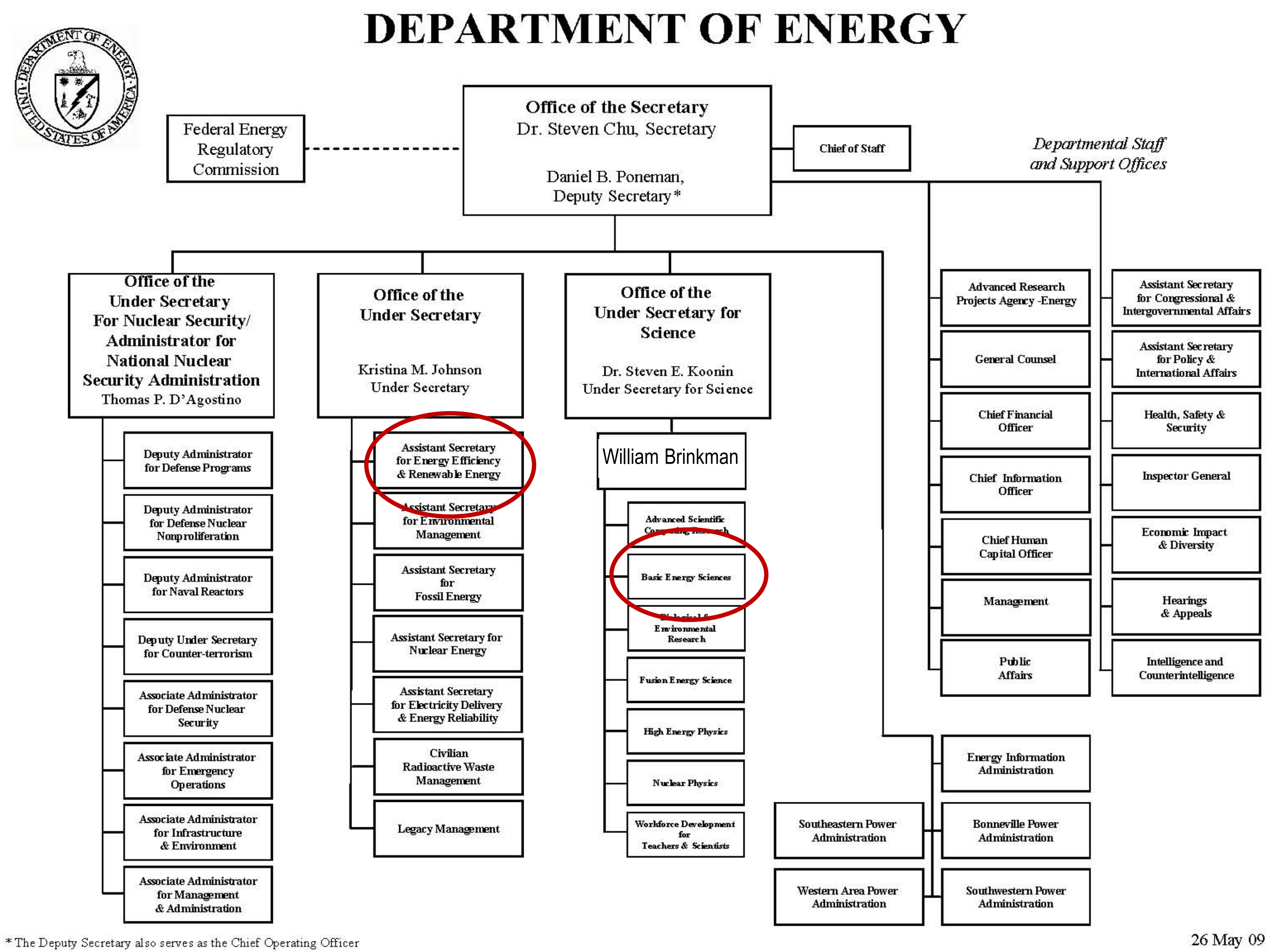
Office of Science
Basic Energy Sciences

2010 DOE Hydrogen & Vehicle Technologies
Merit Review and Peer Evaluation Meeting

June 7, 2010

Linda Horton
Director, Materials Science and Engineering Division
Office of Basic Energy Sciences

DOE – From Fundamental Science to Technology Research



Basic Energy Sciences Mission

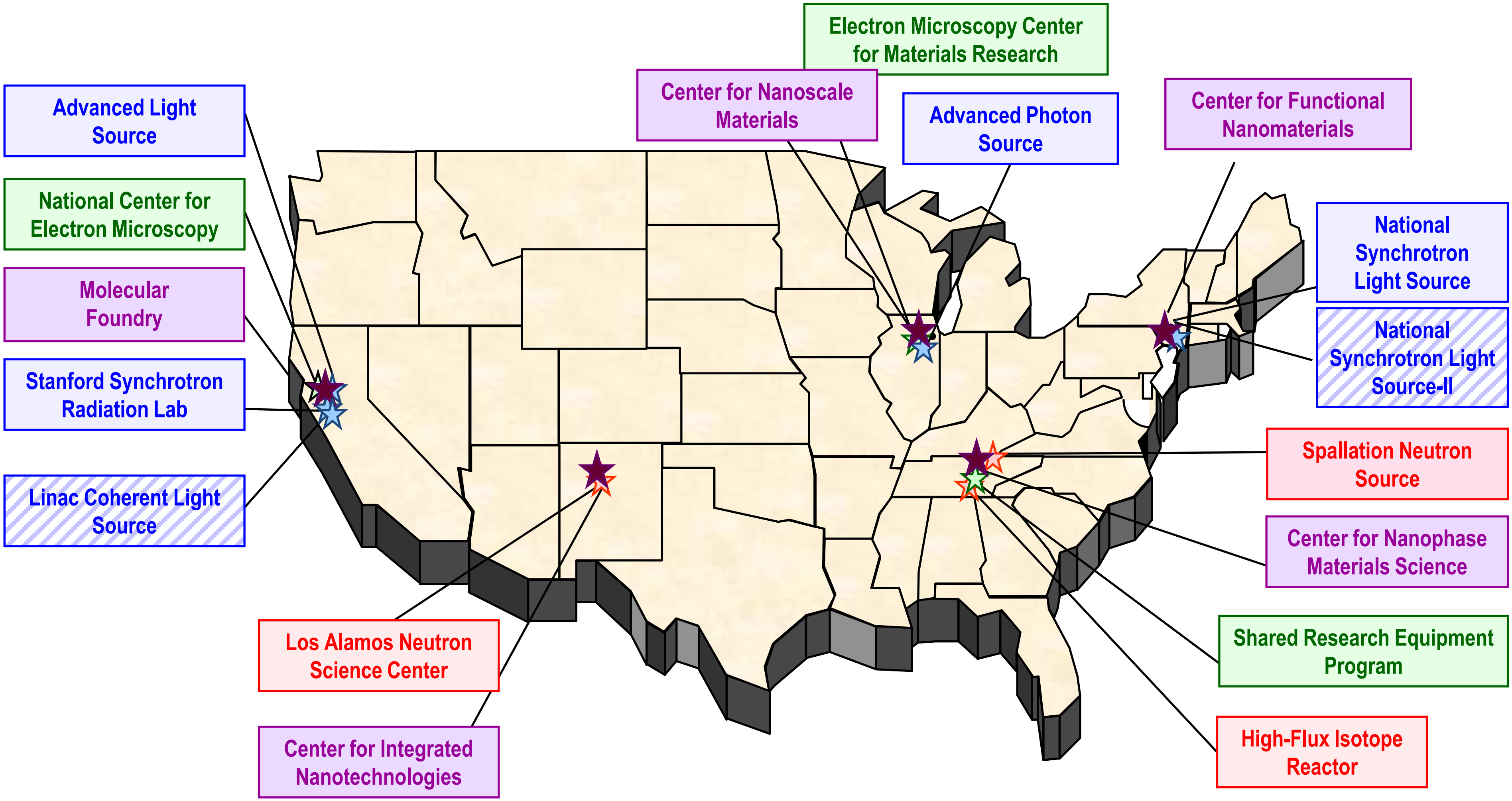
Mission:

- Fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels
- Provide the foundations for new energy technologies to support DOE's missions in energy, environment, and national security
- Plan, construct, and operate world-leading scientific user facilities for the Nation

Priorities:

- Discover and design new materials and molecular assemblies with novel function, through atom-by-atom and molecule-by-molecule control
- Conceptualize, calculate, and predict processes underlying physical and chemical transformations
- Probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials and chemical systems
- To foster integration of the basic research with research in the DOE technology programs and NNSA

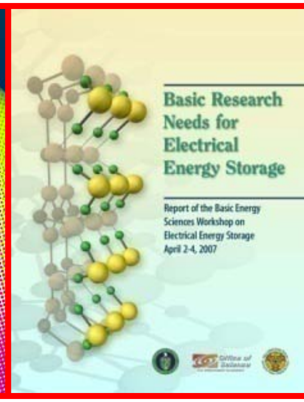
BES Scientific User Facilities: Resources for Materials Research

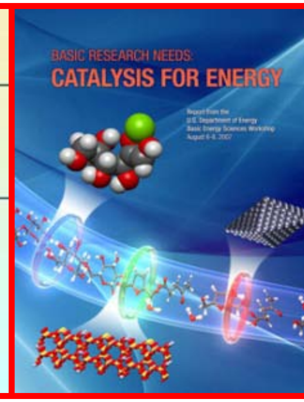


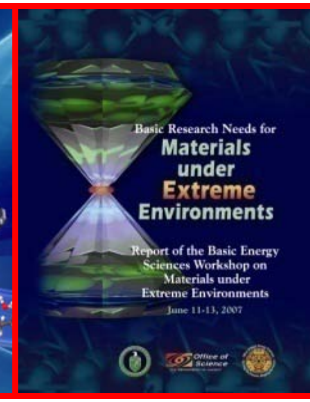
- 4 Synchrotron Radiation Light Sources
- Linac Coherent Light Source (Under construction)
- 3 Neutron Sources
- 3 Electron Beam Microcharacterization Centers
- 5 Nanoscale Science Research Centers

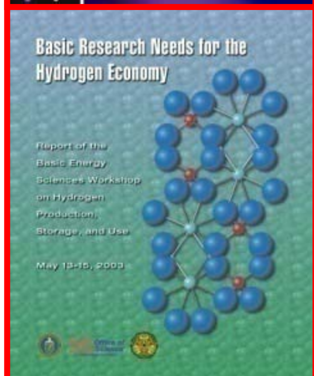
U.S. DEPARTMENT OF ENERGY | Office of Science

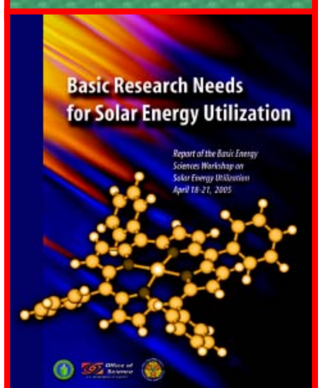
Strategies: Ten "Basic Research Needs …" Workshops

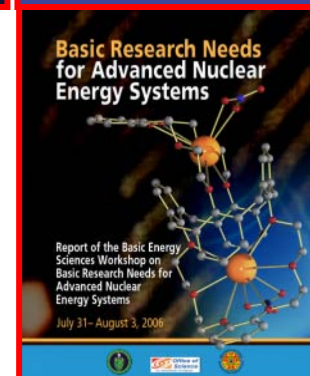


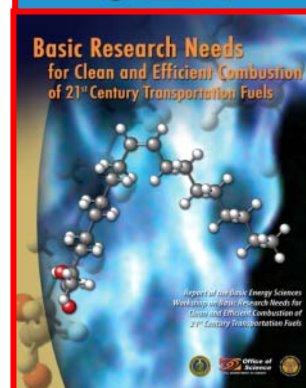








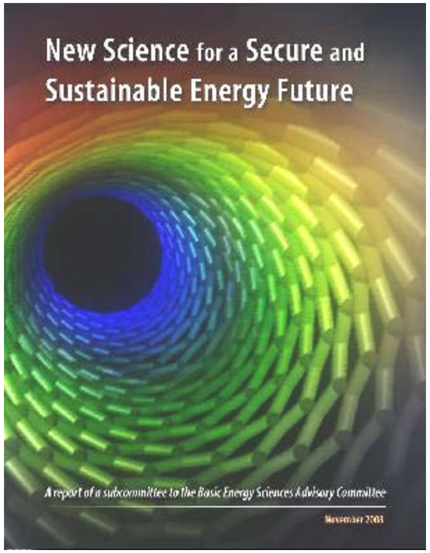




- Hydrogen Economy
- Solar Energy Utilization
- Superconductivity
- Solid State Lighting
- Advanced Nuclear Energy Systems
- Clean and Efficient Combustion of 21st Century Transportation Fuels
- Geosciences: Facilitating 21st Century Energy Systems
- Electrical Energy Storage
- Catalysis for Energy Applications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

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

New Science for a Secure and Sustainable Energy Future



Goals :

- Make fuels from sunlight
- Generate electricity without carbon dioxide emissions
- Revolutionize energy efficiency and use

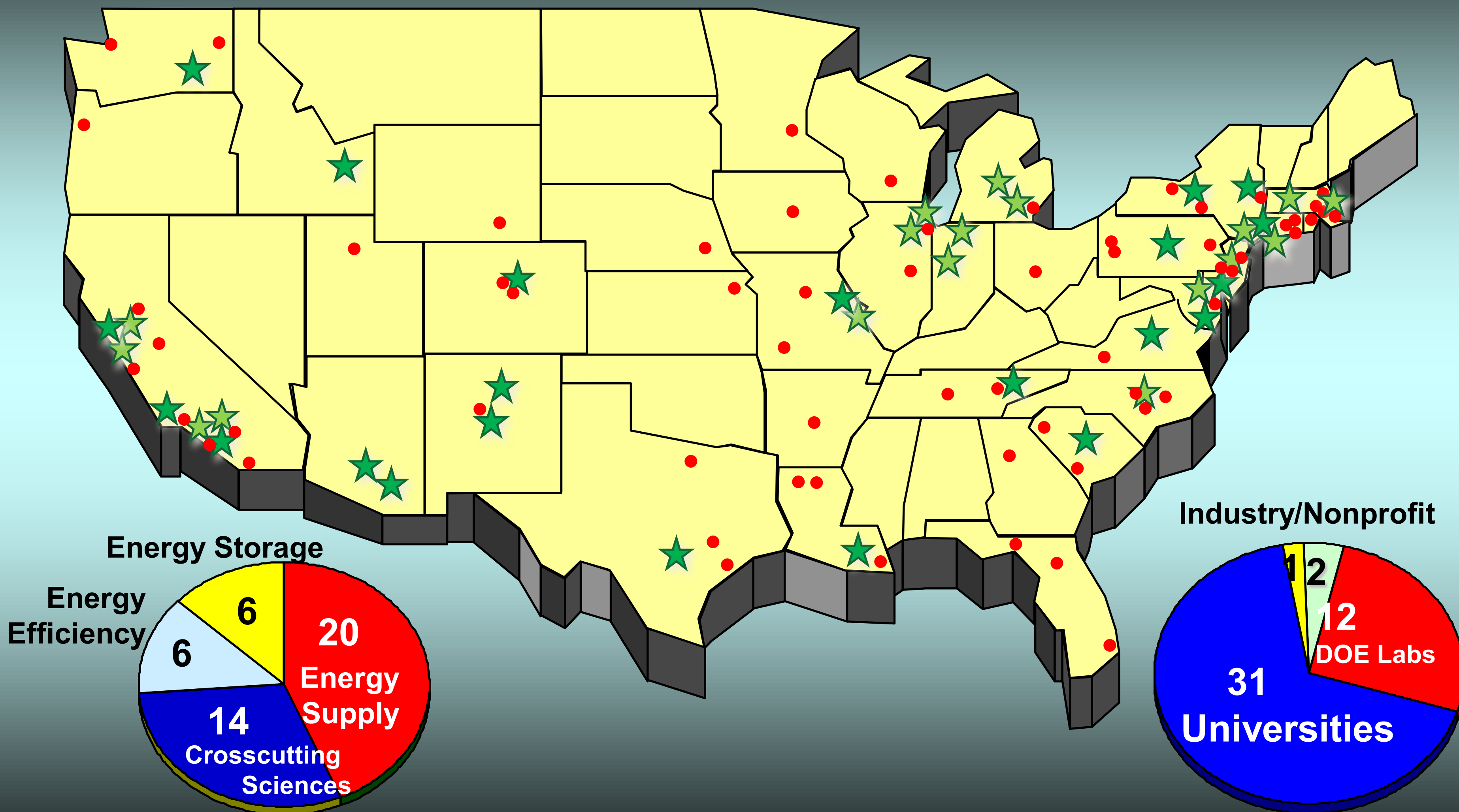
Recommendations:

- Work at the intersection of control science and complex functional materials
- Increase the rate of discoveries
- Establish "dream teams" of talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery
- Recruit the best talent through workforce development to inspire today's students and young researchers to be the discoverers, inventors, and innovators of tomorrow's energy solutions

Energy Frontier Research Centers

46 centers awarded, representing 102 participating institutions in 36 states plus D.C

Energy Frontier Research Center Locations (★ Leads; • Participants)



By Topical Category

By Lead Institution

DOE Energy Innovation Hubs

Three new Hubs launched in FY 2010 with SC-BES leading the Fuels from Sunlight Hub

Modeled after the Office of Science Bioenergy Research Centers, the Energy Innovation Hubs focus on critical energy technology challenges by building creative, highly-integrated research teams that can accomplish more, faster, than researchers working separately.

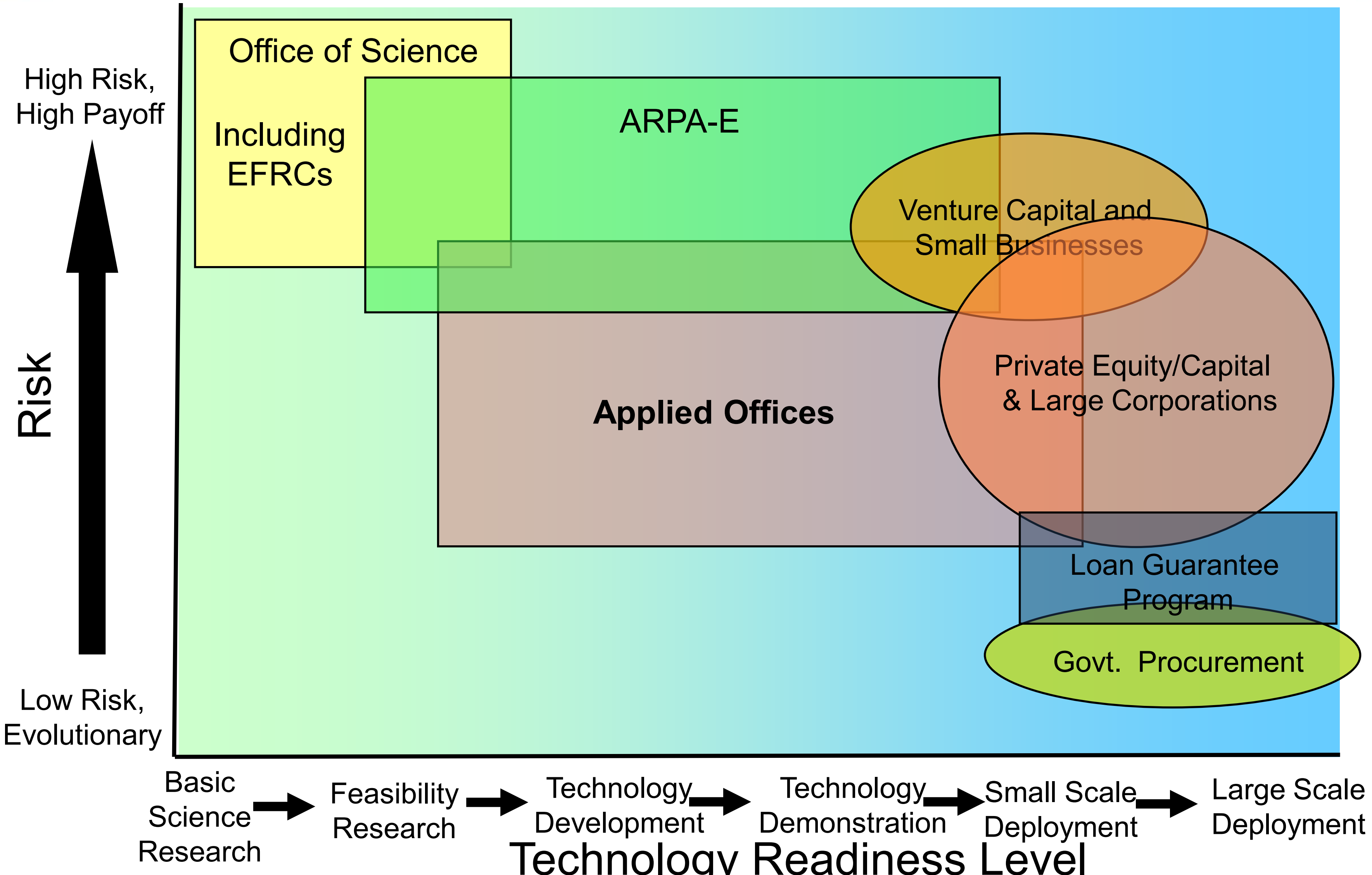
FY 2010 Hubs tackle three important energy challenges:

1. **Production of fuels directly from sunlight (SC)**
2. **Energy-efficient building systems design (EERE)**
3. **Modeling and simulation of advanced nuclear reactors (NE)**

The Fuels from Sunlight Hub will accelerate the development of a sustainable commercial process for the conversion of sunlight directly into energy-rich chemical fuels, likely mimicking photosynthesis, the method used by plants to convert sunlight, carbon dioxide, and water into sugar.

To access the Fuels from Sunlight FOA (reference number DE-FOA-0000214) go to: https://www.fedconnect.net/FedConnect/PublicPages/PublicSearch/Public_Opportunities.aspx and search for "Fuels from Sunlight" in the search box (note that the search flag should be set to "Title" or "Title/Description").

Energy Innovation Profile



DOE Office of Science Early Career Research Program and Graduate Fellowships

Early Career Research Program: ~70 Awards in FY 2010

Purpose: To support individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science

Eligibility: Within 10 years of receiving a Ph.D., either untenured academic assistant professors on the tenure track or full-time DOE national lab employees

Graduate Fellowships: ~160 Awards in FY 2010

Purpose: To educate and train a skilled scientific and technical workforce in order to stay at the forefront of science and innovation and to meet our energy and environmental challenges

Eligibility: Candidates must be U.S. citizens and a senior undergraduate or first or second year graduate student pursuing advanced degrees in areas of physics, chemistry, mathematics, biology, computational sciences, areas of climate and environmental sciences important to the Office of Science and DOE mission

Basic Sciences Underpinning Technology

- **Coordination between basic science and applied research and technology is an important mechanism by which to translate transformational discoveries into practical devices**

