DOE Hydrogen Program Merit Review and Peer Evaluation Meeting

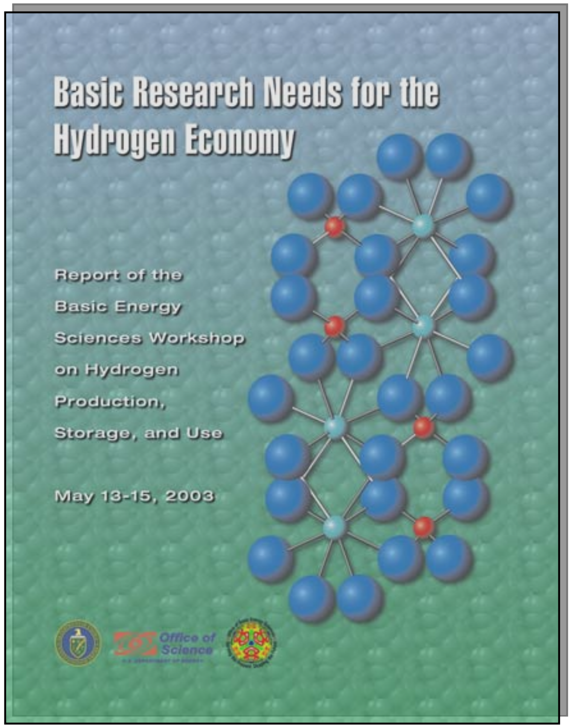
Basic Research Needs for the Hydrogen Economy

New Research Activities in DOE's Office of Basic Energy Sciences

Harriet Kung
Director, Materials Sciences and Engineering Division
Office of Basic Energy Sciences
Office of Science
U.S. Department of Energy

23 May 2005

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."

Workshop Chair:	Millie Dresselhaus	(MIT)
Associate Chairs:	George Crabtree	(ANL)
	Michelle Buchanan	(ORNL)

Challenges for the Hydrogen Economy

From the Report* of the National Research Council, 2004

"The committee believes that for hydrogen-fueled transportation, the four most fundamental technological and economic challenges are :

1. To develop and introduce cost-effective, durable, safe, and environmentally desirable fuel cell systems and hydrogen storage systems.
2. To develop the infrastructure to provide hydrogen for the light-duty vehicle user.
3. To reduce sharply the costs of hydrogen production from renewable energy sources, over a time frame of decades.
4. To capture and store ("sequester") the carbon dioxide byproduct of hydrogen production from coal.

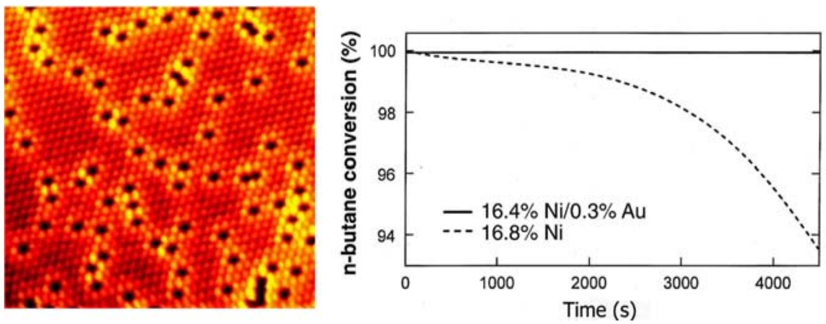
Basic and applied research and development are needed to address the challenges identified.
Basic research will contribute most to challenges 1 and 3.

*THE HYDROGEN ECONOMY: OPPORTUNITIES, COSTS, BARRIERS, AND R&D NEEDS
Committee on Alternatives and Strategies for Future Hydrogen Production and Use
NRC Board on Energy and Environmental Systems, Division on Engineering and Physical Sciences

Priority Research Areas in Hydrogen Production

Fossil Fuel Reforming

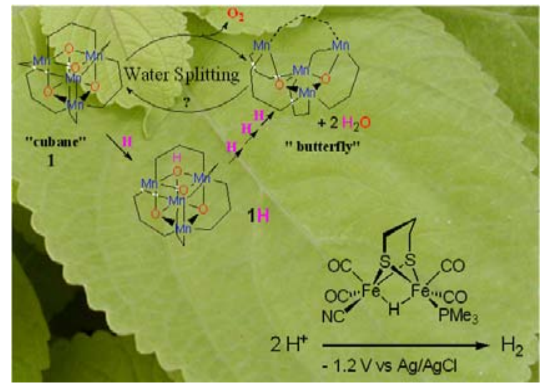
Catalysis; membranes; theory and modeling; nanoscience



Ni surface-alloyed with Au to reduce carbon poisoning

Bio- and Bio-inspired H_2 Production

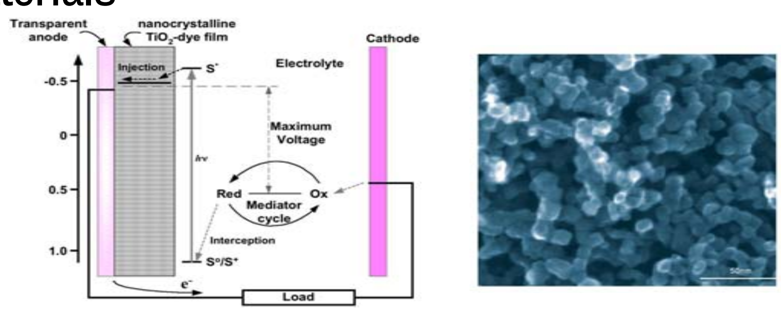
Biological enzyme catalysis; nanoassemblies; bio-inspired materials and processes



