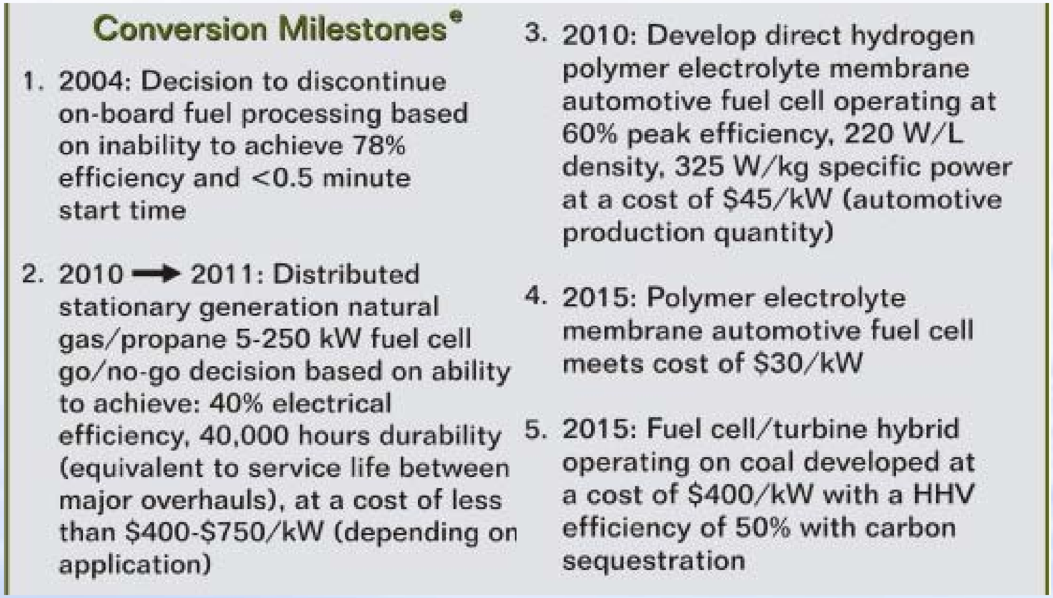


Storage Milestones

1. 2007: Downselect hydrogen storage options with potential to meet 2010 targets
2. 2010: Develop and verify on-board storage systems achieving: 6% by weight capacity and 1,500 watt hours/liter energy density at a cost of $4.00/kWh of stored energy
3. 2015: Develop and verify on-board storage systems achieving: 9% by weight capacity, 2,700 watt hours/ liter, and $2.00/kWh

Conversion (Fuel Cells) Milestones and Decision Points

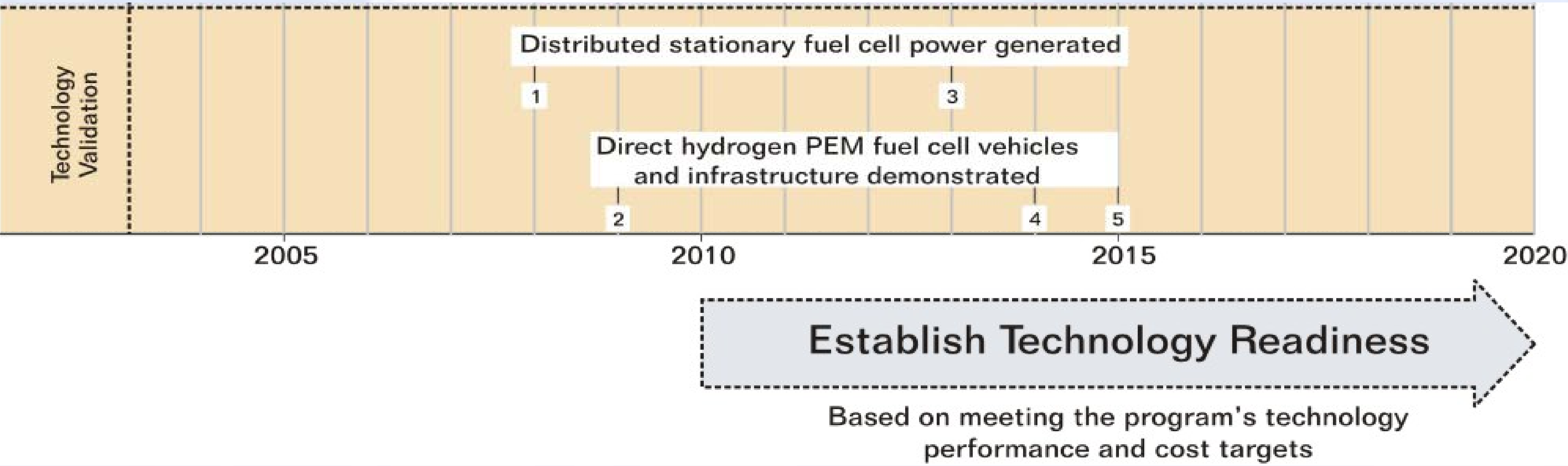




Conversion Milestones[e]

1. 2004: Decision to discontinue on-board fuel processing based on inability to achieve 78% efficiency and <0.5 minute start time
2. 2010 ➞ 2011: Distributed stationary generation natural gas/propane 5-250 kW fuel cell go/no-go decision based on ability to achieve: 40% electrical efficiency, 40,000 hours durability (equivalent to service life between major overhauls), at a cost of less than $400-$750/kW (depending on application)
3. 2010: Develop direct hydrogen polymer electrolyte membrane automotive fuel cell operating at 60% peak efficiency, 220 W/L density, 325 W/kg specific power at a cost of $45/kW (automotive production quantity)
4. 2015: Polymer electrolyte membrane automotive fuel cell meets cost of $30/kW
5. 2015: Fuel cell/turbine hybrid operating on coal developed at a cost of $400/kW with a HHV efficiency of 50% with carbon sequestration