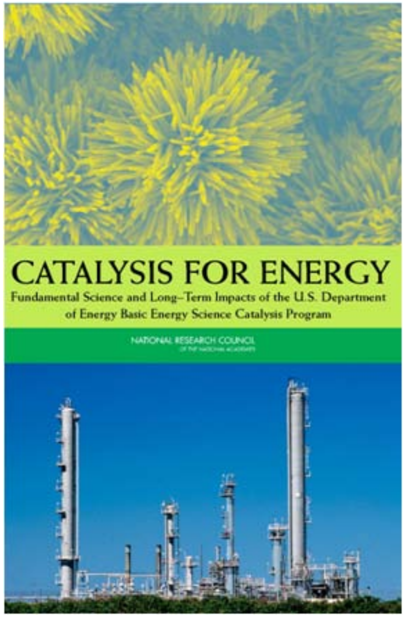
- **Many activities facilitate cooperation and coordination between BES and the technology programs**
  - Joint efforts in strategic planning (e.g., Basic Research Needs workshops)
  - Solicitation development
  - Reciprocal staff participation in proposal review activities
  - Joint program contractors meetings
  - Joint Small Business Innovative Research (SBIR) topics
  - Participation by BES researchers at the Annual Merit Review

- **Co-funding and co-siting of research by BES and DOE technology programs at DOE labs or universities, is a proven approach to close integration of basic and applied research through sharing of resources, expertise, and knowledge of research breakthroughs and program needs**

BES-EERE-Industry: Platinum Monolayer Electrocatalysts Brookhaven National Laboratory

1. Use-inspired BES research on electrochemical interfaces leads to discovery of a new class of nano-catalysts.
2. The EERE fuel cell program supports the development of the new catalysts for fuel cell applications.
3. Industrial support via Cooperative Research and Development Agreements demonstrate synthesis scale up and excellent performance in fuel cell tests.
4. New BES research now turns to catalysts for ethanol fuel cells.

   - BES user facilities – the National Synchrotron Light Source (NSLS) and Center for Functional Nanomaterials (CFN) – provided key characterization capabilities (x-ray absorption spectroscopy and advanced microscopy).
   - This work was featured as one of the 10 most impactful research efforts in the NAS review of the BES Catalysis Science Program.



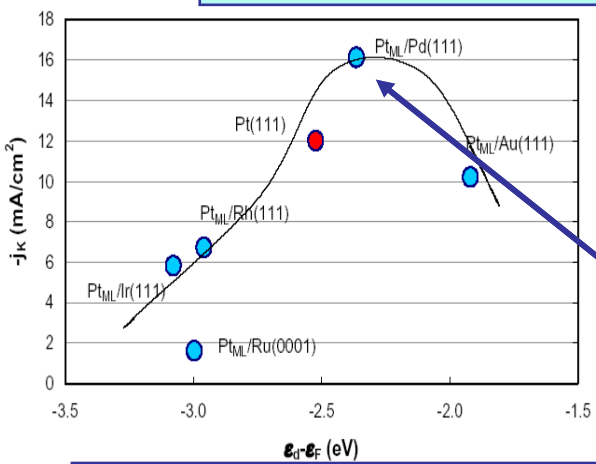
Radoslav Adzic and co-workers, Chemistry Department, Brookhaven National Laboratory

Platinum Monolayer Electrocatalysts

BES-supported research 1992-present at Brookhaven National Laboratory

Fundamental studies of electrocatalysis:
Oxygen reduction reaction (ORR) – mechanism, structure/activity

Insight (2000): Platinum monolayers are promising catalysts

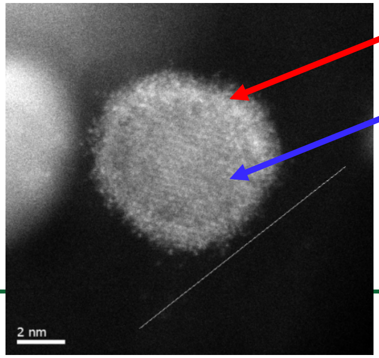


Substrate tunes catalytic activity of Pt overlayer:
- -Catalytic activity correlates to O binding energy
- -Optimum at intermediate binding: volcano plot
- -Stability can also be tuned

Pt monolayer on Pd(111) high ORR activity

Strategy: address critical cost and stability limits of fuel cell ORR catalysts

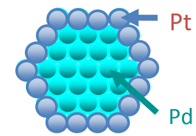
Nanostructured core-shell electrocatalysts
- active monolayer puts all Pt atoms at interface
- substrate core tunes activity & stability



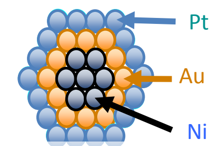
Platinum Monolayer Electrocatalysts

EERE-supported research 2003-present at Brookhaven National Laboratory

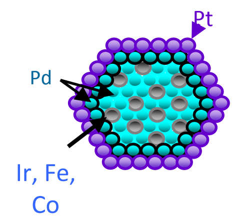
1. Several classes: tune properties & reduce cost
2. Atomic-level characterization *in situ* (XAS), *ex situ* (microscopy), density functional theory (DFT)
3. Atomic-level control syntheses fine-tune Pt-core interactions and control morphology
4. Activity, Stability and Fuel Cell tests



Pt monolayer on Pd nanoparticles



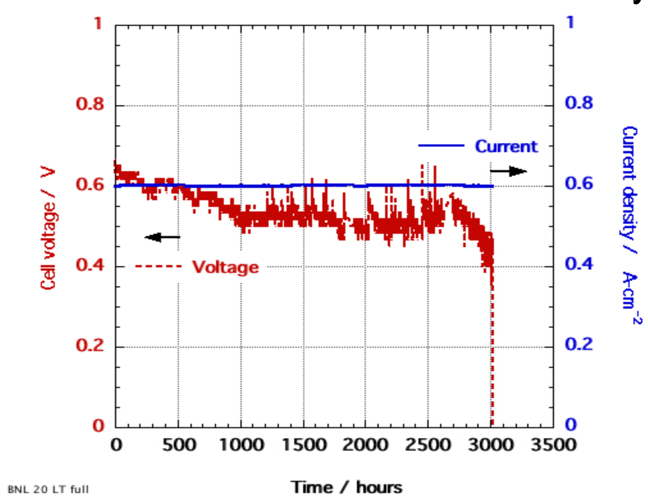
Pt on non-noble metal – noble metal core-shell;



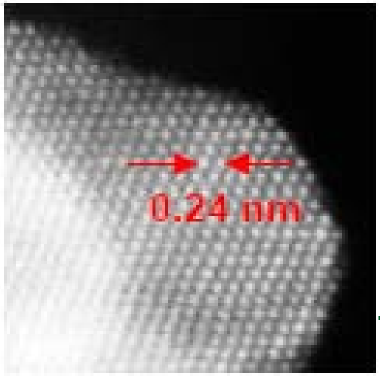
Pt on nanoparticles with interlayer of Pd

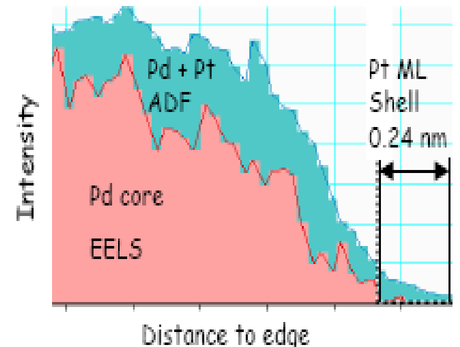
Catalytic Activity improved 5x-20x per wt Pt

Durability improved: multiple thousand hours in Los Alamos National Laboratory tests



Characterization: atomic imaging of one monolayer of Pt shell on Pd-core nanoparticles using microscopy capabilities at Center for Functional Nanomaterials





Electron Energy Loss Spectroscopy

Platinum Monolayer Electrocatalysts

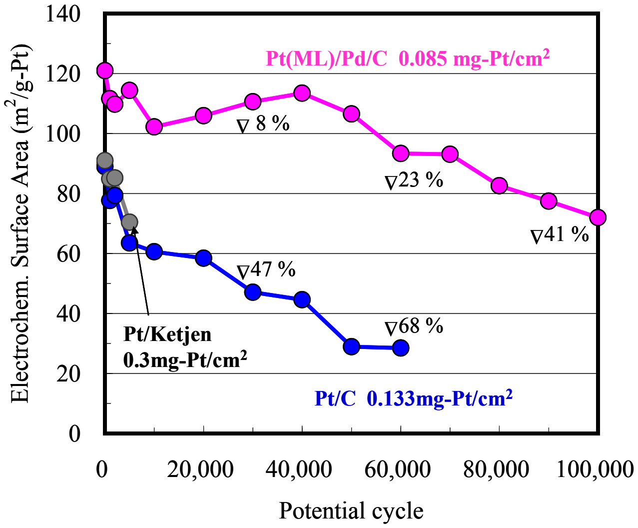
CRADAs with industry 2005-present at Brookhaven National Laboratory