Synthetic catalysts for water oxidation and hydrogen activation

Solar Photoelectrochemistry/Photocatalysis

Understanding physical mechanisms; novel materials; theory and modeling; stability of materials

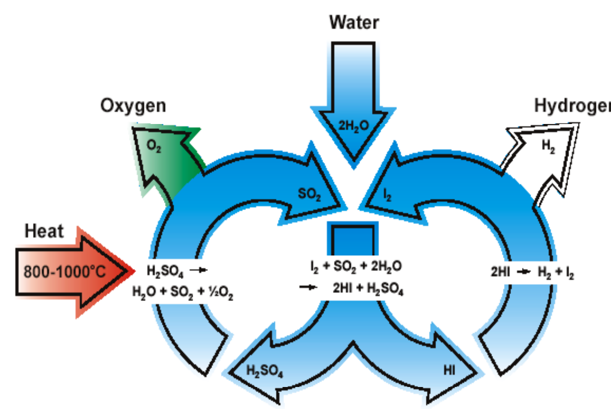


Dye-Sensitized solar cells

Nuclear and Solar Thermal Hydrogen

Thermodynamic data and modeling; novel materials; membranes and catalysts

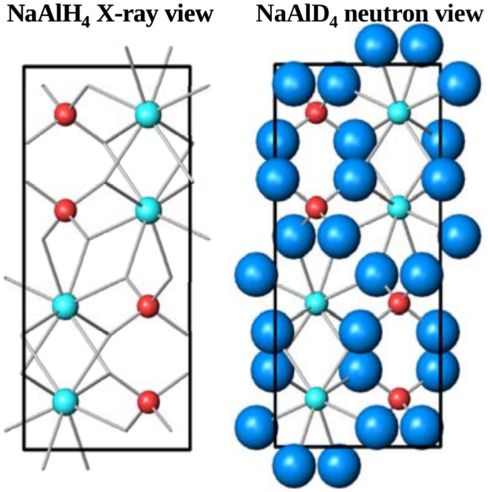
High T operation places severe demands on reactor design and on materials



