U.S. Department of Energy
Hydrogen Program

Office of Science
Basic Energy Sciences

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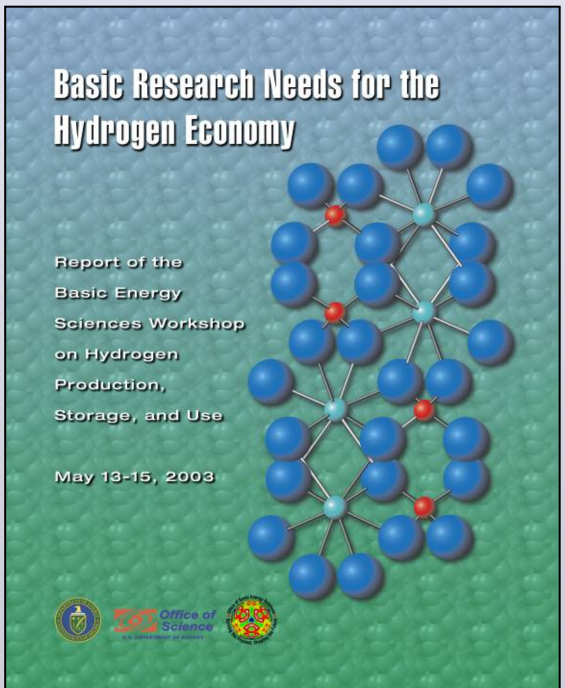
Office of Basic Energy Sciences

2008 DOE Hydrogen Program
Merit Review and Peer Evaluation Meeting

June 9, 2008

Goal and Objectives

The Office of Basic Energy Sciences within DOE held a workshop in May, 2003 on Basic Research Needs for the Hydrogen Economy, which formed the scientific basis for our solicitations in 2004 and 2007.



"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."

http://www.sc.doe.gov/bes/reports/files/NHE_rpt.pdf

2005: BES-HFI Initiative Awards
*$64.5M total; $21.5M annual***

Novel Materials for Hydrogen Storage
(17 projects, $19.8M*)

Universities:
- MIT[1]
- Washington
- Pennsylvania
- Colorado School of Mines
- Georgia Tech
- Louisiana Tech
- Missouri-Rolla
- Georgia
- Tulane
- Southern Illinois

DOE Labs:
- Ames
- Brookhaven
- Lawrence Berkeley
- Oak Ridge
- Pacific Northwest
- Savannah River

Membranes for Separation, Purification, & Ion Transport
(16 projects, $12.3M*)

Universities:
- Utah
- Clemson
- Carnegie Mellon
- Rensselaer
- Lehigh
- Pennsylvania
- Case Western Reserve
- Tennessee
- Vanderbilt
- CalTech
- Rochester
- North Carolina
- Cornell

DOE Labs:
- Lawrence Berkeley
- Los Alamos
- Pacific Northwest

Design of Catalysts at the Nanoscale
(18 projects, $15.8M*)

Universities:
- Pittsburgh
- Tufts
- MIT
- Wisconsin
- California-Santa Barbara
- Wyoming
- Yale
- Texas A&M
- Johns Hopkins
- Illinois[1]
- Texas Tech
- Arizona State

DOE Labs:
- Argonne
- Stanford Linear Accelerator Ctr
- Brookhaven
- Sandia
- Oak Ridge

Solar Hydrogen Production
(13 projects, $10M*

Universities:
- Colorado State
- Cal Tech
- Arizona
- California-Santa Cruz
- Penn State[1]
- Purdue
- Washington
- Virginia Tech

Industry:
- Nanoptek Corp.