Technology Validation Milestones and Decision Points



Distributed stationary fuel cell power generated

Direct hydrogen PEM fuel cell vehicles and infrastructure demonstrated

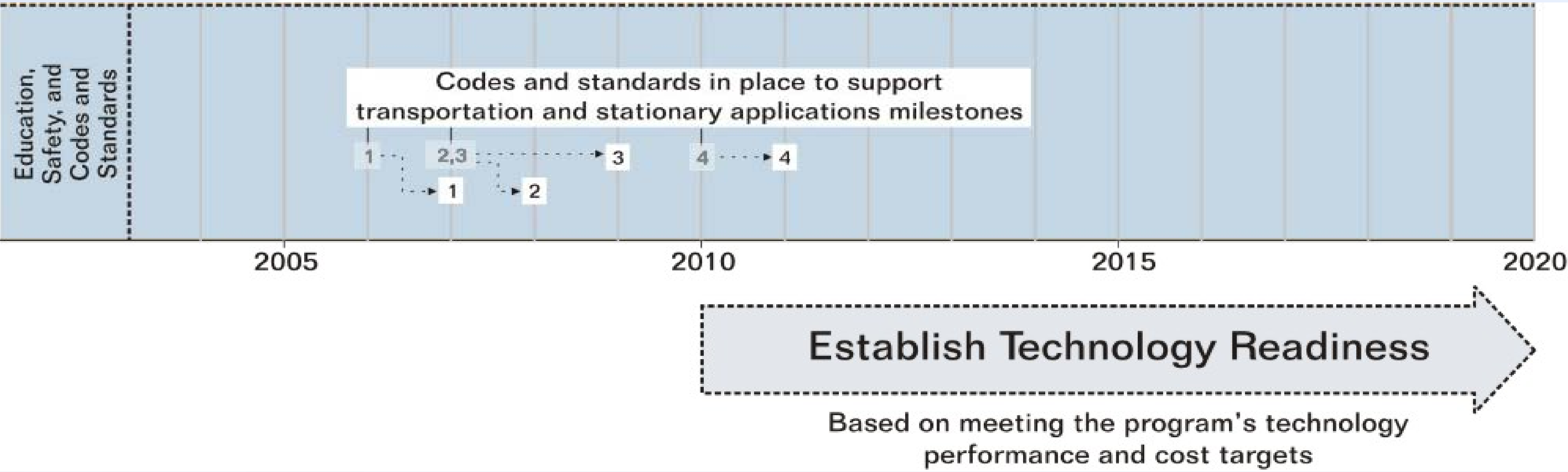
Establish Technology Readiness

Based on meeting the program's technology performance and cost targets

Validation Milestones

1. 2008: Validate stationary fuel cell system that co-produces hydrogen and electricity at 20,000 hours durability with 32% efficiency at a cost of $1500/kW or less
2. 2009: Validate polymer electrolyte membrane fuel cell vehicles at multiple sites, achieving 2,000 hours durability, a 250-mile range, and $3.00/gge of hydrogen
3. 2013: Validate stationary fuel cell system that co-produces hydrogen and electricity at 40,000 hours durability with 40% efficiency at a cost of $750/kW or less
4. 2014: Validate PEM fuel cells on operational vehicles in different climatic conditions that can be produced for $45/kW when produced in quantities of 500,000
5. 2015: Validate polymer electrolyte membrane fuel cell vehicles achieving 5,000 hours durability (service life of vehicle) and a 300-mile range

Education, Safety, and Codes and Standards Milestones and Decision Points



Codes and standards in place to support transportation and stationary applications milestones

Establish Technology Readiness

Based on meeting the program's technology performance and cost targets

Education, Safety, and Codes and Standards Milestones[e]

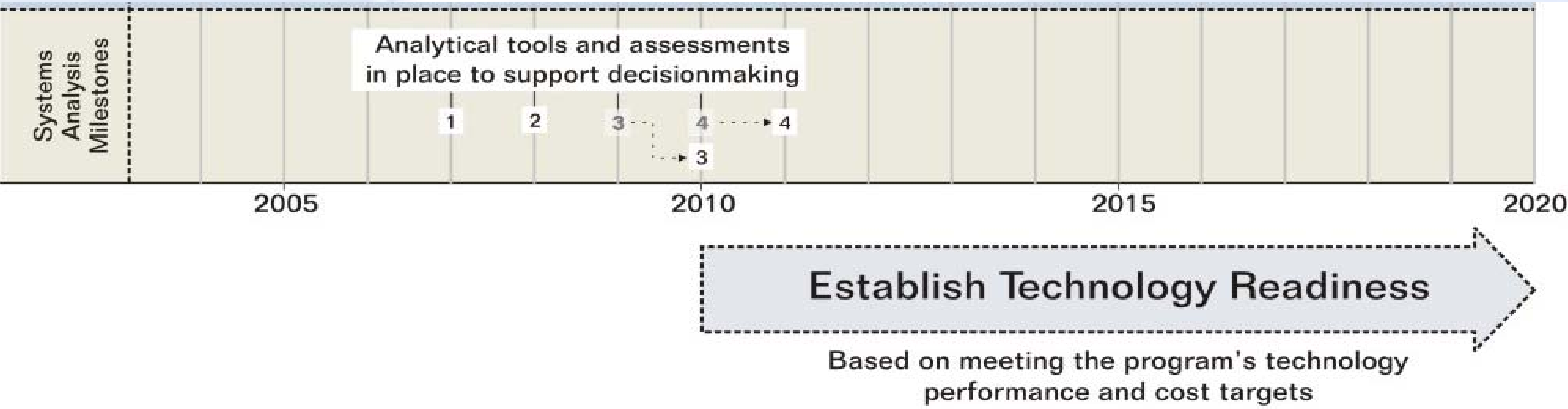
1. 2006 → 2007: Facilitate publishing domestic and international hydrogen quality standards and publish initial set of basic safety training materials