Scale-up, fuel cell testing: Toyota, GM, UTC Fuel Cells, Battelle

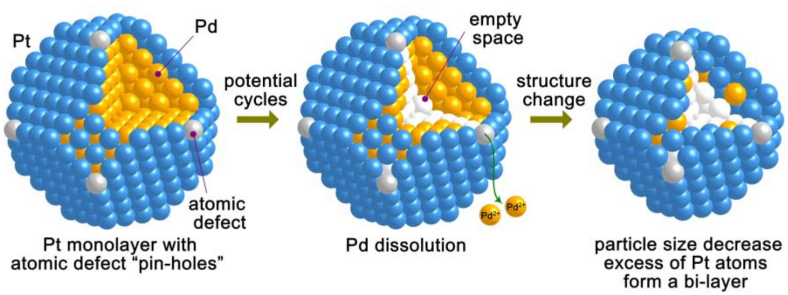
1. Demonstrate efficient, reproducible synthesis of gram quantities of Pt_{ML}
2. Fuel cell tests, performance, stability, potential cycling

Synthesis: e.g., Demonstrate scale-up to 50 gram batches of high-activity nanostructured core-shell electrocatalysts (with Toyota).

Performance: High activity, improved stability in MEA-level cycling. Scale-up will enable full fuel cell stack testing.



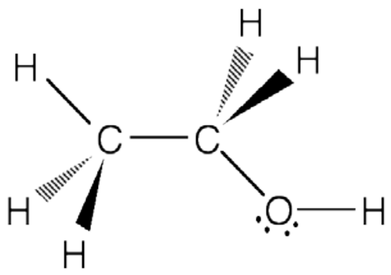
Understand improved stability: Evidence that Pd core acts as 'sacrificial electrode' for Pt shell.



Status: Core-shell nanocatalysts currently promising route to Polymer Electrolyte Membrane (PEM) fuel cell commercialization

Platinum Monolayer Electrocatalysts

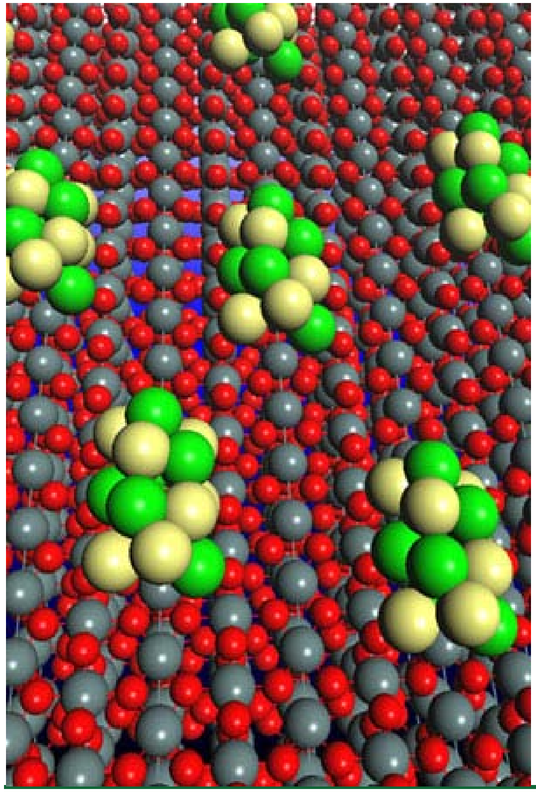
New BES research on catalysts for ethanol fuel cells Brookhaven National Laboratory



Challenge: *stable, selective and energy-efficient C-C oxidation in a fuel cell with fuel molecules containing C-C, C-O, C-H bonds.*

- Model of a ternary electrocatalyst for ethanol oxidation consisting of platinum-rhodium clusters on a surface of tin dioxide. For the first time, this catalyst can split the carbon-carbon bond selectively at a fuel cell anode

- Hydrogen adsorbate binds through the hollow Rh-Pt site, all other species bind through the bare Rh sites; the cluster structure forces the formation of a cyclic intermediate that results in C-C bond breakage

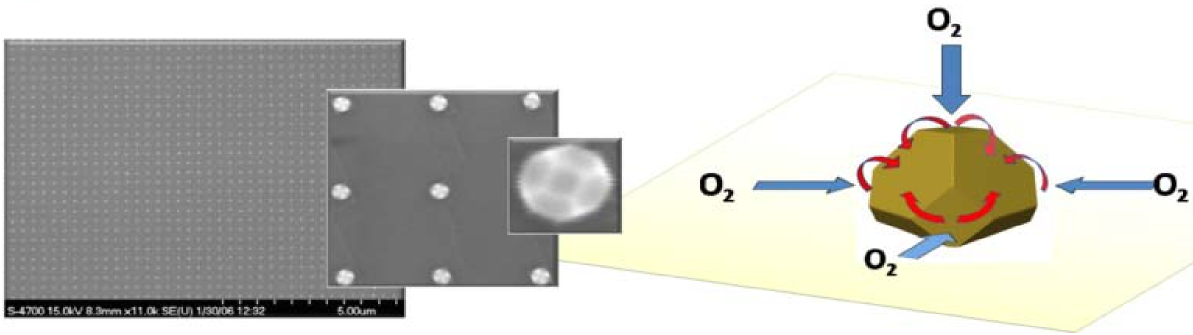


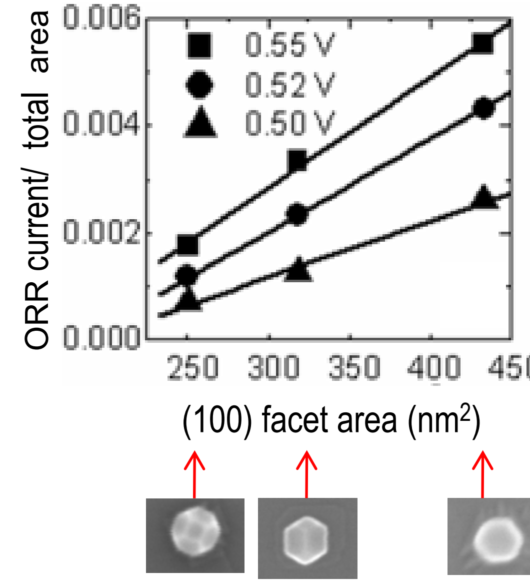
BES-supported critical advances: use of characterization techniques at National Synchrotron Light Source and Center for Functional Nanomaterials and molecular modeling techniques to understand the role of bimetallic cluster structure, support structure, electronic structure, and charge transfer on the mechanism of C-C splitting and oxidation.