DOE Labs:
- Brookhaven
- Pacific Northwest
- National Renewable Energy

Bio-Inspired Materials and Processes
(6 projects, $7M*)

Universities:
- Penn State
- Washington
- North Carolina State
- Georgia
- Pennsylvania

DOE Labs:
- National Renewable Energy

In 2006 a small number of additional awards were issued, bringing the BES HFI funding to a total of $32.4M/yr

* Over three years

[1] Selected for 2 awards

**This represents new funding, bringing the total BES funding of Hydrogen research to $29.2M/yr

2007: BES-HFI Initiative Awards
$12.5M total; $3.9M annual

Novel Materials for Hydrogen Storage
(8 projects, $6.5M*)

Universities:
- Missouri-Columbia
- California-Santa Barbara
- Florida International
- Rutgers
- California-Davis
- South Florida
- Northwestern

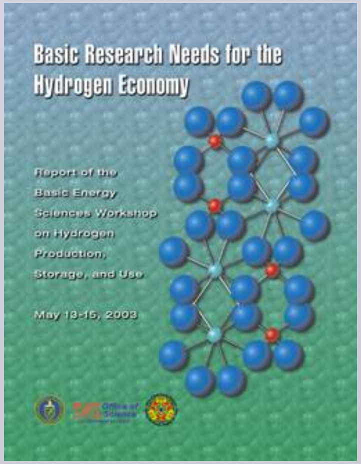
DOE Labs:
- Oak Ridge

Design of Catalysts at the Nanoscale
(7 projects, $6.0M*)