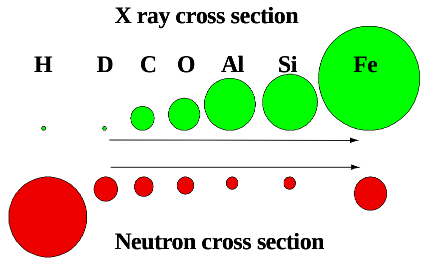
Source: BES Hydrogen Workshop Report

Priority Research Areas in Hydrogen Storage

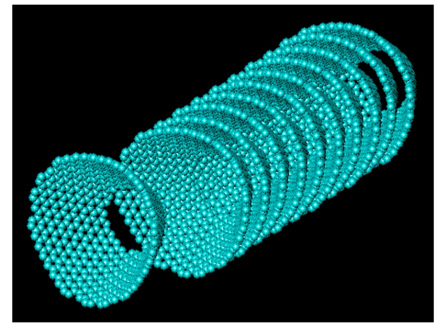
Novel and Nanoscale Materials



Complex metal hydrides can be recharged on board the vehicles

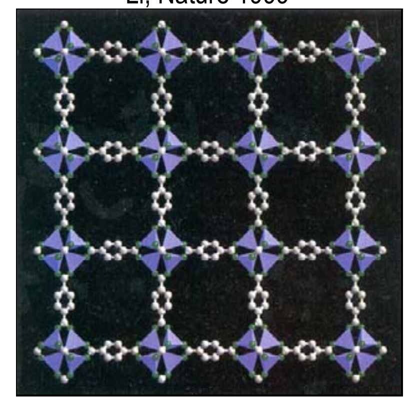


Neutron imaging of hydrogen

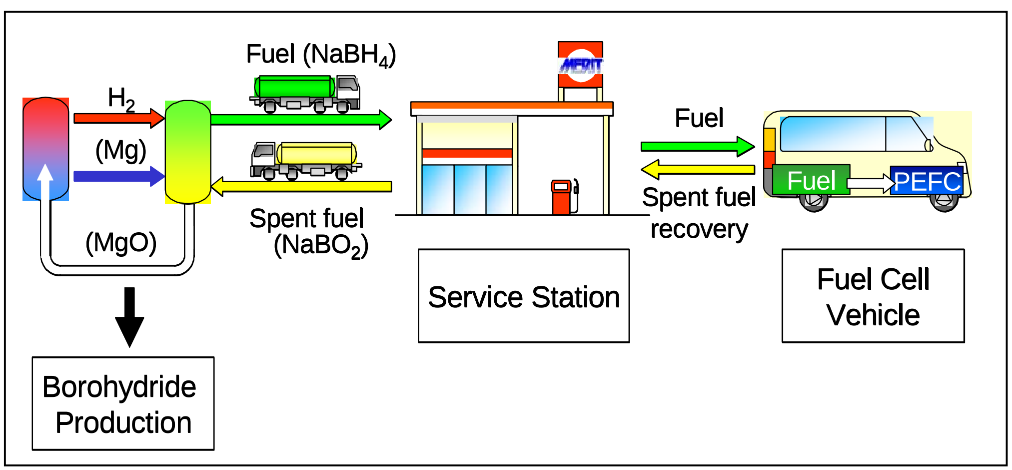


Cup-stacked carbon Nanofiber

Li, Nature 1999



Nanoporous inorganic-organic compounds

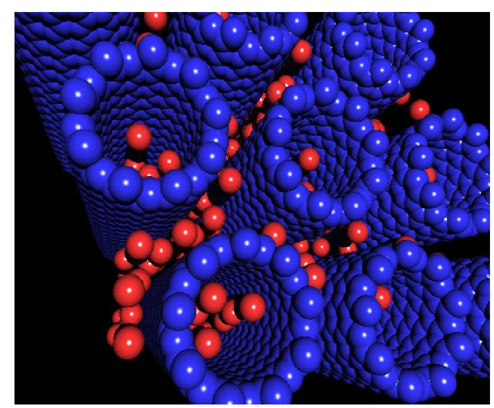


Chemical hydrides will need off-board regeneration

Theory and Modeling

To Understand Mechanisms, Predict Property Trends, Guide Discovery of New Materials

H Adsorption in nanotube array

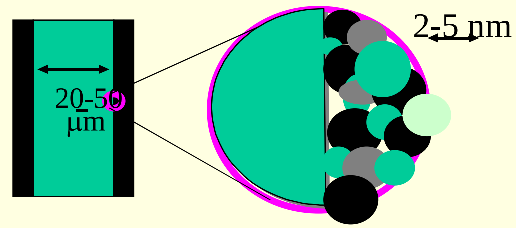


Source: BES Hydrogen Workshop Report

Priority Research Areas in Fuel Cells

Electrocatalysts and Membranes

Non-noble metal catalysts; designed triple-percolation electrodes

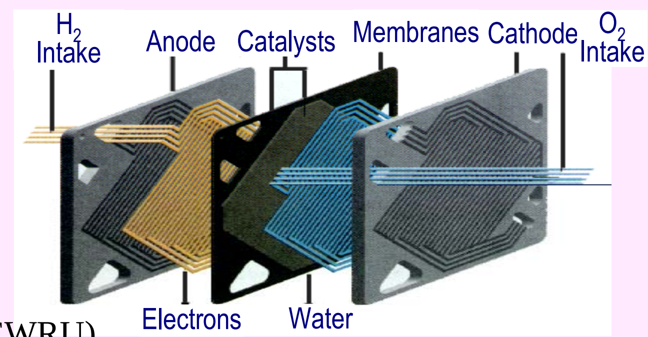


Controlled design of triple percolation nanoscale networks: ions, electrons, and porosity for gases

Low temperature fuel cells

'Higher' temperature membranes; degradation mechanisms; tailored nanostructures

Internal view of a PEM fuel cell

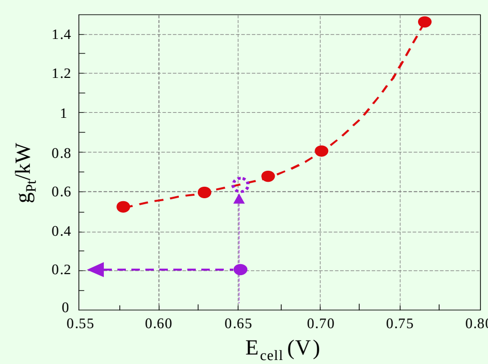


Source: T. Zawadzinski (CWRU)

Solid Oxide Fuel Cells

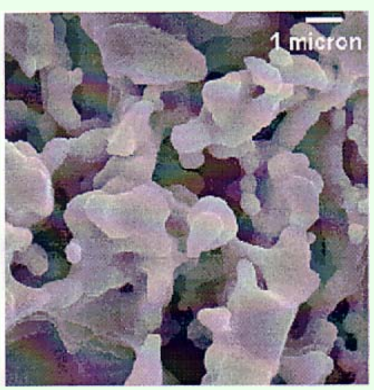
Theory, modeling, and simulation; new materials; novel synthesis; in-situ diagnostics

Mass of Pt Used in the PEMFCs — a Critical Cost Issue



Source: H. Gasteiger (General Motors)

