U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences
Research Priorities and Strategic Planning

John C. Miller, Acting Director
Chemical Sciences, Geosciences, and Biosciences Division
Office of Basic Energy Sciences
Office of Science, Department of Energy

EERE Annual merit Review
May 13, 2013
Washington, D.C.

Basic Energy Sciences Overview

U.S. DEPARTMENT OF **ENERGY**

Secretary
Ernest Moniz (nominated)

Deputy Secretary
Daniel B. Poneman

Advanced Research Projects Agency – Energy
Eric Rohlfing (Acting Dep. Dir.)

Under Secretary for Nuclear Security/Administrator for National Nuclear Security Administration
Vacant

- Defense Nuclear Nonproliferation
- Defense Programs
- Naval Reactors
- Counter-terrorism
- Defense Nuclear Security
- Emergency Operations
- Environmental Management Legacy Management

Under Secretary for Science
Vacant

Office of Science
Patricia Dehmer
Acting Director

- Basic Energy Sciences — Harriet Kung
- High Energy Physics — James Siegrist
- Advanced Scientific Computing Research — Barbara Helland (acting)
- Nuclear Physics — Tim Hallman
- Biological & Environ. Research — Sharlene Weatherwax
- Fusion Energy Sciences — Ed Synakowski
- SBIR/STTR — Manny Oliver
- Workforce Develop. for Teachers & Scientists — Patricia Dehmer (A)

Under Secretary
Vacant

- Energy Efficiency & Renewable Energy — David Danielson
- Fossil Energy — Christopher Smith (A)
- Nuclear Energy — Peter Lyons
- Electricity Delivery & Energy Reliability — Pat Hoffman

Office of Basic Energy Sciences

Harriet Kung, Director
Wanda Smith, Administrative Specialist

BES Budget and Planning
- Bob Astheimer, Senior Technical Advisor
- Margie Davis, Financial Management
- Donetta Herbert, Financial Management

BES Operations
- Dawn Adin, AAAS Fellow
- Kerry Gorey, Program Support Specialist
- Robin Hayes, Program Manager
- Natalia Melcer, Program Manager
- Katie Perine, Program Analyst / BESAC
- Ken Rivera, Laboratory Infrastructure / ES&H

Materials Sciences and Engineering Division

Linda Horton, Director
Teresa Crockett, Program Analyst
Vacant

Materials Discovery, Design, and Synthesis
Arvind Kini
Vacant, P.A.

- Materials Chemistry — Craig Henderson, Michael Sennett
- Biomolecular Materials — Mike Markowitz
- Synthesis and Processing Science — Bonnie Gersten
- Technology Coordination Program Management — Craig Henderson, John Vetrano

Condensed Matter and Materials Physics
Jim Horwitz
Marsophia Agnant, P.A.

- Experimental Condensed Matter Physics — Andy Schwartz
- Theoretical Condensed Matter Physics — Jim Davenport
- Physical Behavior of Materials — Refik Kortan
- Mechanical Behavior and Radiation Effects — John Vetrano

Scattering and Instrumentation Sciences
Helen Kerch
Cheryl Howard, P.A.

- X-ray Scattering — Lane Wilson
- Neutron Scattering — Thiyaga P. Thiyagarajan
- Electron and Scanning Probe Microscopies — Jane Zhu
- Experimental Program to Stimulate Competitive Research (DOE EPSCoR) — Tim Fitzsimmons

Scientific User Facilities Division

James Murphy, Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

Operations
- X-ray and Neutron Scattering Facilities — Peter Lee, Jim Rhyne
- NSRCs and EBMCs* — Peter Lee, Vacant, ☆ Tof Carim
- Accelerator and Detector Research — Eliane Lessner
- Facilities Coordination; Metrics; Assessment — Van Nguyen

* Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers

Construction
- National Synchrotron Light Source-II — Phil Kraushaar
- Facilities Upgrades and MIE** Projects — Joe May, Phil Kraushaar

** Major Items of Equipment

Chemical Sciences, Geosciences, and Biosciences Division

John Miller, Acting Director
✦ Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-Leon, Program Assistant

Fundamental Interactions
Michael Casassa
Robin Felder, P.A.