U.S. DEPARTMENT OF ENERGY | Office of Science

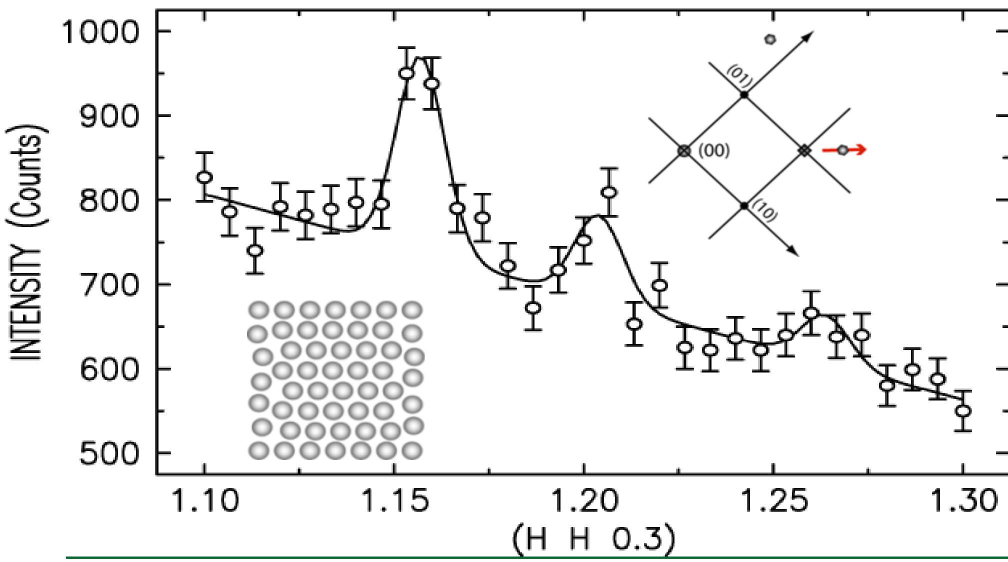
R. Adzic, et al., Nature Materials 8, 325 (2009)

Catalytic Mechanisms Elucidated with Pt Nanoparticle Arrays





Arrays of replicated Pt nanoparticles were tested in $HClO_4$ for oxygen reduction reaction (ORR) activity. Distinct substrate orientations produced particles with differing ratios of (111) to (100) facet area. Each array exhibits nanoparticles of nearly identical size, shape, and orientation.



- The (100) nanofacet is found by synchrotron x-ray experiments to have partial 'hex'-surface reconstruction, known for inducing catalytic activity in large (100) surfaces.
- ORR is proportional to the area of 1st step adsorbing (100) facets, while activation energies match those of the final steps found on active (111) surfaces.
- High activity of the particles are explained by nanoscale crossover of intermediates.

U.S. DEPARTMENT OF ENERGY | Office of Science

V Komanicky, H Iddir, K-C Chang, A Menzel, G Karapetrov, D Hennessy, P Zapol, H You, *J. Am. Chem. Soc.* **131**, 5732 (2009)

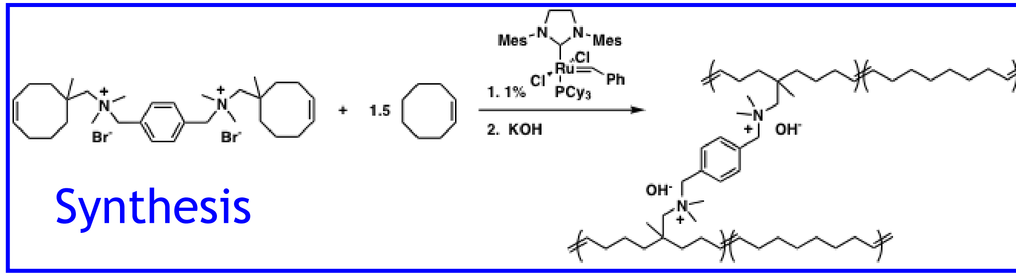
New Strategies for Fuel Cell Membranes

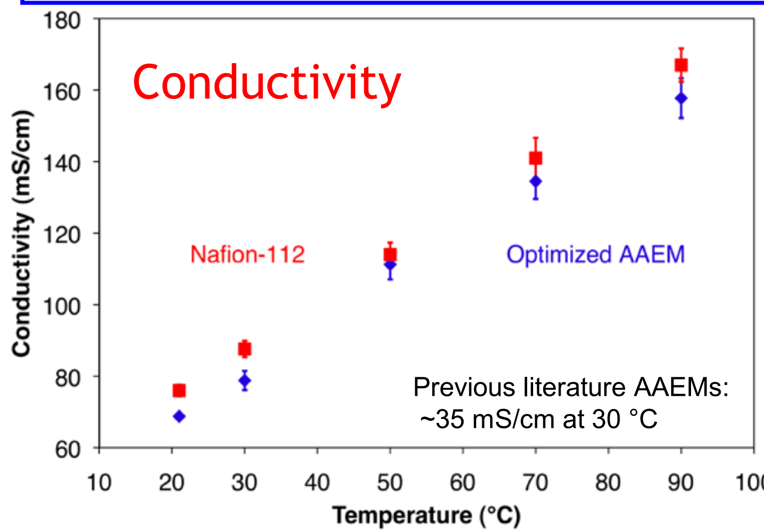
Fuel cells operating under alkaline conditions offer significant efficiency benefits, especially for the oxygen reduction reaction. This requires a switch from proton conducting membranes to hydroxide anion exchange membranes.

Previous synthesis efforts have resulted in membrane materials with low hydroxide ion conductivity and poor mechanical properties.

Using advanced synthesis and designed precursors (based on cyclooctenes substituted with tetraalkylammonium cations) they have prepared membranes with high conductivity; matching, and even surpassing (when normalized to the mobilities of H^+ and OH^-) Nafion® and with outstanding mechanical properties.

The high conductivity is enabled by the high ionic content while the mechanical properties derive from cross-linking.

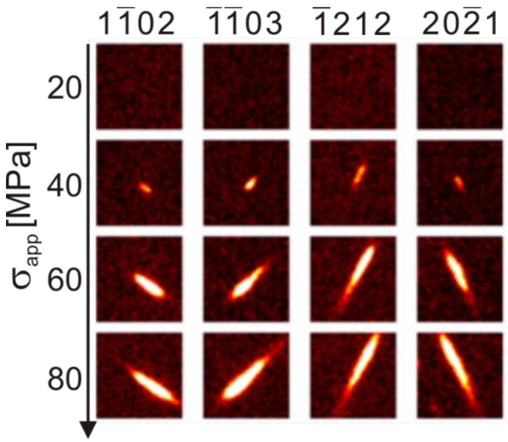


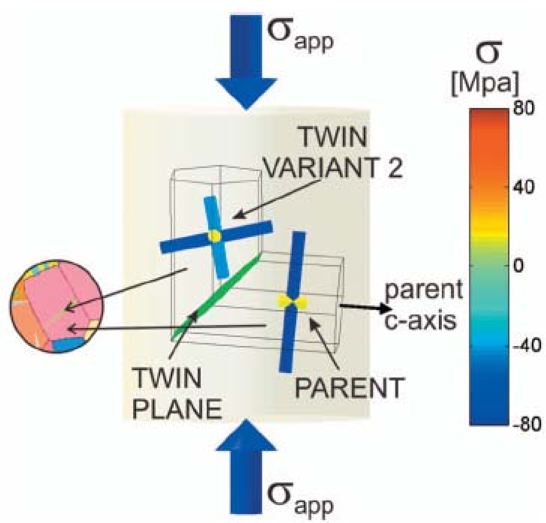


Outstanding Mechanical Properties!

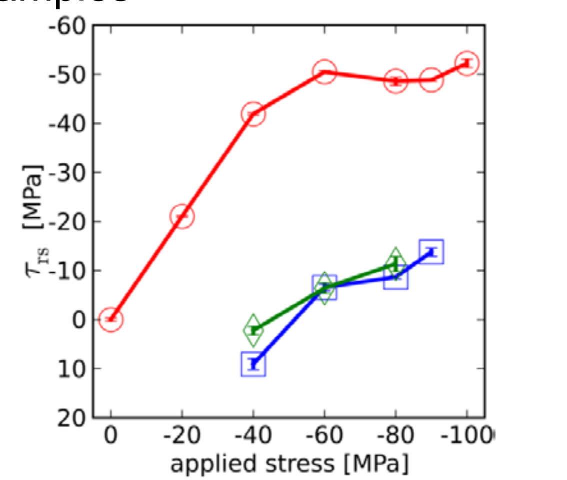
NJ Robertson, HA KostalikIV, TJ Clark, PF Mutolo, HD Abruña and GW Coates, JACS 132 (2010), p. 3400

In-Situ Measurements of Stress Distribution during Twinning of the Magnesium Alloy AZ31





- Crystallographic twinning is a strain accommodation mechanism in hexagonal close-packed (HCP) such as Mg alloys used in lightweight vehicles
- Twinning transformations are stress induced and lead to characteristic hardening rates, texture evolution and internal stress distributions and therefore an important part of advanced constitutive modeling of HCP deformation.
- 3D X-ray diffraction (3DXRD) at the Advanced Photon Source was utilized to measure internal stresses in-situ during compression of AZ31 samples
- Shear stress vs applied stress plot shows the stress state of the twin is drastically different from the parent grain
- Elucidates the relationship between the twin shear transformation and the constraints from the parent grain