Universities:
- Virginia
- Georgetown
- Ohio State
- Arizona State

DOE Labs:
- Argonne
- Brookhaven
- Pacific Northwest

* Over three years

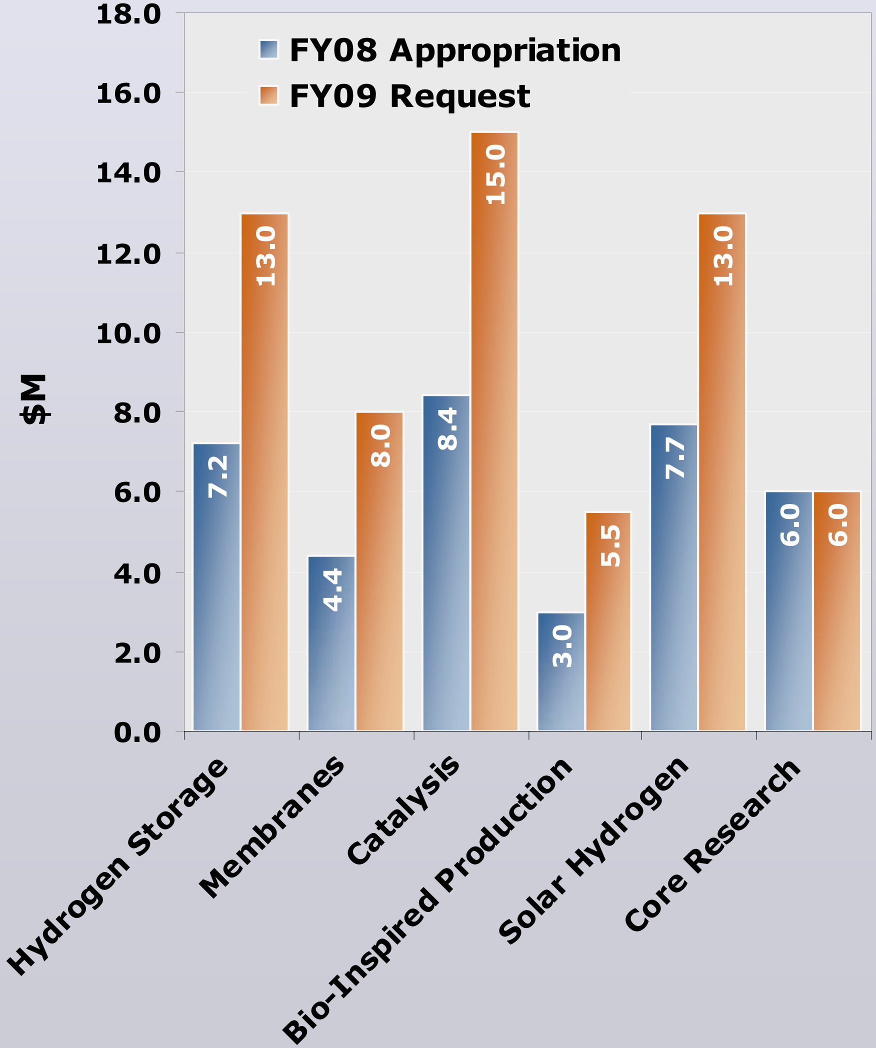


In 2006 BES issued another solicitation for basic research in hydrogen. A total of 502 pre-proposals were received, 249 selected for submission of a full proposal, and 229 full proposals were received and reviewed by peer-review panels. Due to a reduction in anticipated HFI funding for FY07 only 15 new proposals were initiated with a concentration in the areas of Hydrogen Storage and Nanoscale Catalysts. No additional money for the HFI was appropriated to BES in FY08 so the remaining 214 proposals were declined.

Budget

FY2009 Budget Request = $60.4M

FY2008 Budget = $36.4M



Emphasis

Continued focus on critical basic research needs for the hydrogen economy:

- Hydrogen Storage
- Membranes
- Nanoscale Catalysts
- Bio-Inspired Hydrogen Production
- Solar Hydrogen Production

The Scientific Opportunities in BES

Identified in The “Basic Research Needs …” Workshop Series, *Identifying Basic Research Directions for Today’s and Tomorrow’s Energy Technologies*

Basic Research Needs for a Secure Energy Future (BESAC)

- **Basic Research Needs for the Hydrogen Economy**
- Basic Research Needs for Solar Energy Utilization
- Basic Research Needs for Superconductivity
- Basic Research Needs for Solid State Lighting
- Basic Research Needs for Advanced Nuclear Energy Systems
- Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels
- Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems
- Basic Research Needs for Electrical Energy Storage
- Basic Research Needs for Catalysis for Energy Applications
- Basic Research Needs for Materials under Extreme Environments

www.science.doe.gov/bes/reports/list.html

Important Recurring Themes from the Workshops

Control of materials properties and functionalities through electronic and atomic design

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- “Control” of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designer catalysts
- Designer interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation

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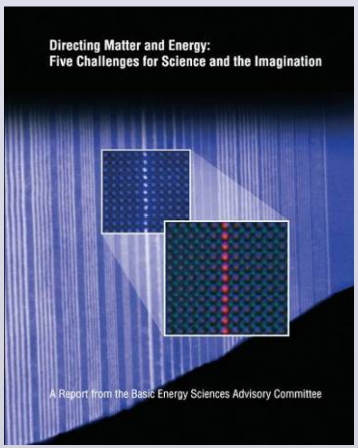
One Additional Workshop: Science Grand Challenges

How does nature execute electronic and atomic design? How can we?

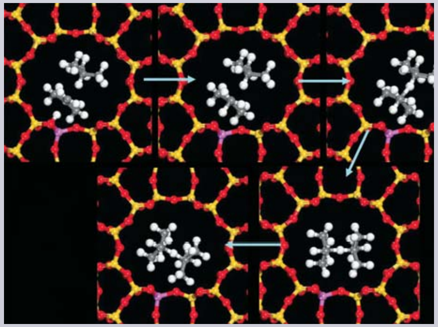
Directing Matter and Energy: Five Challenges for Science and the Imagination