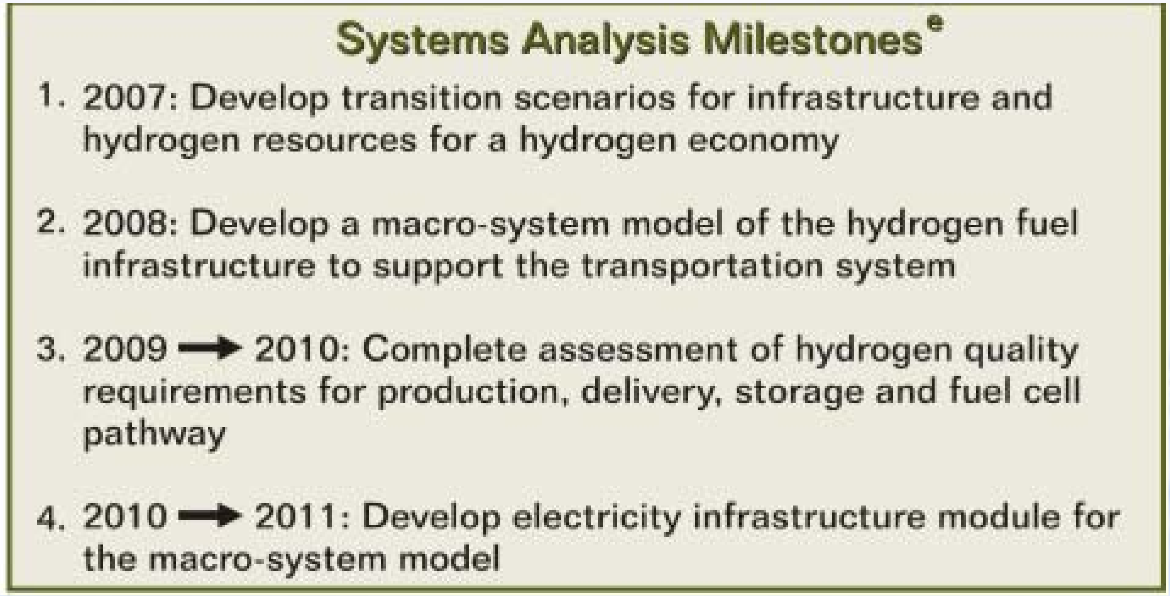
2. 2007 → 2008: Publish initial Best Practices manual for hydrogen safety

3. 2007 → 2009: Education program for safety and code officials in place

4. 2010 → 2012: Initial set of technical codes and standards in place to support demonstrations, commercialization decisions and regulatory standards

Systems Analysis
Milestones and Decision Points





Systems Analysis Milestones[e]

1. 2007: Develop transition scenarios for infrastructure and hydrogen resources for a hydrogen economy
2. 2008: Develop a macro-system model of the hydrogen fuel infrastructure to support the transportation system
3. 2009 → 2010: Complete assessment of hydrogen quality requirements for production, delivery, storage and fuel cell pathway
4. 2010 → 2011: Develop electricity infrastructure module for the macro-system model

Evaluation
and
Coordination

Program Evaluation

Annual Program Merit Review & Peer Evaluation

- Projects are rated by peers. Reviewers come from National Labs, Industry, and universities.
- Rating Criteria: relevance, approach, progress & tech transfer

FreedomCAR & Fuel Partnership

- Includes automobile and energy companies
- Technical Teams provide input on technical milestones & system needs, and review/evaluate projects:
    - ➔ Hydrogen Production
    - ➔ Hydrogen Delivery
    - ➔ Hydrogen Storage
    - ➔ Fuel Cells
    - ➔ Hydrogen Codes & Standards
    - ➔ Fuel Pathway Integration

National Academy of Sciences

- NAS reviews the program priorities & technical milestones, and evaluates progress toward achieving them.

Extensive External Coordination

Hydrogen R&D Task Force (Interagency - OSTP lead)

- Key mechanism for collaboration among 8 Federal agencies
- Provides guidance for agency research directions
- Identifies key areas for interagency collaboration

Federal/State/local (Example)

- California Fuel Cell Partnership
- California Hydrogen Highway Network

International Partnership for the Hydrogen Economy

- Accelerates the development of hydrogen and fuel cell technologies to improve their energy, environmental and economic security.
- Provides a mechanism to organize, coordinate and implement effective, efficient, and focused international RD&D and commercial utilization activities
- Provides forum for advancing policies and common codes & standards
- Educates/informs stakeholders and the general public on H_2

Next Steps

Next Steps

- Coordinate R,D&D Plan and priorities within DOE & DOT to make consistent with Posture Plan, EPACT 2005, and NAS recommendations
- Continue to implement relevant provisions of EPACT 2005
- Strengthen existing interagency coordination to ensure Federal investments in are leveraged to maximum extent.
- Identify opportunities to work more closely with emerging state-led initiatives to advance hydrogen infrastructure development.
- Complete and publish the DOE Hydrogen Program Safety Plan and the DOE Hydrogen Program Risk Management Plan.
- Promote sharing of safety-related information and maintain database of safety “learnings.”
- Increase awareness of the nation’s regulatory framework of energy, economic, and environmental policies at federal, state & local levels, and work with agencies to coordinate the timing of policy instruments and regulatory actions to meet market requirements.
- Continue DOT and DOE participation in the development of Global Technical Regulations for fuel cell light duty vehicles.
- Strengthen international cooperation on hydrogen-related R,D&D programs and on development of interoperable codes & standards through IPHE