- Atomic, Molecular, and Optical Sciences — Jeff Krause
- Gas Phase Chemical Physics — Wade Sisk
- Condensed Phase and Interfacial Molecular Science — Gregory Fiechtner
- Computational and Theoretical Chemistry — Mark Pederson

Photochemistry and Biochemistry
Gail McLean
Vacant, P.A.

- Solar Photochemistry — Mark Spitler
- Photosynthetic Systems — Gail McLean
- Physical Biosciences — Robert Stack
- Fuels from Sunlight Energy Innovation Hub — Rich Greene, Vacant

Chemical Transformations
John Miller
Vacant, P.A.

- Catalysis Science — Paul Maupin, Raul Miranda
- Separations and Analysis — Larry Rahn
- Heavy Element Chemistry — Philip Wilk
- Geosciences — Nick Woodward

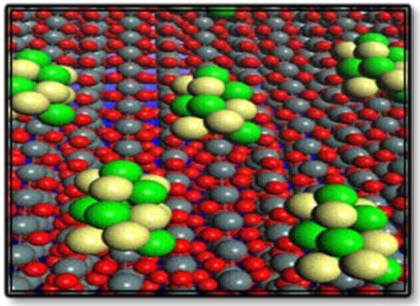
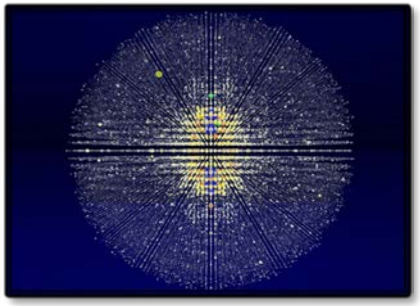
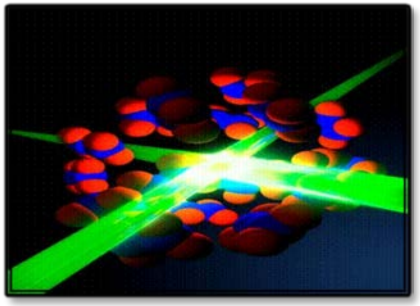
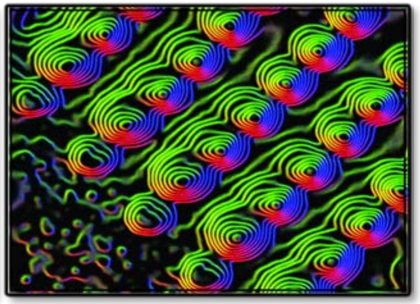
LEGEND
- ✦ On detail to ARPA-E
- ☆ On detail to OSTP
- P.A. Program Assistant

Basic Energy Sciences 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

BES Research — Science for Discovery & National Needs
Three Major Types of Funding Modality

increasing progression of scientific scope and level of effort

- **Core Research**

  Single-investigator, small groups, and targeted larger programs

  - Enable seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, and aspects of geosciences and biosciences. Scientific discoveries at the frontiers of these disciplines establish the knowledge foundation to spur future innovations and inventions.

- **Energy Frontier Research Centers**

  $2-5 million-per-year research centers; multi-investigator and multi-disciplinary

  - Harness the most basic and advanced discovery research in a concerted effort to accelerate the scientific breakthroughs needed to create advanced energy technologies. Bring together critical masses of researchers to conduct fundamental energy research in a new era of grand challenge science and use-inspired energy research.