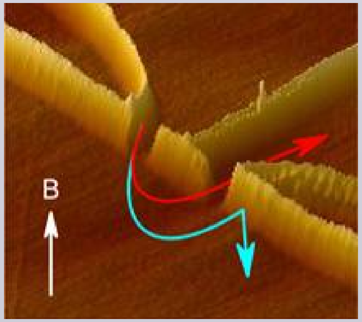
- **Control the quantum behavior of electrons in materials**
  Imagine: Direct manipulation of the charge, spin and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun's energy into fuel through artificial photosynthesis.
- **Synthesize, atom by atom, new forms of matter with tailored properties**
  Imagine: Create and manipulate natural and synthetic systems that will enable catalysts that are 100% specific and produce no unwanted byproducts, or materials that operate at the theoretical limits of strength and fracture resistance, or that respond to their environment and repair themselves like those in living systems
- **Control emergent properties that arise from the complex correlations of atomic and electronic constituents**
  Imagine: Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO_2 from atmospheric gases yet maintain high throughput.
- **Synthesize man-made nanoscale objects with capabilities rivaling those of living things**
  Imagine: Master energy and information on the nanoscale, leading to the development of new metabolic and self-replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision measurement tools as in molecular rulers, and defect-tolerant electronic circuits
- **Control matter very far away from equilibrium**
  Imagine: Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere.

The Essential Role of Basic Science in Addressing the Energy Problem

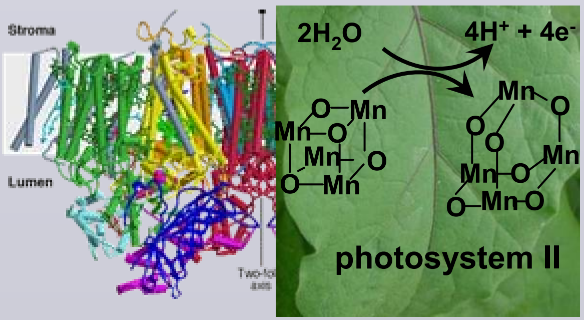
- Today's energy technologies and infrastructure are rooted in 20th Century technologies and 19th Century discoveries—internal combustion engine, electric lighting, alternating current.
- Current fossil energy sources, current energy production methods, and current technologies cannot meet the energy challenges we now face.
- We need transformational discoveries and truly disruptive technologies.
- 21st Century technologies will require the ability to direct and control matter down to the molecular, atomic, and quantum levels.



Computed mechanism for the catalytic coupling of two four-carbon molecules to create an eight-carbon, fuel-like molecule



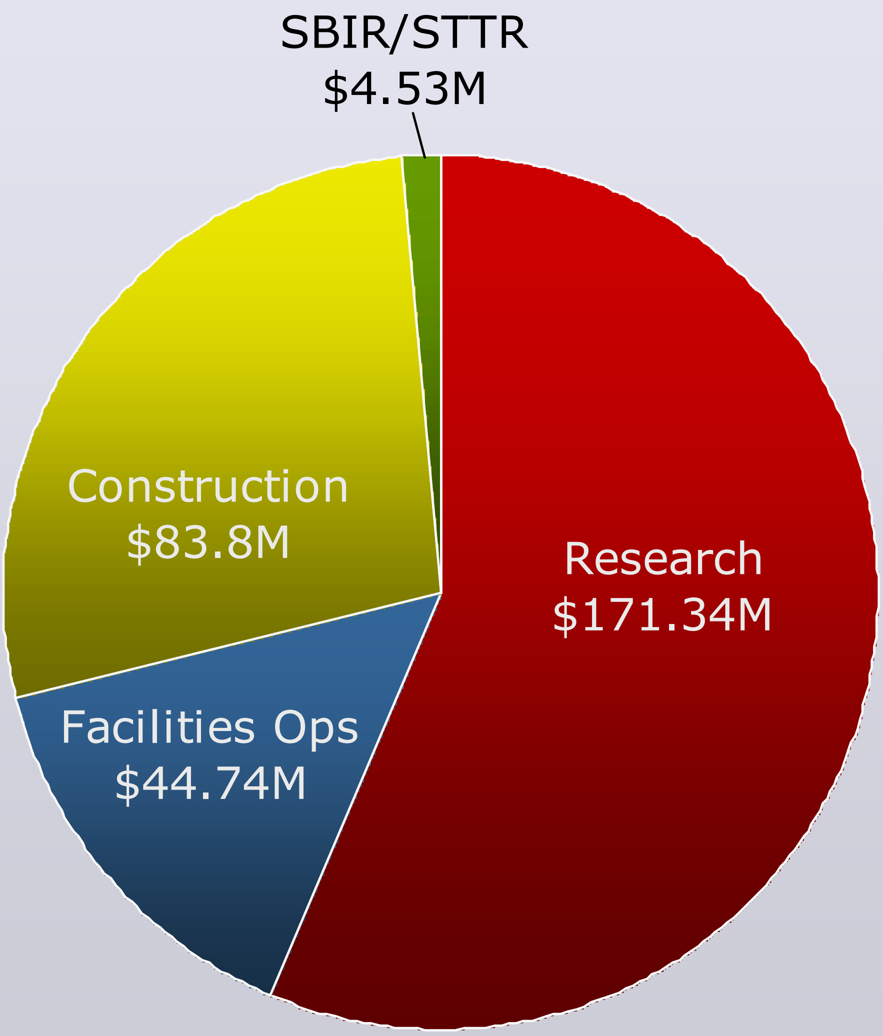
Separating electrons by their spin for "spintronics" and other applications of electron control.