For More Information

hydrogen.energy.gov

U.S. DEPARTMENT OF ENERGY

Hydrogen Program

hydrogen.energy.gov

- Hydrogen Production
- Hydrogen Delivery
- Hydrogen Storage
- Hydrogen Manufacturing
- Conversion/ Fuel Cells
- Applications/ Technology Validation
- Safety
- Codes & Standards
- Education
- Basic Research
- Systems Analysis
- Systems Integration

Announcements

Register now for the 2006 Annual Merit Review

News

DOE Releases New Analysis Tools for Hydrogen Delivery Technologies
DOE's H2A Analysis Group recently developed two H2A delivery models: the H2A Delivery Components Model and the H2A Delivery Scenario Model.
April 26, 2006 More >

DOE Seeks Public Comment on Draft Paper on the Potential Roles of Ammonia in a Hydrogen Economy
A draft paper that identifies, evaluates, and summarizes the key issues and advantages and disadvantages associated with ammonia for on-board vehicular hydrogen storage is now available for public comment.
April 25, 2006 More >

New Resource Offers Analytical Data and Tools
The Hydrogen Analysis Resource Center provides well-documented, reliable data for hydrogen-related calculations, modeling, and other analytical activities.
March 31, 2006 More >

President's Hydrogen Fuel Initiative

2005 A
Review a
Evaluation
(released 9/0

National E
Policy
(PDF 3.05 MB)

DOE Strategic Plan

Introductory fact sheets available in the web site library

All hard copy documents, fact sheets, CDs, etc. can be ordered free-of-charge

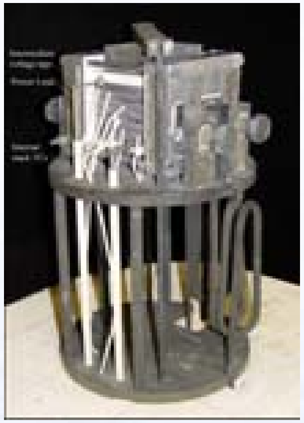
Additional Information

Nuclear Hydrogen Initiative Focus and Goals

Focus: Hydrogen production technologies that are compatible with nuclear energy systems and do not produce greenhouse gases

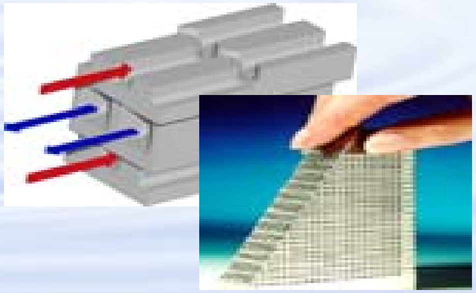
Research Focus Areas

- Thermochemical Systems
- High-Temperature Steam Electrolysis
- Reactor/Process Interface Technologies



Major Program Milestones

- FY 2008: Operate of laboratory-scale hydrogen production experiments
- FY 2011: Select hydrogen production technology for Next Generation Nuclear Plant (per Energy Policy Act)
- FY 2014: Operation of pilot-scale hydrogen production experiments
- FY 2019: Demonstrate commercial-scale hydrogen production system for use with nuclear reactors



Hydrogen from Coal

Goals

Facilitate the transition to a sustainable hydrogen economy through the use of coal, our largest domestic fossil resource

Objectives

Production: Central Pathway

- **By 2015, demonstrate a 60% efficient, zero-emission, coal-fueled hydrogen and power co-production facility that reduces the cost of hydrogen by 25% compared to current coal-based technology.**

Production: Alternative Hydrocarbon Pathway

- **By 2011, an alternative hydrocarbon pathway and reforming system for sub-central/decentralized hydrogen from coal is available.**

Technology Challenges

- **Reduce cost/improve efficiency**
  - **Clean synthesis gas production**
  - **H_2 separation & purification**
  - **Process intensification**
- **Capture and store carbon**
- **Integrate technologies into FutureGen**

FY05 Basic Research : Solicitation & Research Highlights

Basic Research Needs for the Hydrogen Economy

Report of the Basic Energy Sciences Workshop on Hydrogen Production, Storage, and Use