  Started in FY 2009

- **Energy Innovation Hubs**

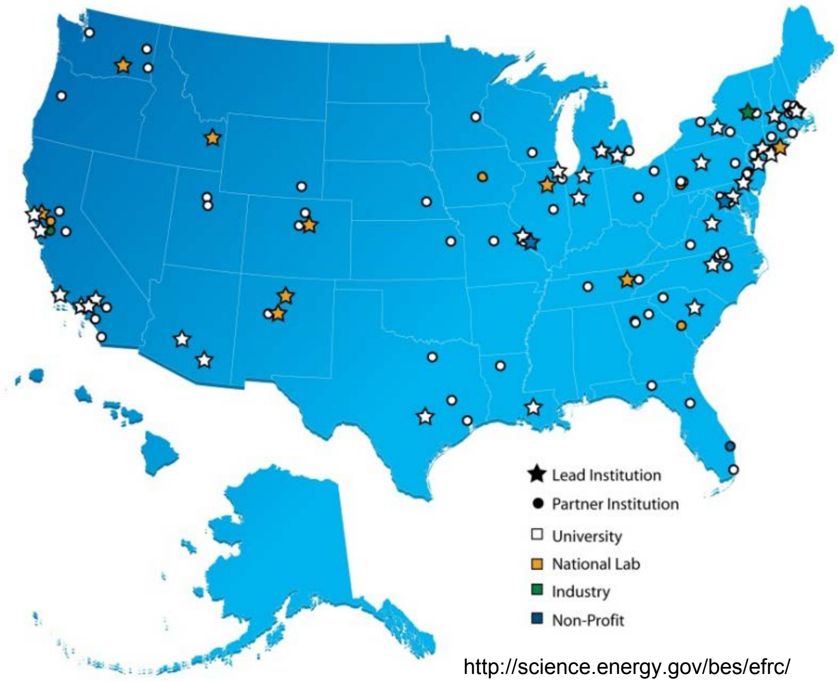
  $25 million-per-year research centers focus on co-locating and integrating multi-components, multi-disciplinary research with technology development to enable transformational energy applications.

  Started in FY 2010

Energy Frontier Research Centers Update

Participants:

- **46** EFRCs in **35** States + Washington D.C.
- ~**850** senior investigators and
  ~**2,000** students, postdoctoral fellows, and technical staff at ~**115** institutions
- >**250** scientific advisory board members from **13** countries and >**40** companies



http://science.energy.gov/bes/efrc/

Progress to date (~3.5 years funding):

- >**3,400** peer-reviewed papers including >**110** publications in *Science* and *Nature*
- **18** PECASE and **11** DOE Early Career Awards
- >**200** patent/patent applications, plus an additional >**60** invention disclosures and at least **30** licenses
- At least **60** companies have benefited from EFRC research
- EFRC students and staff now work in: >**195** university faculty and staff positions;
  >**290** industrial positions;
  >**115** national labs, government, and non-profit positions

Energy Frontier Research Centers Recompetition in FY2014

- The initial 46 EFRCs were funded for 5-years beginning in FY 2009: 30 EFRCs were funded annually at about $100M; 16 were fully funded by Recovery Act support
- For FY 2014, funding continues at $100M plus one-time funding of $68.7M
- Solicitation will request both renewal and new EFRC applications including:
  - Areas of energy-relevant research identified by recent BES and BESAC workshops
  - Research to advance the rate of materials and chemical discovery
  - Mesoscale science
- Selection of awards will be based on rigorous peer review of applications of the proposed research
  - Renewal awards will include assessment of the progress during the first 5-year award
- Renewal and new awards will maintain a balanced EFRC portfolio for grand challenge and use-inspired energy research

Fuels from Sunlight Hub
Joint Center for Artificial Photosynthesis (JCAP)

Mission

Develop a solar-fuels generator scalable to manufacture, from earth-abundant elements, that uses only sunlight, water, and carbon dioxide in the robust production of fuels

JCAP Team

Carl Koval, Director (CalTech); Nate Lewis, Founding Director and Chief Scientist (CalTech); two Assistant Directors; about 150 staff

Space

- JCAP North at LBNL: 14,000 sq. ft. leased space
- JCAP South at Caltech: 18,500 sq. ft. in renovated Jorgensen Lab Building (by Caltech & initial startup funds from DOE)

Funding & Oversight

- Up to $122 million over five years
- External reviews in 2011, 2012; scheduled at both sites for April 2013