YSZ Electrolyte for SOFCs

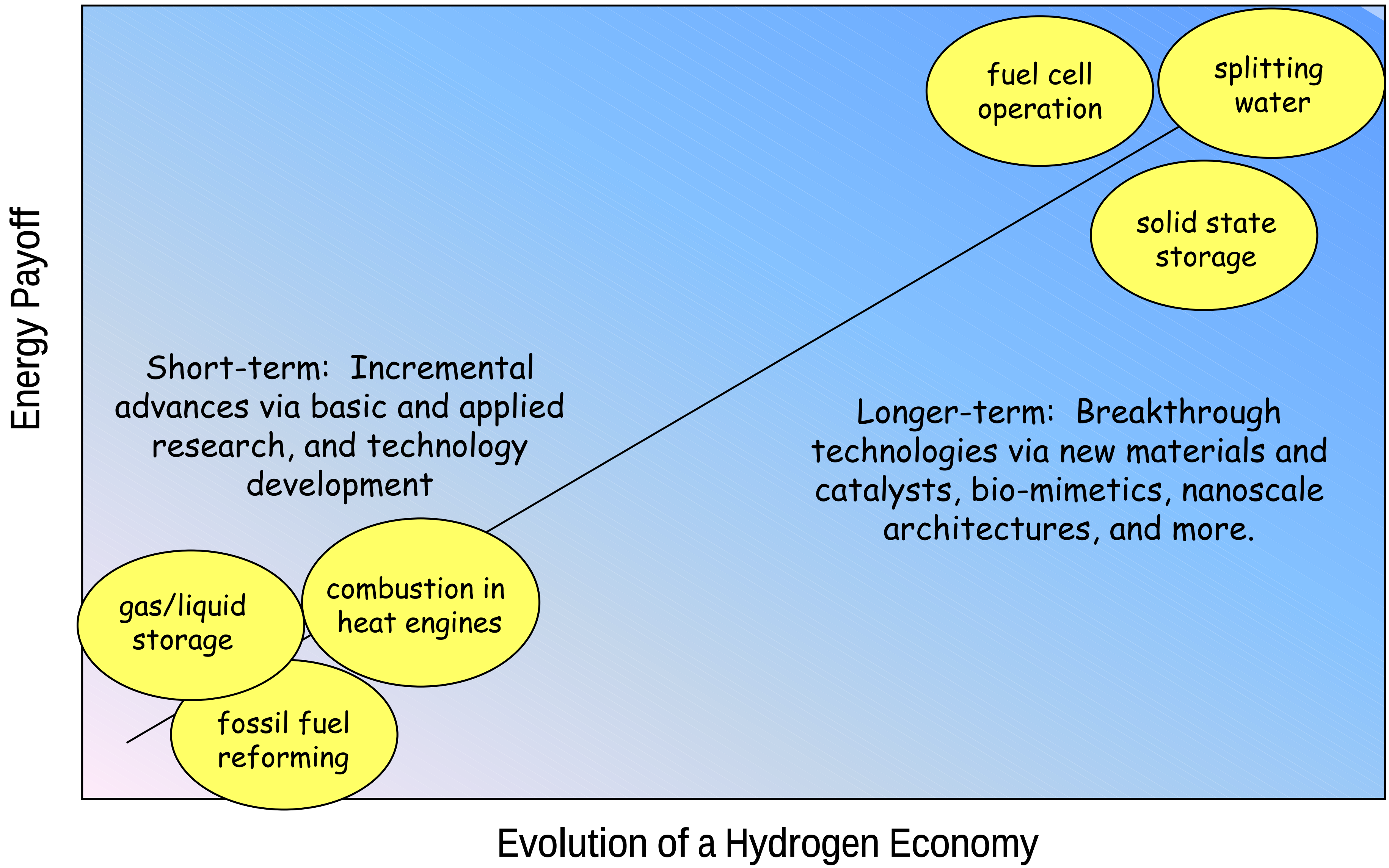


Tailored Porosity

Source: R. Gorte (U. Penn)

Source: BES Hydrogen Workshop Report

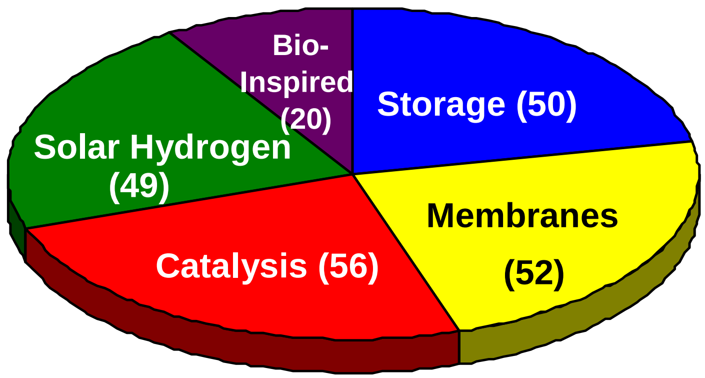
Summary: Research for Short-term Showstoppers and Long-term Grand Challenges



BES Solicitation for Basic Research for Hydrogen Fuel Initiative

- Two solicitations (one for grants and one for FFRDCs) were issued in April 2004. FFRDCs were limited to six submissions as leading institution. There was no limit on the number of submissions for universities.

- 668 qualified preproposals were received by July 15, 2004 in the following five categories.
  - *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*



Full Proposals Submitted

- 227 full proposals were received by January 4, 2005.

- Approximately $21.5 million in new funding will be awarded in FY 2005.

Timeline

January 4, 2005	Full proposals due
February – April, 2005	Proposal Peer Review
April – May, 2005	DOE assessment of review and selection of awards
June – July 2005	Awards made

Timeline of BES Solicitation for Basic Research for Hydrogen Fuel Initiative

Jan. | April | July | Oct. | Jan. | April | July

FY2004 | FY 2005

2/2004
FY2005 Budget Request
New Funding For Basic Research in SC-BES Announced

4/2004
BES Hydrogen Solicitations Issued

7/2004
668 3-page Preproposals Received

9/2004
261 Preproposals Selected for Full Proposal Submission

1/2005
227 Full Proposals Received

6/2005
Awards Announced

Awards are expected to be announced on time

Coordination within DOE on the Hydrogen Fuel Initiative

- For the EERE hydrogen storage/ hydrogen production solicitations
  - BES staff: (1) provided recommendations on scientific scope of the Grand Challenge solicitations; (2) assisted in developing the external peer review panels of experts; and (3) served as federal reviewers on the award selection panels.
- For the BES basic research solicitation
  - DOE technology program offices (EERE, FE, and NE) reviewed research topical areas.
  - Staff from technology offices were part of the preproposal review process.
  - DOE Hydrogen Program Manager (Steve Chalk) were informed of the SC preproposal award selections.
- The Annual DOE Hydrogen Program Review involves EERE, SC, FE, and NE.
- The Annual BES Hydrogen Program Contractors' Meeting will be collocated with the DOE Hydrogen Program Review.
- EERE, SC, FE, and NE coordinate regularly on formulation of program management and operations plans