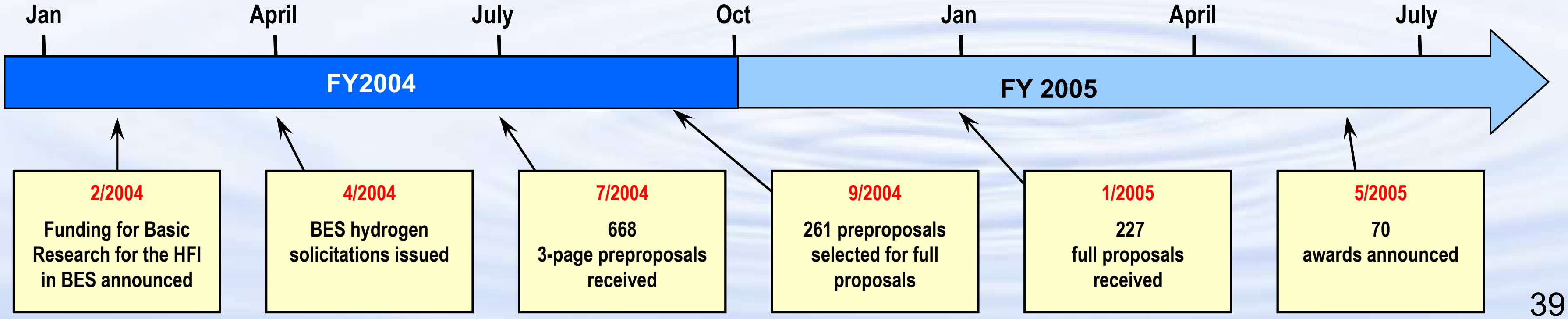
May 13-15, 2003

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

> *"Bridging the gaps that separate the hydrogen- and fossil-fuel based economies in cost, performance, and reliability goes far beyond incremental advances in the present state of the art. Rather, fundamental breakthroughs are needed in the understanding and control of chemical and physical processes involved in the production, storage, and use of hydrogen. Of particular importance is the need to understand the atomic and molecular processes that occur at the interface of hydrogen with materials in order to develop new materials suitable for use in a hydrogen economy. New materials are needed for membranes, catalysts, and fuel cell assemblies that perform at much higher levels, at much lower cost, and with much longer lifetimes. Such breakthroughs will require revolutionary, not evolutionary, advances. Discovery of new materials, new chemical processes, and new synthesis techniques that leapfrog technical barriers is required. This kind of progress can be achieved only with highly innovative, basic research."*

FY05 solicitation based on the five priority research areas identified by the workshop report:

- 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



2/2004
Funding for Basic Research for the HFI in BES announced

4/2004
BES hydrogen solicitations issued

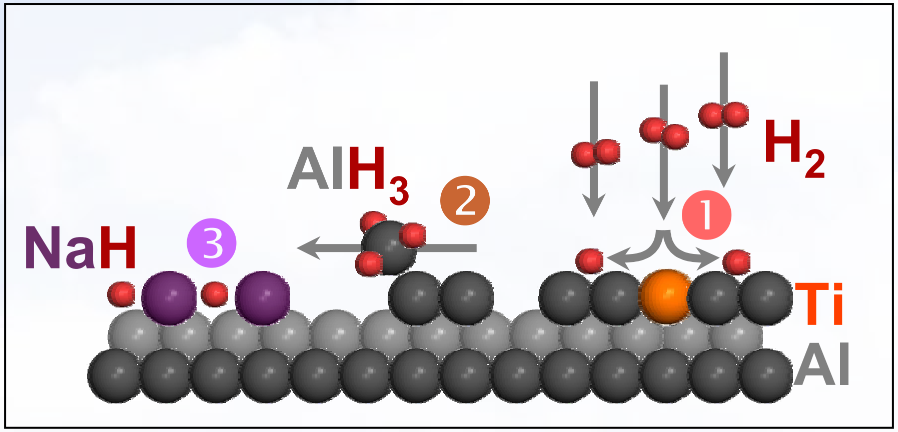
7/2004
668
3-page preproposals received

9/2004
261 preproposals selected for full proposals

1/2005
227
full proposals received

5/2005
70
awards announced

Hydrogen Storage: Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides



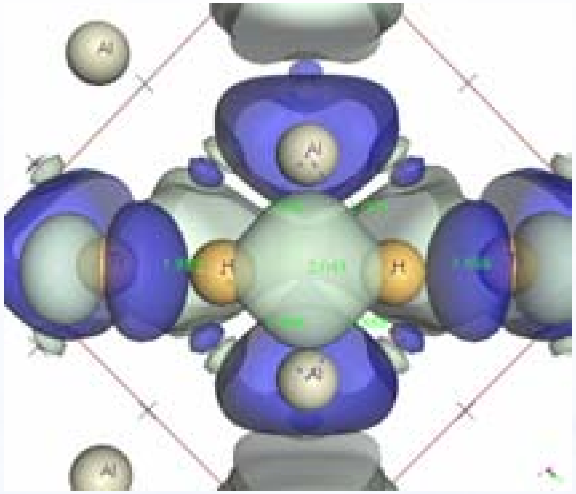
- Titanium-doped sodium alanate ($NaAlH_4$) is the only known complex hydride material that stores hydrogen reversibly at moderate temperature and pressure. A quantitative understanding of the atomic-scale mechanisms underlying the facile reversible hydrogen storage is needed.

Key: Hydrogenation ("fueling") reaction

❶ Di-hydrogen (H2) adsorption & dissociation
❷ Formation & diffusion of mobile surface species
❸ Solid state reaction with sodium hydride (NaH).

Key step in the hydrogenation of $NaAlH_4$ identified

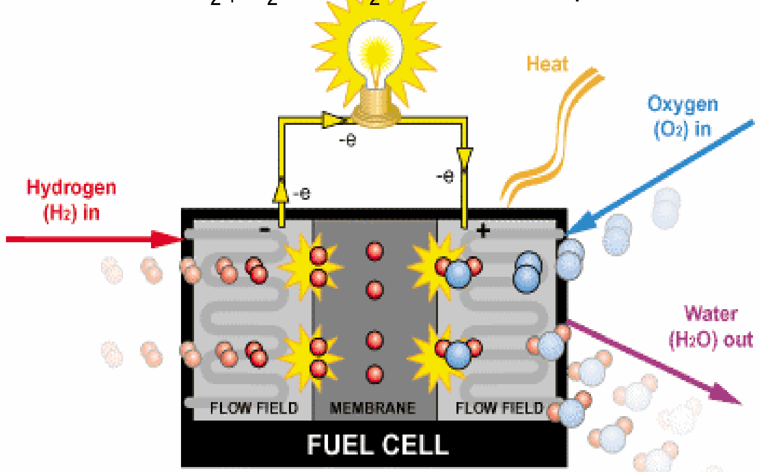
- A specific Ti:Al complex near the (001) surface of Al in the hydrogen-depleted storage material has been predicted by atomistic first-principles theory to be highly efficient in dissociating di-hydrogen (H_2) to atomic-H, part ❶ of the "fueling" reaction to hydrogen-rich $NaAlH_4$.
- This finding is an important step toward understanding how Ti catalysts enable fast hydrogen uptake and release in $NaAlH_4$. It demonstrates how catalysts may be used to enhance reaction rates in other candidate materials for the storage of hydrogen, a fundamental requirement in a future hydrogen economy.