Goals & Lasting Legacies

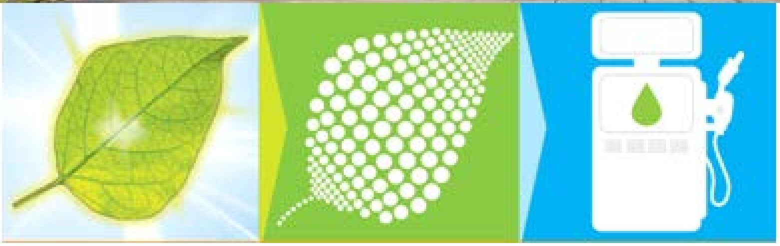
- Produce fuel from the sun 10x more efficiently than crops
- Library of fundamental knowledge
- Research prototype solar-fuels generator
- Develop the science and the critical expertise for a solar fuels industry

Milestones

2013: Establish benchmarking capabilities to compare large quantities of catalysts and light absorbers under standard conditions. Progress:
- Benchmarking protocols established for thin films, plan to benchmark over 40 catalytic thin films.
- As of March 2013, more than 20 films evaluated

2014: Design the first prototypic devices for testing components (catalysts, light harvesters, membranes, interfaces, etc.) as an integrated system

Jorgensen Laboratory Building



Batteries and Energy Storage Hub
Joint Center for Energy Storage Research (JCESR)

Mission
Science to enable next generation batteries—beyond lithium ion—and energy storage for the grid and for transportation

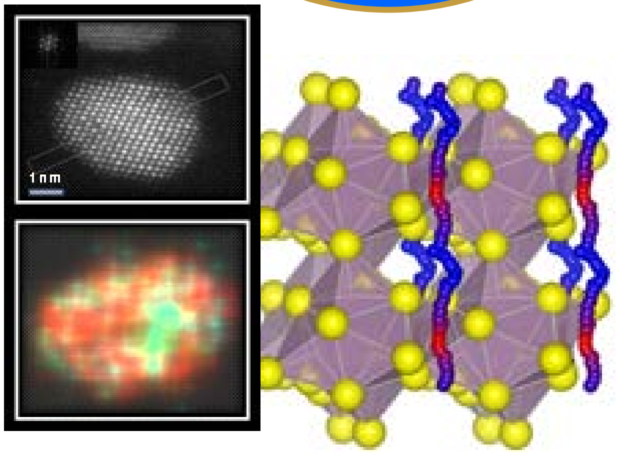
JCESR Team
George Crabtree, Director (ANL); 5 national labs, 5 universities, 4 industry partners, and 2 individual members' institutions

Space
- ANL Electrochemical Discovery Laboratory will provide lab and office space for use by all JCESR Institutions.
- State of Illinois has provided $5M for a new JCESR building with state-of-the-art laboratory and meeting space

Funding & Oversight
- Up to $120 million over five years
- Management review (PY1), Annual external S&T reviews (PY2-5)

Goals & Lasting Legacies
- 5x Energy Density, 1/5 Cost, within 5 Years
- Library of fundamental knowledge
- Research prototype batteries for grid and transportation
- New paradigm for battery development

Initial Milestones
2013-2014:
- Bring suite of experimental tools to full operation.
- Design new architectures of electrode/working ion combinations
- Begin the development of an electrolyte database to predict the design of new electrolytes



JCESR will use nanoscience tools and theoretical approaches to enable next generation energy storage