Bio-inspired nanoscale assemblies – self-repairing and defect-tolerant materials and selective and specific chemical reactivity.

Summary of FY09 BES Budget Increases

Of the $298.3M increase in the requested FY09 budget for BES, $161M is slated for new research. Approximately $100M of this will go towards funding Energy Frontier Research Centers and the rest towards single PI or small-group awards through our Core Programs. **Research in Hydrogen, totaling $60.4M in FY09, will be an important part of both.**



Energy Frontier Research Centers

Tackling our energy challenges in a new era of science

Energy Frontier Research Centers will bring together the skills and talents of multiple investigators to enable research of a scope and complexity that would not be possible with the standard individual-investigator or small-group award.

The DOE Office of Science, Office of Basic Energy Sciences, announced the Energy Frontier Research Centers (EFRCs) program. Pending appropriations, up to $100M will be available in FY2009 for EFRC awards that are $2–5 million/year for an initial 5-year period. Universities, labs, nonprofits, and for-profit entities are eligible to apply.

Energy Frontier Research Centers will pursue fundamental research that addresses both energy challenges and science grand challenges in areas such as:

- Solar Energy Utilization
- Catalysis for Energy
- Electrical Energy Storage
- Solid State Lighting
- Superconductivity
- Bioenergy and biofuels
- Geosciences for Nuclear Waste and CO_2 Storage
- Advanced Nuclear Energy Systems
- Combustion of 21st Century Transportation Fuels
- **Hydrogen Production, Storage, and Use**
- Materials Under Extreme Environments

EFRC Funding Opportunity Announcement was published on April 4, 2008. See: http://www.sc.doe.gov/bes/EFRC.html

Single-Investigator and Small-Group Research

Tackling our energy challenges in a new era of science

- Pending appropriations, up to $60M will be available for single-investigator and small-group awards in FY2009.
- BES seeks applications in two areas: grand challenge science and energy challenges identified in one of the Basic Research Needs workshop reports.
- Awards are planned for three years, with funding in the range of $150-300k/yr for single-investigator awards and $500-1500k/yr for small-group awards (except as noted below)
- Areas of interest include:
  - ***Grand challenge science:*** ultrafast science; chemical imaging, complex & emergent behavior
  - ***Tools for grand challenge science:*** midscale instrumentation; accelerator and detector research (awards capped at $5M over 3-year project duration)
  - ***Use inspired discovery science:*** basic research for electrical energy storage; advanced nuclear energy systems; solar energy utilization; **hydrogen production, storage, and use**; other basic research areas identified in BESAC and BES workshop reports with an emphasis on nanoscale phenomena
- For full details see: http://www.sc.doe.gov/bes/SISGR.html

2008 Progress & Accomplishments

Research Highlights

- Hydrogen Storage
- Catalysis
- Membranes
- Solar Hydrogen
- Bio-inspired and Biomimetic Hydrogen Production