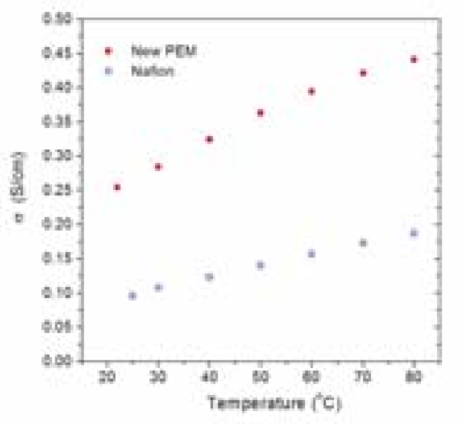
Molecular orbital model showing the Ti-doped Al surface with hydrogen. The model shows the highest occupied molecular orbital (HOMO) configuration after the H_2 adsorption and spontaneous dissociation of the H-H bond. Light/dark blue represents different signs of the orbital.

Membranes: Micro- & Nano-Patterning Boost Power Output and Miniaturization of Fuel Cells

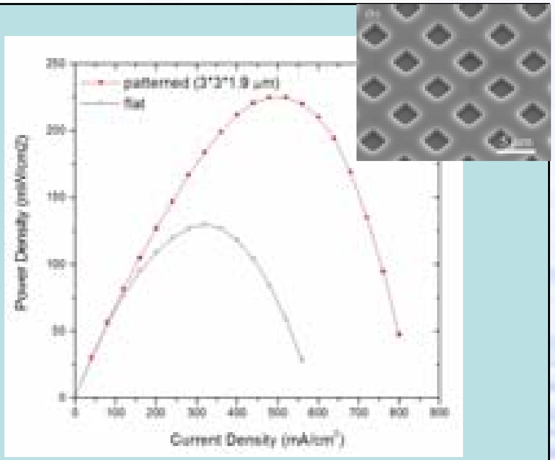
Fuel Cells: $2H_2 + O_2 \rightarrow 2H_2O$ + electrical power + heat



Membrane conducts protons from anode to cathode



New “liquid PEMs” have higher acid content and therefore higher conductivity than Nafion™



Lithographically patterned “liquid PEMs” lead to higher surface area of the membrane and the catalyst, and therefore, to higher power density of fuel cell

Traditional fuel cell proton exchange membranes (PEMs) such as Nafion™ , the current gold standard, have limitations:

- Have lower-than-desirable conductivity
- Require high humidity for optimal operation, which reduces durability
- Difficult to process, requiring high temperature melt extrusion, followed by exhaustive hydrolysis
- Has smooth surfaces and thus low active surface areas

New Photochemically cured “liquid PEMs” was recently developed:

- Liquid precursors converted directly into membranes
- Can be cured into any desired shape including very thin films
- Can be chemically cross-linked

  Enables higher acid content

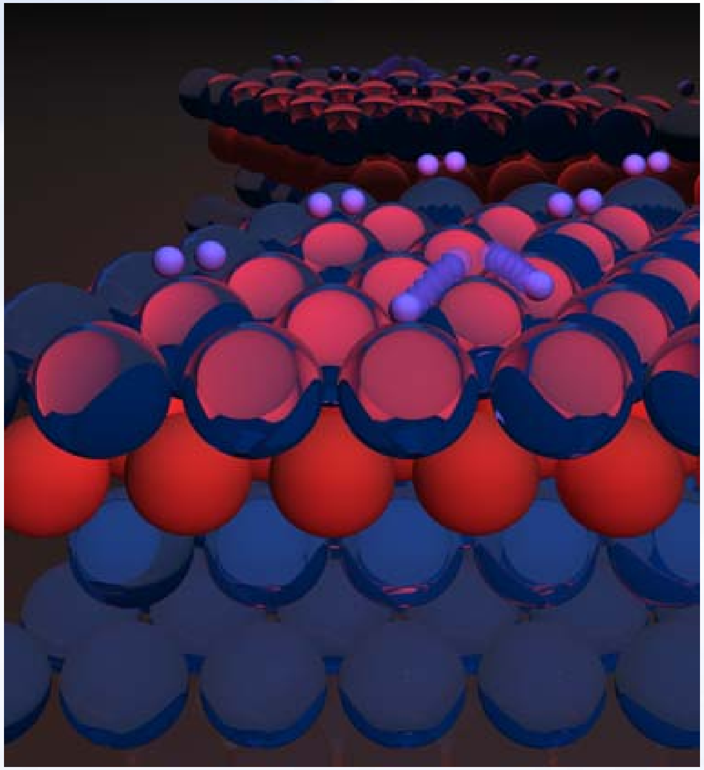
  ~ 250% increase in conductivity demonstrated

  Result in higher durability and better performance at lower humidity
- Can be patterned into high-surface area PEMs by soft lithography and micro-molding techniques

  ~ 200% increase in power density

  Could lead to significant size/weight reduction

Catalysts: Predicting Catalysts for Hydrogen Production, Storage or Fuel-Cell Utilization