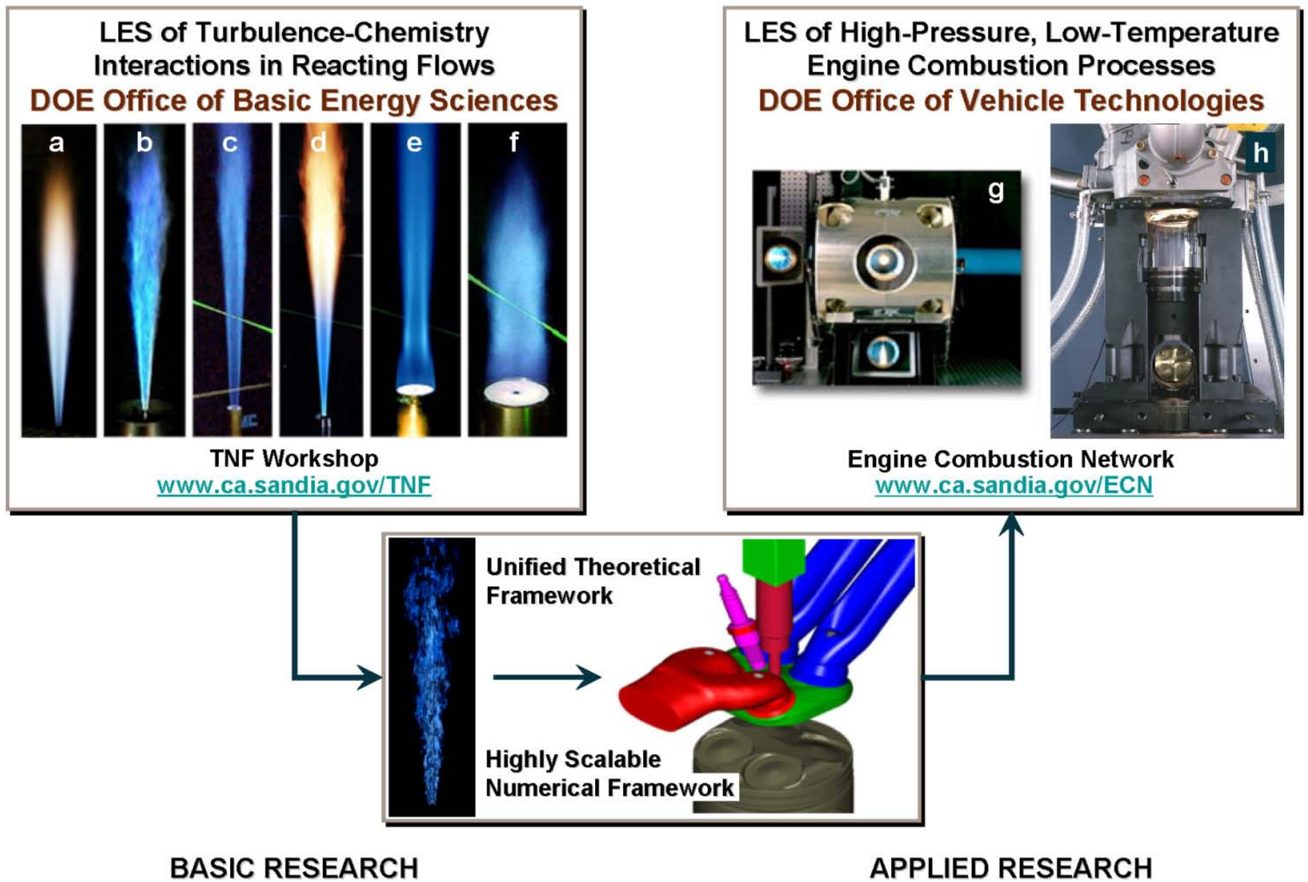


Upper line (red) - parent phase
Lower two lines (blue and green) -twin phase

Aydiner, Bernier, Blausen, Lienert, Tomé and Brown, “Evolution of stress in individual grains and twins in a magnesium alloy aggregate,” ***Physical Review B*** *80*, 024113 (2009)

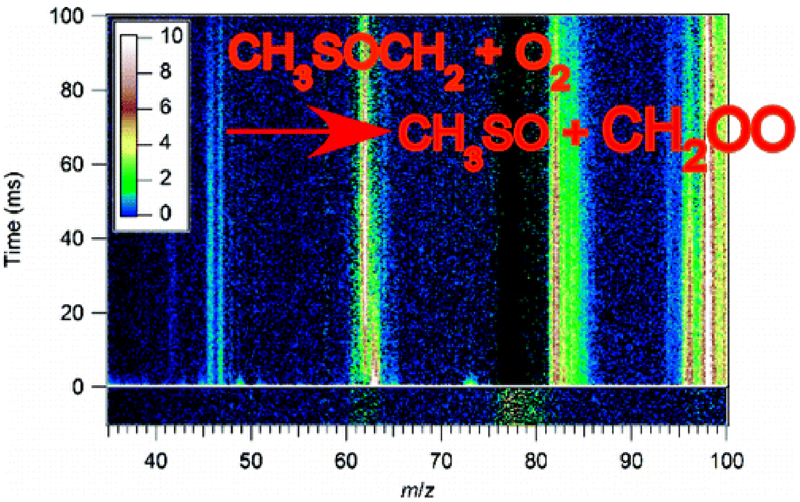
Combustion Research Facility - BES – EERE/VTP Collaborations

Large Eddy Simulations (LES)



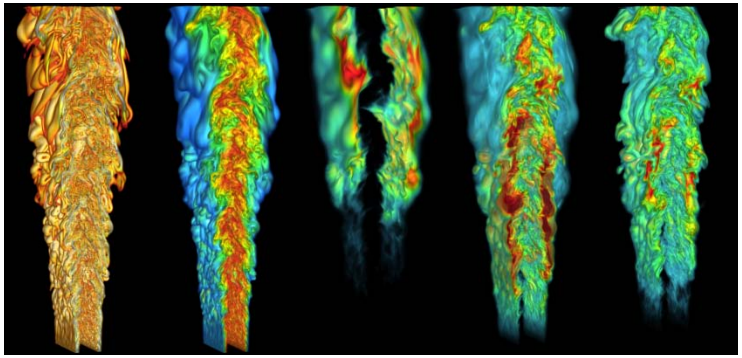
Joe Oefelein, SNL/CRF, jointly funded by BES and EERE

Highlights from the Combustion Research Facility



Detection and characterization of combustion intermediates

- Scientists from CRF, LLNL, LBNL & UC Berkeley directly detected the primary Criegee intermediate, formaldehyde oxide (CH_2OO)
- Paves the way for spectroscopic detection of CH_2OO, and places the elusive goal of direct measurement of highly excited CH_2OO in flames within reach. (J. Am. Chem. Soc., 2008, 130 (36), pp 11883–11885)



DNS of Turbulent C_2H_4/air Jet Flame in a Heated Air Coflow, left to right: mixing rate, mixture fraction, OH, CH_2O, and HO_2 mass fractions

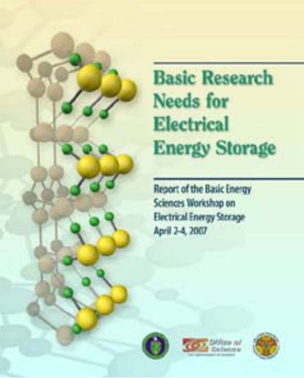
Turbulent Combustion Models

- Direct Numerical Simulation (DNS) (Jackie Chen) and Large Eddy Simulations (Joe Oefelein) codes show excellent scaling to thousands of processors, and they are working with DOE's Advanced Scientific Computing Scientific Discovery through Advanced Research (SciDAC) centers to facilitate development of data analysis tools
- CRF researchers have won INCITE awards every year of program. Current award: 67M cpu-hr at ORNL

A proposed, new FY 2011 SC/BES **Energy Innovation Hub for Batteries and Energy Storage** ($34,020K) will address the critical research issues and will include:

- **Design of advanced materials architectures**: design of low-cost materials that are self-healing, self-regulating, failure tolerant, and impurity tolerant
- **Control of charge transfer and transport:** control of electron transfer through designer molecules; electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity
- **Development of probes of the chemistry and physics of energy storage:** tools to probe interfaces and bulk phases with atomic spatial resolution and femtosecond time resolution
- **Development of multi-scale computational models**: computational tools to probe physical and chemical processes in storage devices from the molecular scale to system scale

Batteries and Energy Storage: Critical Issues in Research



A Unified Research Framework for Transportation and Stationary End-use

How can we approach theoretical energy densities?