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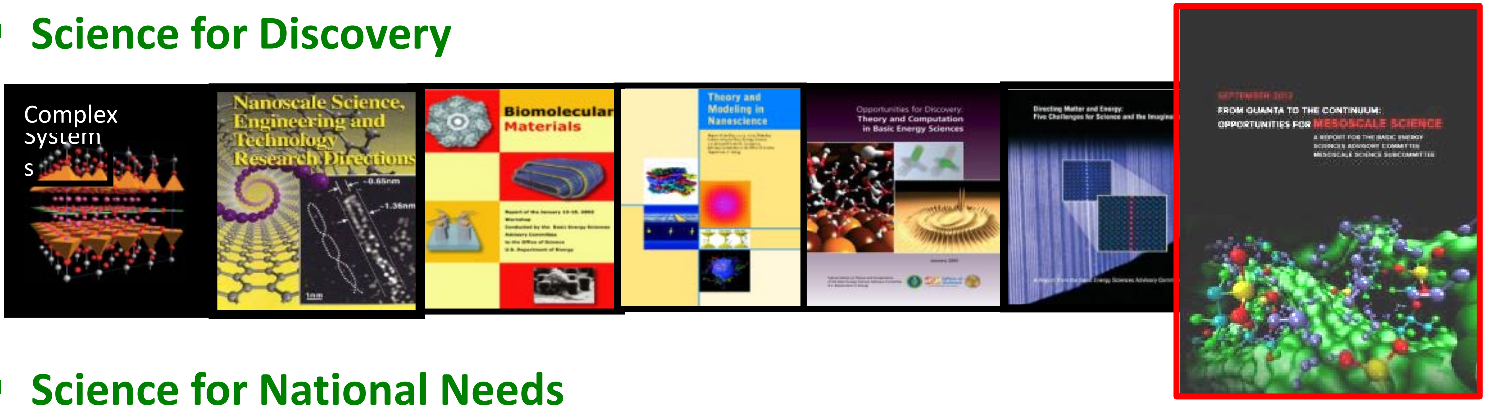
Strategic Planning in BES