Roles of BES and EERE in Hydrogen Research: Differences

BES

- "Use-inspired" basic research to advance fundamental knowledge
- Focus on fundamental understanding
- Emphasis on science at the nanoscale to understand, predict, fabricate, and control novel or "designer" materials
- Strong ties with BES core research programs
- Deliverables: Knowledge widely disseminated, with the goal of impacting future directions in basic and applied research and technology development

EERE

- Applied research for technology development
- Focus on technical targets
- Emphasis on the development, performance, cost reduction and durability of materials and components
- Strong ties with industrial collaborations and with systems analysis and integration
- Deliverables: Materials and/or components for hydrogen and fuel cell technologies that meet performance and cost targets

Roles of BES and EERE in Hydrogen Research: Similarities

BES

- "Use-inspired" basic research to advance fundamental knowledge
- Focus on fundamental understanding
- Emphasis on science at ... understand, predict, fab... novel or "designer" ma...
- Strong ties with BES co... programs
- Deliverables: Knowledge widely disseminated, with the goal of impacting future directions in applied research and technology development

EERE

- Applied research for technology/prototype development
- Focus on technical targets
- ... development, ...t reduction and durability ...omponents for fuel cells
- ...ndustrial collaborations ...s analysis and integration
- Deliverables: Materials and/or components for hydrogen and fuel cell technologies that meet performance and cost targets

Both BES and EERE employ:

- Modeling and simulation
- Synthesis and characterization
- "Outside-the box" approaches

External Coordination and Outreach on Basic Research for the Hydrogen Fuel Initiative

- Hydrogen symposia at:
  - American Physical Society March Meeting (March 22-26, 2004)
  - American Chemical Society National Meeting (March 28 - April 1, 2004)
  - Materials Research Society Fall Meeting (November 29 - December 3, 2004)

- MIT mini-course on hydrogen research by Dresselhaus
  - Lecture notes posted at: web.mit.edu/mrschapter/

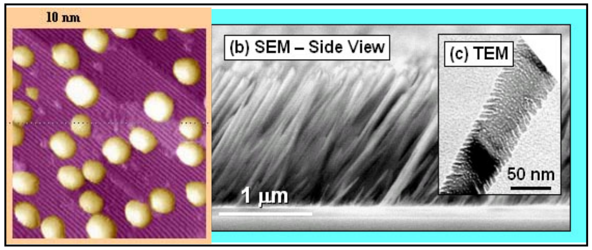
- Physics Today and IUMRS Facets articles on basic research needs for a hydrogen economy by Crabtree, Dresselhaus, and Buchanan

- Message delivered at Jim Lehrer Newshour interview, newspaper interviews, and NPR interview

- International activities
  - Participated in multi-lateral and bi-lateral hydrogen meetings - IPHE, US/European Commission, US/Canada, US/India, US/United Kingdom, IEA Hydrogen Coordination Group
  - Topics of Discussion: hydrogen production, carbon sequestration, storage, delivery, fuel cells, codes and standards, economic/cost modeling

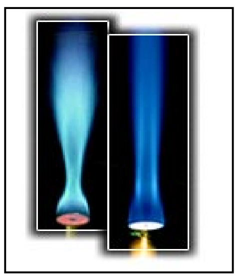
- Interagency coordination via the OSTP Hydrogen R&D Task Force
  - Developed Taxonomy of Research Directions to facilitate interagency coordination
  - BES leads the “Fundamental Research” subgroup to develop 10-year interagency coordination plans
  - Participation by DOC, DOD, DOE, DOT, DOS, EPA, NASA, NIST, NSF, USDA

BES-Supported Research Related to Hydrogen

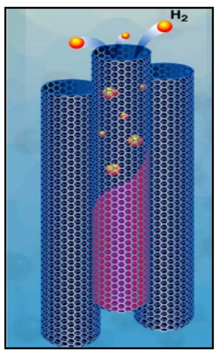


New synthetic catalysts facilitate the production of hydrogen

Goal: To Obtain a fundamental understanding of atomic/molecular level interactions and reactions associated with hydrogen production, storage, and use.



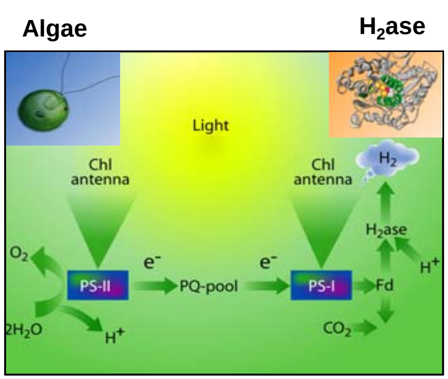
NOx formation in hydrogen and hydrocarbon flames



Nanotubes for hydrogen storage

Major areas of current research:

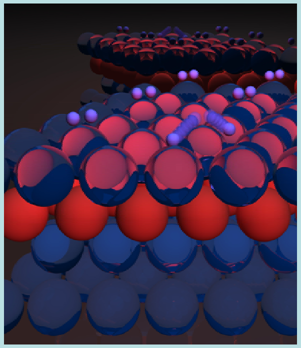
- Catalysts and mechanisms related to hydrogen production
- Electrochemical energy conversion mechanisms and materials research for fuel cells
- Modeling of hydrogen combustion for NOx minimization
- Hydrogen storage- hydrides, nanofibers, and nanotubes
- **Biological mechanisms of generation and metabolism**