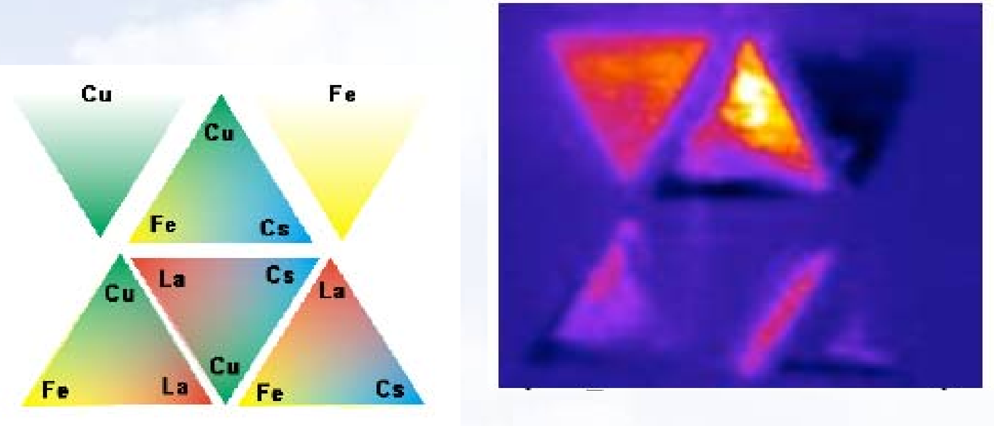


Theoretical calculation of molecular hydrogen undergoing dissociation over near-surface alloys.

- Small purple spheres: **hydrogen**
- Blue spheres: **platinum** atoms
- Red spheres: **nickel** atoms
- **Bicolor** blue and red spheres: platinum atoms whose electronic properties have been dramatically altered by the underlying nickel.

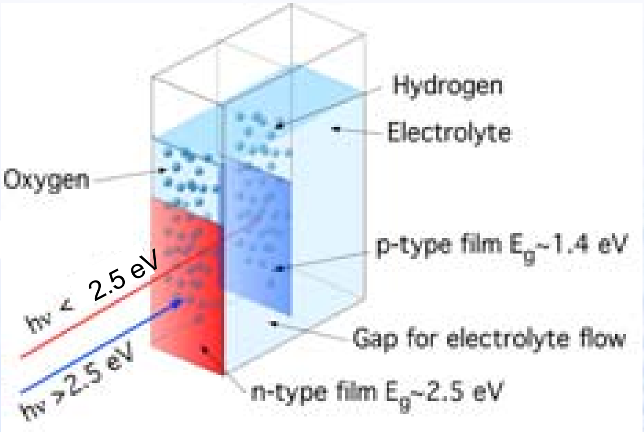
- Production of hydrogen from biomass or fossil fuels at the large scales commensurate with future demands of a hydrogen-fuel economy calls for low-temperature, highly efficient and durable catalysts, non-existent today.
- New structures and compositions are now being predicted *a priori*, rather than searched empirically, thanks to recent advances in computational quantum chemistry and molecular dynamics.
- Near-surface alloys of two transition metals are unnatural structures that have recently been discovered through calculations. Single metallic layers of one metal embedded within a matrix of another metal have the requisite properties for low-energy hydrogen scission and recombination. No natural materials or homogeneous alloys display BOTH of these properties simultaneously.
- Nickel within platinum, as an example, can attach atomic hydrogen as weakly as inert metals like copper and gold, while simultaneously it can dissociate molecular hydrogen as rapidly as noble metals like platinum and rhodium. Experimental validation has demonstrated the feasibility of this new concept.
- Several families of new alloys with novel architectures and compositions have been identified as potentially suitable for hydrogen reactions, and await experimental validation. This is a rare instance in which theoretical catalysis precedes experiments.
- This study may lead to breakthroughs in the challenging technologies of rapid hydrogen storage and release at room temperature, or selective extraction of hydrogen from natural gas at low temperature, or high-activity hydrogen electrodes for fuel cells.

Solar Hydrogen Production: The Search for the Ideal Mixed-Metal Oxide Photoelectrode



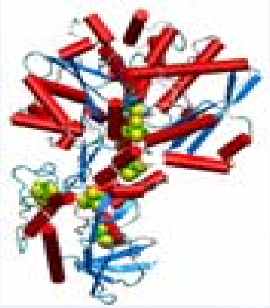
Ink jet patterning of metal oxides

Operational cell for solar water splitting

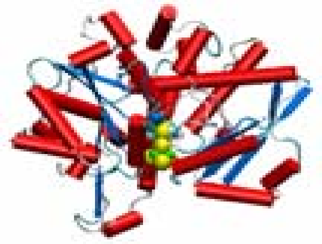


- Solar water splitting by semiconductor electrodes is the ideal method for production of hydrogen fuel.
- A novel high-throughput search seeks to move beyond known single-oxide semiconductors which are inefficient at water splitting in order to find a semiconductor with the band gap of 1.6eV to 2.0 eV needed for simultaneous hydrogen and oxygen evolution.
- This search follows the lead of high temperature superconductors, such as tetrametallic $HgBa_2CaCu_2O_{6+\alpha}$, by seeking compound metal oxides for water splitting that contain up to four different metals. Some metals are found to provide structure and stability, some the color of light absorption, while others are added for charge compensation and recombination suppression.
- The high throughput search is made possible with the use of a three-cartridge ink jet printer where the cartridges are filled with different metal nitrate precursor solutions. Many thousands of candidate compositions of metal oxide semiconductors can be screened.
- A triangular pattern with all possible variations of the three metal inks is printed on a conductive glass where each position contains a different combination of metals. The triangle is scanned point by point with a laser to assess the potential of each combination for water splitting.