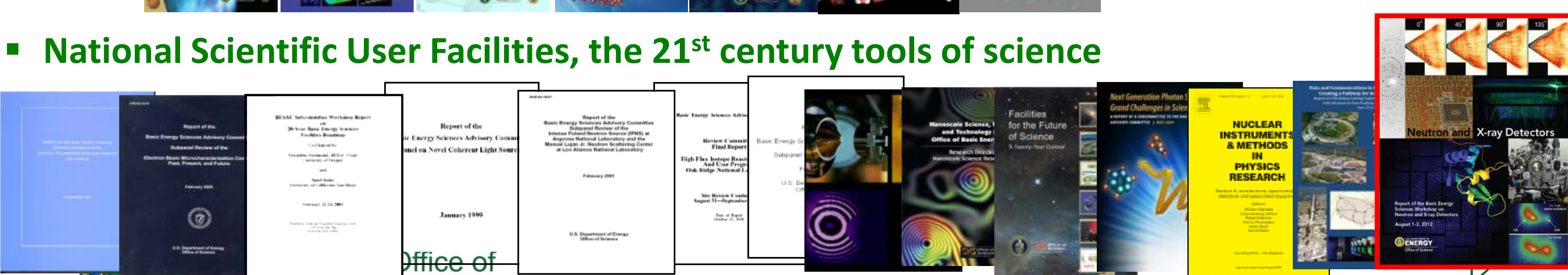
BES Strategic Planning Activities

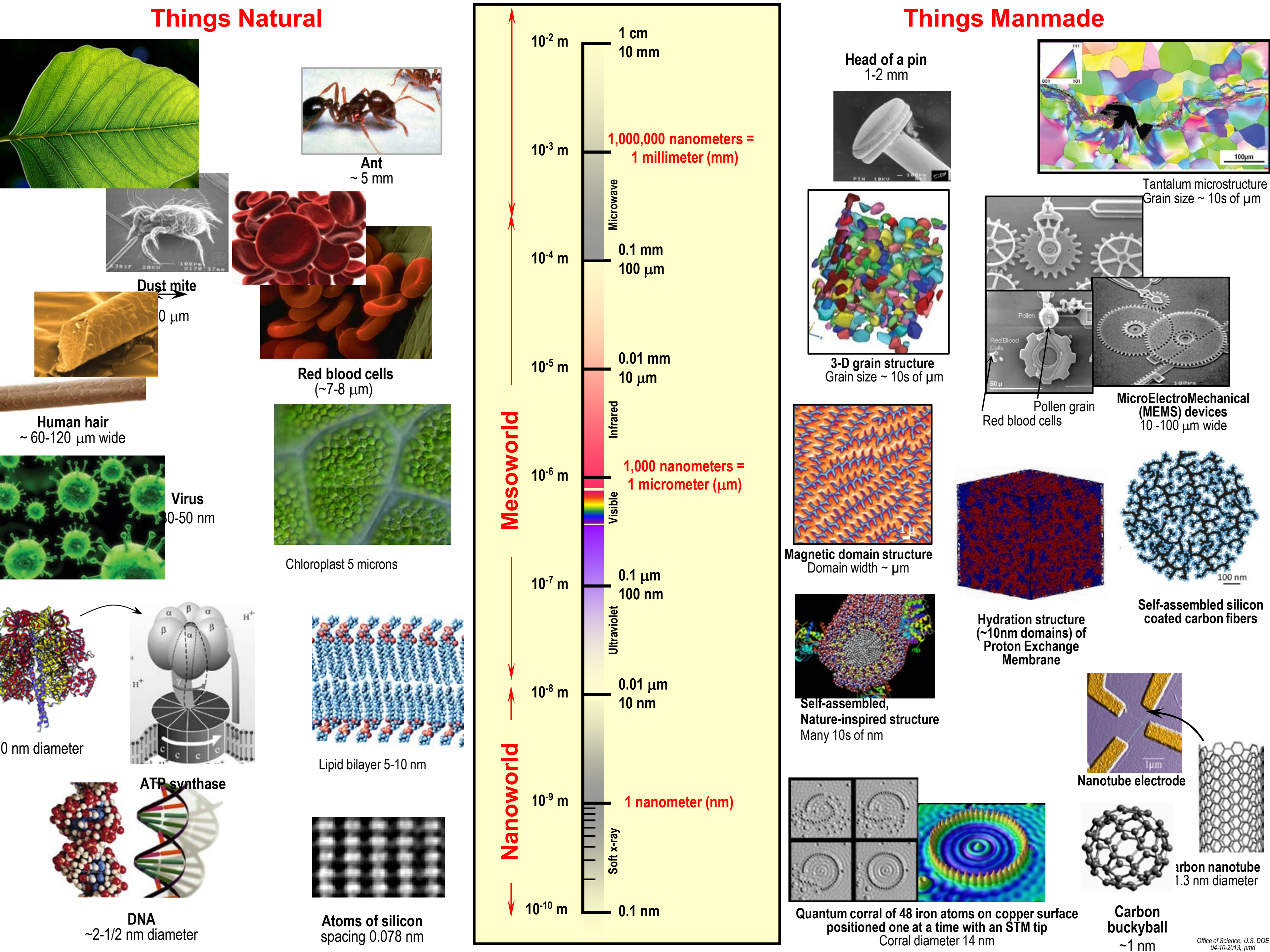
- Science for Discovery



- Science for National Needs

- National Scientific User Facilities, the 21st century tools of science





Things Natural
Ant
~ 5 mm
Dust mite
0 µm
Red blood cells
(~7-8 µm)
Human hair
~ 60-120 µm wide
Virus
30-50 nm
Chloroplast 5 microns
0 nm diameter
ATP synthase
Lipid bilayer 5-10 nm
DNA
~2-1/2 nm diameter
Atoms of silicon
spacing 0.078 nm
10-2 m
1 cm
10 mm
10-3 m
1,000,000 nanometers =
1 millimeter (mm)
Microwave
10-4 m
0.1 mm
100 µm
10-5 m
0.01 mm
10 µm
Infrared
Mesoworld
10-6 m
1,000 nanometers =
1 micrometer (µm)
Visible
10-7 m
0.1 µm
100 nm
Ultraviolet
10-8 m
0.01 µm
10 nm
Nanoworld
10-9 m
1 nanometer (nm)
Soft x-ray
10-10 m
0.1 nm
Things Manmade
Head of a pin
1-2 mm
Tantalum microstructure
Grain size ~ 10s of µm
3-D grain structure
Grain size ~ 10s of µm
Pollen grain
Red blood cells
MicroElectroMechanical
(MEMS) devices
10 -100 µm wide
Magnetic domain structure
Domain width ~ µm
Hydration structure
(~10nm domains) of
Proton Exchange
Membrane
Self-assembled silicon
coated carbon fibers
100 nm
Self-assembled,
Nature-inspired structure
Many 10s of nm
Nanotube electrode
Carbon nanotube
1.3 nm diameter
Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14 nm
Carbon
buckyball
~1 nm
Office of Science, U.S. DOE
04-10-2013, pmd