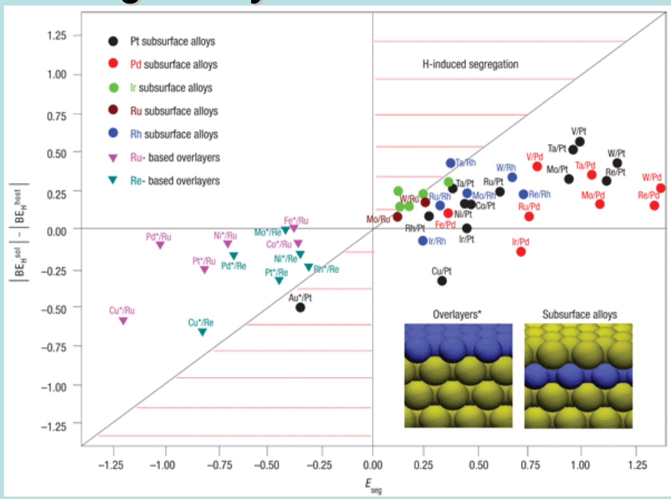


Enzymes in green algae convert water and light to hydrogen

BES-Supported Nano-catalyst Research Related to Hydrogen

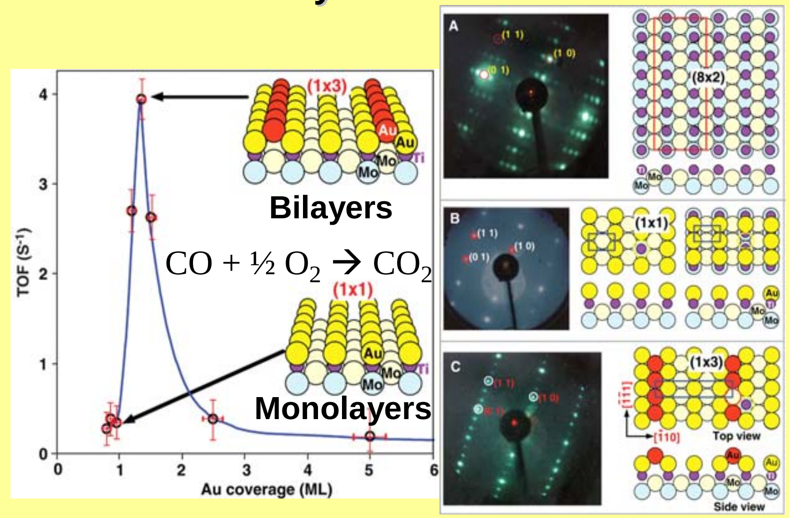
Ab-Initio Design of Near-Surface Alloys for Hydrogen-Bearing Catalysts





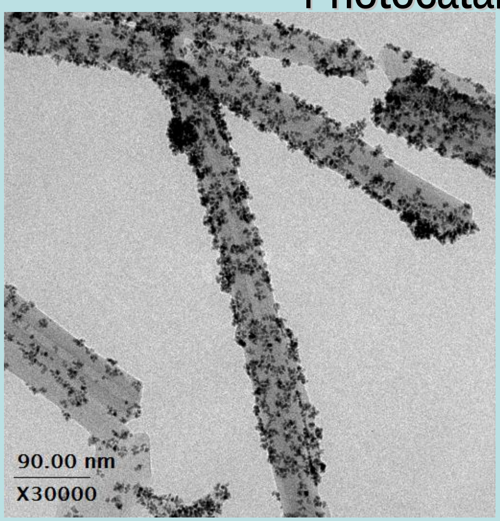
M. Mavrikakis et al., ***Nature Materials*** (2004) (**3:** 810–815)

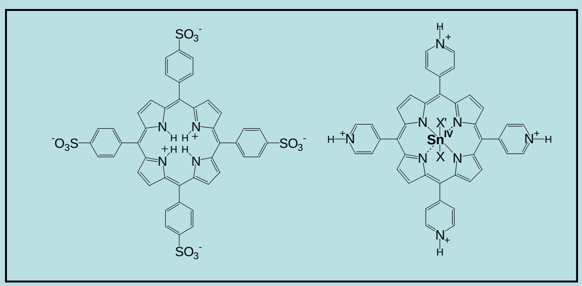
Marvelous Activity of Gold at the Nanoscale



D.W. Goodman et al. (***Science*** 2004 **306**: 252-255).