- Need to know how to design and control energy transfer
- Need to develop novel multi-electron systems
- Need to understand fluid behavior in nanopores

Increased Energy Density

How do we increase the rate of energy utilization and safe storage capacity?

- Need to improve ionic and electrical conductivity
- Need to design simple, stable nanostructures
- Need to understand energy transport

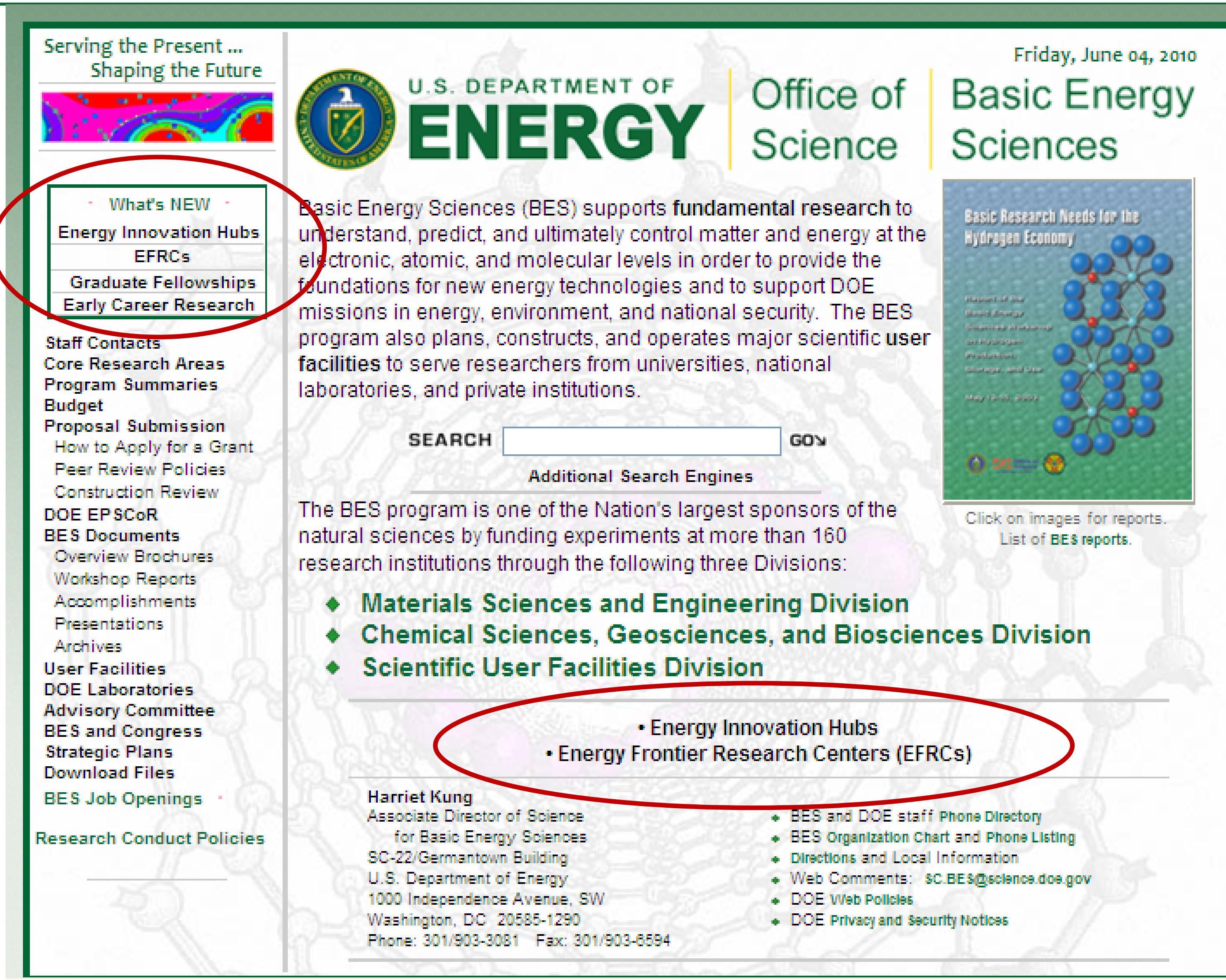
Higher Power

Can we create a system that is close to perfectly reversible?

- Need to understand interfaces and phase stability
- Need to understand system dynamics
- Need to use design new materials and structures

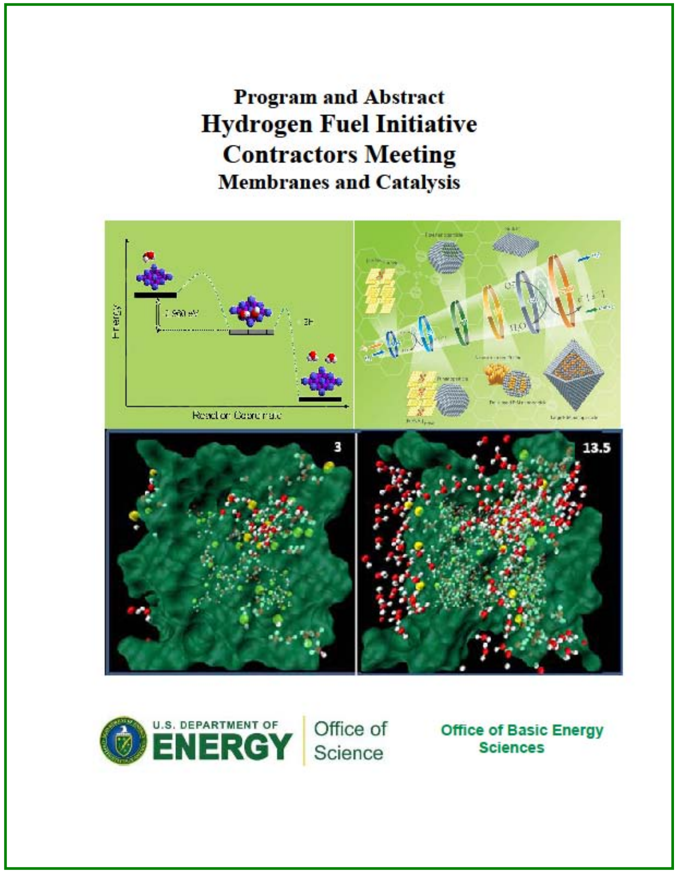
Longer Lifetimes

More Information? www.sc.doe.gov/bes/ *



*** Or just Google "DOE + BES"**

BES Events at the 2010 Annual Merit Review Meeting



BES Hydrogen Contractors' Meeting for Catalysis and Membranes

Thursday, June 10

- 33 Projects
- 18 Presentations
- 15 Posters

Joint Poster Session between BES projects related to **Electrical Energy Storage** and the EERE BATT Program

Monday and Tuesday Evenings June 7-8

Where Can a Battery and Energy Storage Hub Take Us?

- Move science and technology for energy storage forward at a rapid pace to enable transformative developments for reliable energy supply and transportation systems

- Provide a strong linkage between fundamental science, applied technology and end-use communities to create long- and short-term innovations that would not otherwise be achieved

Batteries and Energy Storage Hub:
A research framework for scientific discovery and transformational technologies