Why Mesoscale Science?

September 2012
http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf

"The great scientific advances of the last decade and more, especially at the nanoscale, are ripe for exploitation.

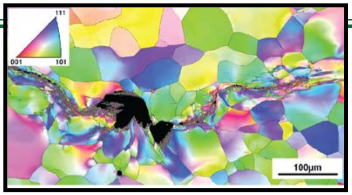
Seizing this opportunity requires mastering the mesoscale, where classical, quantum, and nanoscale science meet.

The functionality that is critical to macroscopic behavior begins to manifest itself not at the atomic or nanoscale but at the mesoscale, where defects, interfaces, and non-equilibrium structures are the norm.

The reward for breakthroughs in our understanding at the mesoscale is the emergence of previously unrealized functionality."

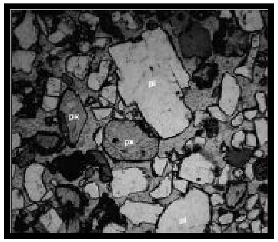
Mesoscale Science - From Quanta to the Continuum

- **Mastering Defect Mesostructure and its Evolution**
  Tracking, modeling and controlling the dynamic evolution of mesoscale defect patterns from their atomic origins to their macroscale impact is critical for extending materials lifetime, designing new generations of functional materials, and creating less expensive, more efficient advanced manufacturing.



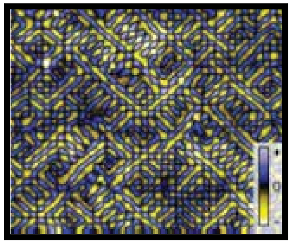
Scanning electron microscope image of pore coalescence in dynamically loaded Tantalum, showing defect evolution

- **Regulating Coupled Reactions and Pathway-dependent Chemical Processes**
  Characterizing and controlling fluid flow and chemical reactions in mesoscale pathways are central to solving energy and environmental challenges such as carbon sequestration, groundwater contamination and cleanup, shale gas extraction, energy storage, separation membranes for fluid and gas purification, and subsurface geological processes.



Pores in sandstone, a sedimentary rock formed by accumulation of many sizes and shapes of mineral and organic grains, may significantly influence transport properties.

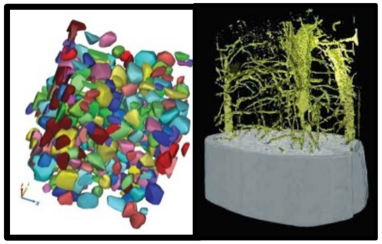
- **Optimizing Transport and Response Properties by Design and Control of Mesoscale Structure**
  Controlling the size and geometry of mesoscale architectures that mediate the interaction of electrons, photons and lattices allows new horizons in materials functionalities spanning thermoelectricity, light absorption and emission, spintronics, and multiferroics, building blocks for innovating next generation energy conversion and information technology.



Spectroscopic scanning tunneling microscope image of the electronic modulation in BSCCO superconductors – a correlated electron material that exhibits self-organized meoscale structure.

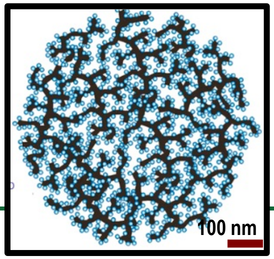
- **Elucidating Non-equilibrium and Many-Body Physics of Electrons**
  Controlling electronic correlation in artificial mesoscale architectures such as quantum dots and nanoparticle arrays adds new dimensions to exploiting functional behaviors from metal-insulator transitions to magnetism and high temperature superconductivity to produce entirely new levels of macroscopic functionality and advanced technology.