Novel Platinum and Gold-Porphyrin Nanotubes: Photocatalytic Water Splitting

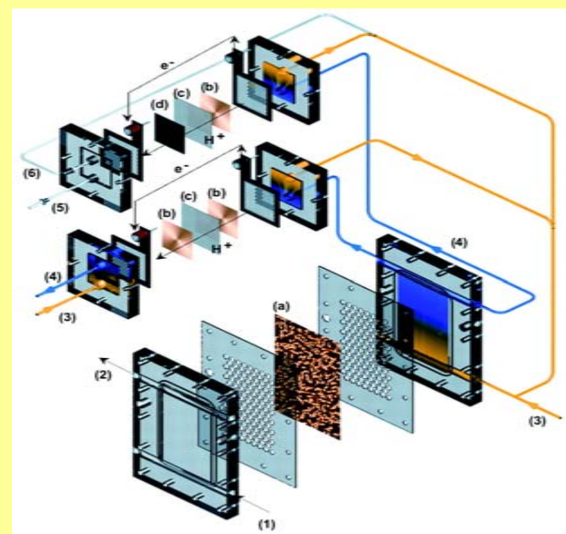




$$2SnP^{-\bullet} + 2H^{+} \xrightarrow{Pt} 2SnP + H_2$$

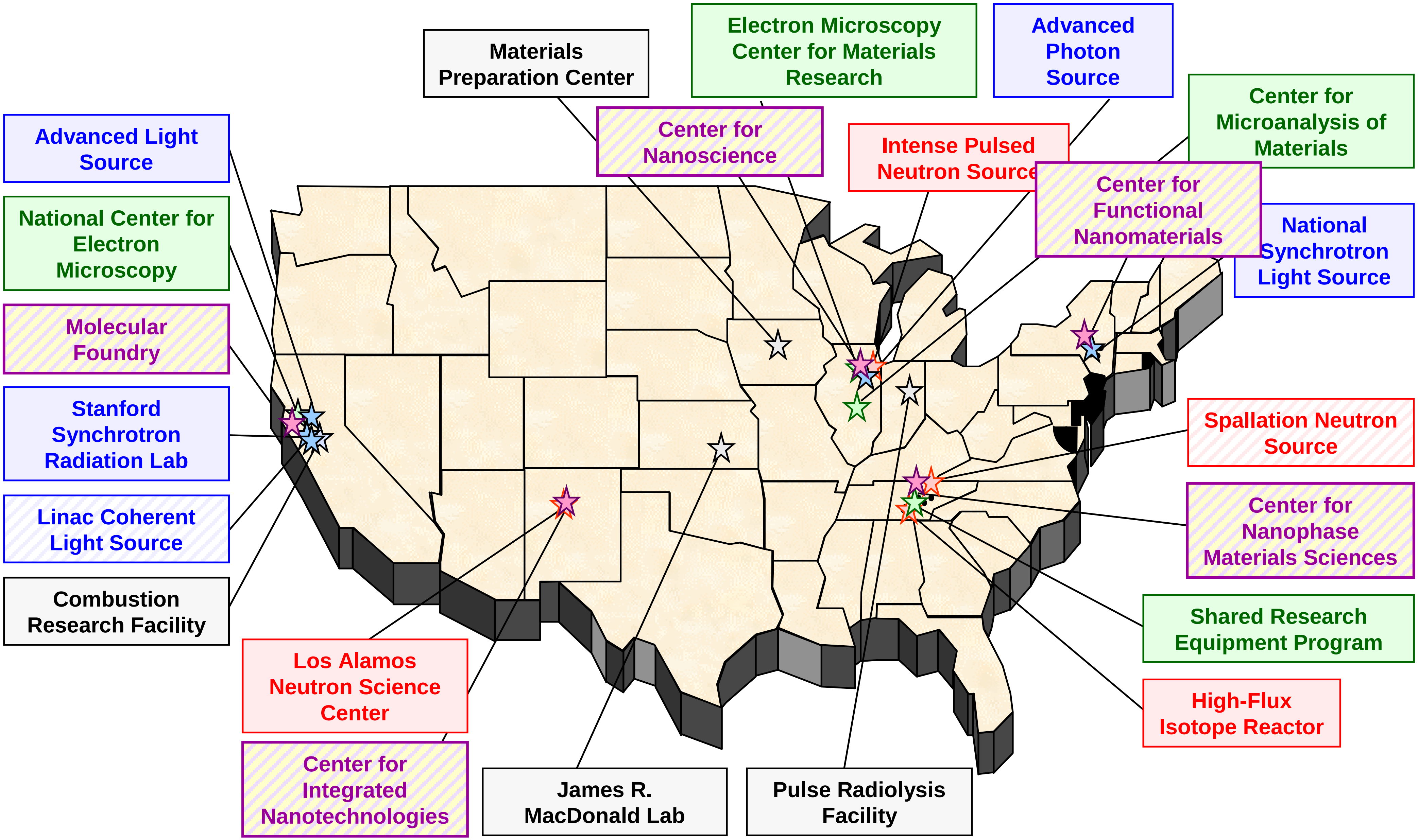
Shelnutt J A., et al., ***J. Am. Chem. Soc.* 2004**, *126*, 635-645.

Gold Nanocatalysts and Polyoxometallates for Biomass-Derived-Hydrogen Fuel Cells



J. Dumesic et al., ***Science*** (2004) **305**:1280-1283

BES Scientific User Facilities



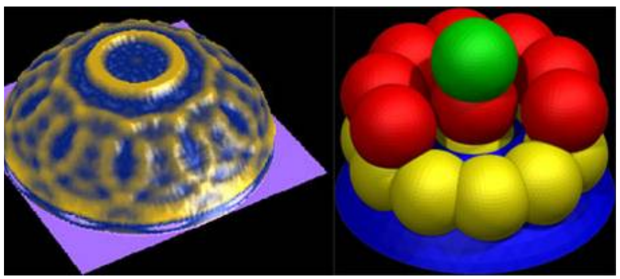
- *4 Synchrotron Radiation Light Sources*
- *Linac Coherent Light Source (PED)*
- *4 High-Flux Neutron Sources (SNS under construction)*
- *4 Electron Beam Microcharacterization Centers*
- *5 Nanoscale Science Research Centers (PED and construction)*
- *4 Special Purpose Centers*

Seeing atoms:

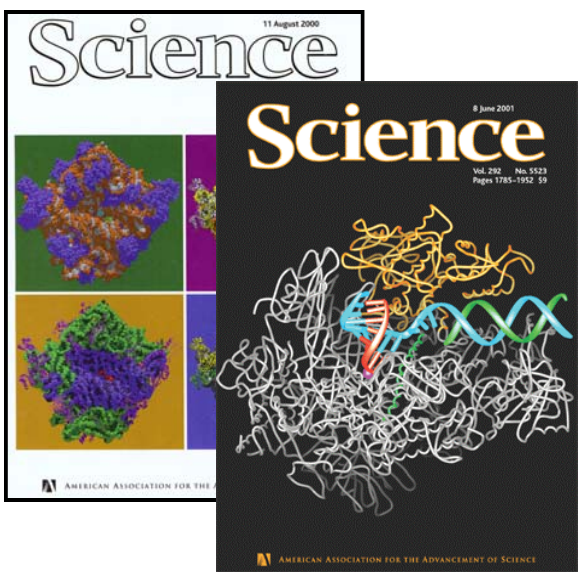
Providing national user facilities for probing materials at the atomic scale

X-ray, neutron, and electron scattering techniques have opened the world of the ultra-small. The next challenge is to open the world of the ultra-fast at this same spatial resolution.

X-ray scattering

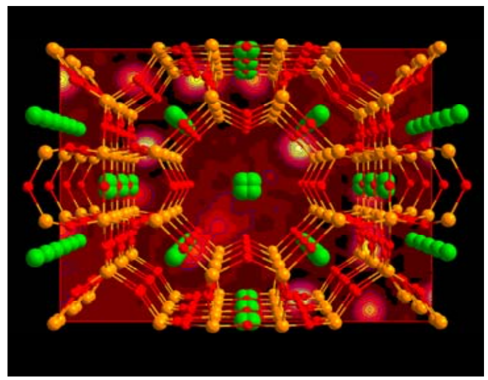


AlNiCo quasicrystal structure

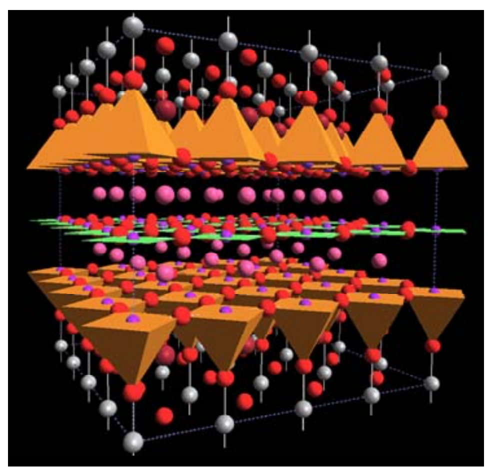


Molecular machines of life

Neutron scattering

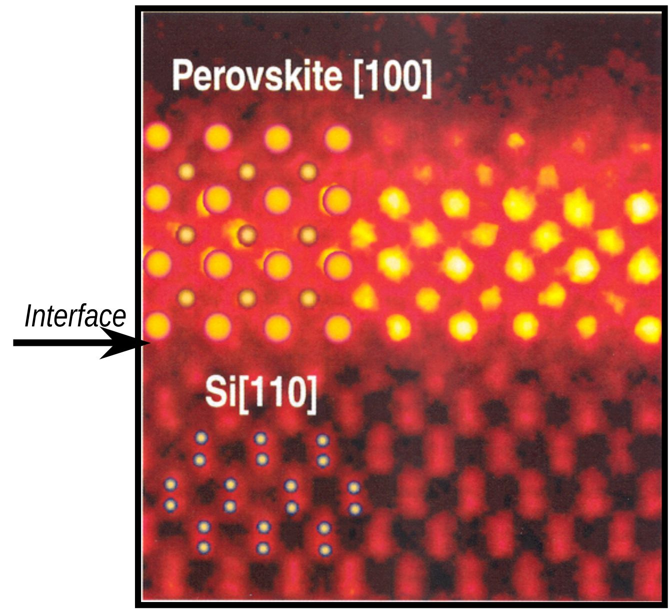


Zeolite catalyst



High Tc superconductor

Electron Scattering



Transmission electron microscope image showing an abrupt interface and low defect density for the ferroelectric $SrTiO_3$ on Si.

BES National User Facilities for Nanoscale Science

Facilities (under Construction) for the Synthesis, Characterization, and Study of Nanoscale Materials

Center for Functional Nanomaterials
(Brookhaven National Laboratory)

Center for Nanoscale Materials
(Argonne National Laboratory)

Molecular Foundry
(Lawrence Berkeley National Laboratory)

Center for Nanophase Materials Sciences
(Oak Ridge National Laboratory)

Center for Integrated Nanotechnologies
(Sandia & Los Alamos National Labs)

Relevant web sites for DOE-SC-BES programs

Core Research Program

http://www.science.doe.gov/bes (Office of Basic Energy Sciences)
http://www.science.doe.gov/grants/ (Sponsored research details)

SBIR/STTR

http://sbir.er.doe.gov/sbir

Major Research Facilities

http://www.sc.doe.gov/bes/BESfacilities.htm
http://www.science.doe.gov/bes/User_Facilities/dsuf/DSUF.htm

DOE Nano Centers

Center For Functional Nanomaterials, Brookhaven National Laboratory
www.cfn.bnl.gov
Center For Integrated Nanotechnologies, Sandia National Laboratories/Los Alamos National Laboratory
cint.sandia.gov or cint.lanl.gov
Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory
www.cnms.ornl.gov
Center for Nanoscale Materials (CNM), Argonne National Laboratory
nano.anl.gov
The Molecular Foundry, Lawrence Berkeley National Laboratory
www.foundry.lbl.gov