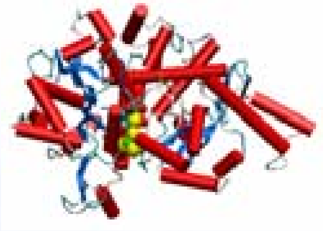
Bio-Inspired Processes: Effects of structure truncation on Oxygen Tolerance of Hydrogenase



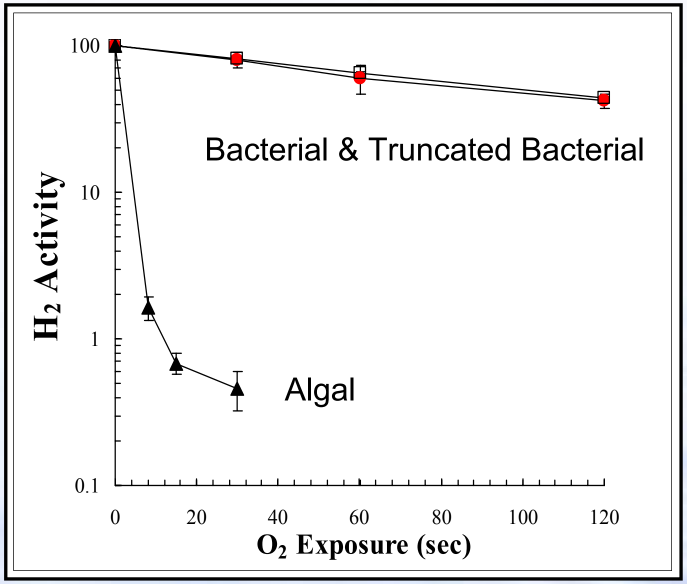
Bacterial



Truncated Bacterial (Genetically Modified)



Algal



- Large scale production of hydrogen by mimicking the processes used by Nature, either in algae or in bacteria, is an attractive strategy.
- While the hydrogenases in algae and bacteria have similar hydrogen production activities, [FeFe]-hydrogenase from bacterium is >100 times more tolerant of oxygen than algal enzyme.
- Natural hydrogenases (e.g., bacterial enzyme) typically have large protein residues surrounding the Fe-S active site, and thus are not robust enough to operate under non-biological conditions.
- A truncated bacterial enzyme with a simpler structure has been developed and exhibited oxygen tolerance similar to natural systems.
- Subtle structural differences between truncated bacterial and algal enzymes provide important insights into the origins of oxygen-tolerance and could guide the design of other bio-mimetic hydrogen production systems.
- Simplified and robust synthetic mimics of bacterial hydrogenase are essential for the development of a commercial hydrogen-producing system that is cost effective, scalable to large production, non-polluting, and self-sustaining.

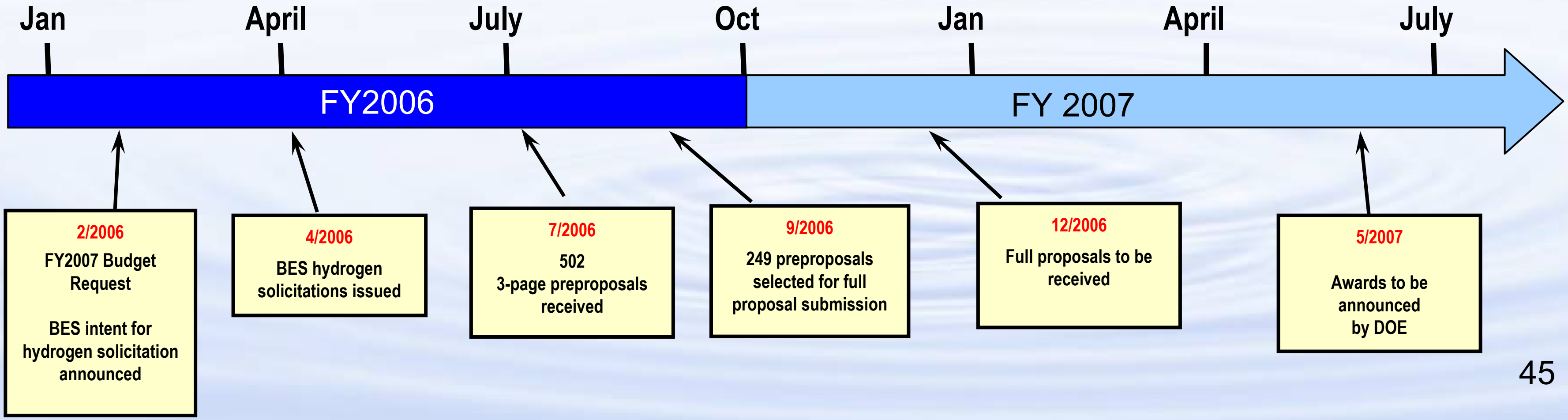
FY07 Basic Research Solicitation

FY07 solicitation focuses on the following three areas:

- Novel materials for hydrogen storage
- Functional membranes
- Nanoscale catalysts

BES received 502 pre-applications and pre-proposals in response to FY 2007 Basic Research for the Hydrogen Fuel Initiative solicitations. Based on the reviews and recommendations of DOE program mangers, principal investigators of 249 submissions have been encouraged to submit full proposals. A breakdown by research category is given in the table at right. Full proposals are expected by December 12, 2006.

	Pre-proposals Received		Pre-proposals Encouraged	
	Grant	Lab	Grant	Lab
Novel materials for hydrogen storage	150	14	74	12
Functional membranes	130	16	62	13
Nanoscale catalysts	175	17	77	11
Total	455	47	213	36
	502		249	



2/2006
FY2007 Budget Request

BES intent for hydrogen solicitation announced

4/2006
BES hydrogen solicitations issued

7/2006
502
3-page preproposals received

9/2006
249 preproposals selected for full proposal submission

12/2006
Full proposals to be received

5/2007
Awards to be announced by DOE