- **Harnessing Fluctuations, Dynamics, and Degradation for Control of Metastable Mesoscale**
  The inherent metastability of complex behaviors in mesoscale biological and human-engineered systems appears on multiple length and time scales that can be exploited to introduce smart, real-time responses to environmental cues, mitigate materials degradation due to defect accumulation, and dramatically extend useful technology life.



X-ray tomagraphy (left) and 3-D coherent imaging (right) are critical tools for mesoscale structural characterization.

- **Directing Assembly of Hierarchical Functional Materials**
  Directed assembly of functional materials in hierarchical mesoscale architectures requires the ability to model, synthesize, and assemble building blocks with motifs that embed information and behavior via anisotropies in chemical make-up, shape, and bonding strength. The integration of disparate material motifs by "top-down" design and "bottom-up" assembly creates a new paradigm in materials synthesis and advanced manufacturing.



Self-assembly of silicon coated carbon fibers for battery electrodes as an energy efficient synthesis approach with organized instead of random mesostructure.

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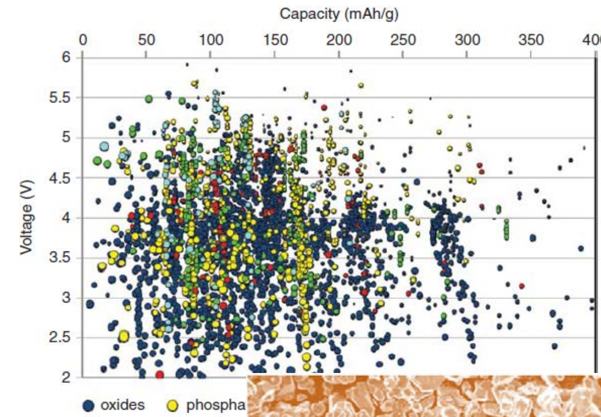
Materials Genome Initiative

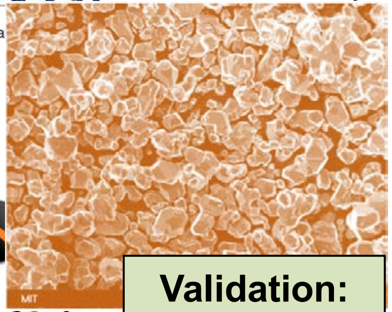
- *The Materials Genome Initiative will create a new era of materials innovation that will serve as a foundation for strengthening domestic industries… and offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.*
- Multiagency Initiative led by the Office of Science and Technology Policy
- DOE role:
  - Software development, building on theory and partnering (BES)
    - Robust, accurate and multiscale in both size and time
  - Validation of software and theory
    - User facilities and broad experimental materials science portfolio
  - Application specific R&D for manufacturing and to develop lightweight, high-strength alloys for automotive (EERE)
- Technical emphasis includes materials for clean energy

Materials and Chemical Processes by Design

- Research to establish design rules to launch an era of predictive modeling, changing the paradigm of materials discovery to rational design.
  - New software tools and data standards to catalyze a fully integrated approach from material discovery to applications
- Discovery of new materials has been the engine driving science frontiers and fueling technology innovations. Research would utilize the powerful suite of tools for materials synthesis, characterization, and simulation at DOE's world-leading user facilities
- Integrated teams to focus on key scientific knowledge gaps to develop new theoretical models
  - Long-term: realization in reusable and broadly-disseminated software
  - Collection of validated experimental and modeling data for broader community use

Prediction: New battery materials starting from first principles theory





Validation: Materials fabrication

MATERIALS PROJECT

http://materialsproject.org/

End Use: Software on-line for general community use

From Basic Energy Science to Technology

Cross-cutting Investments and Coordination

- DOE has increasingly emphasized cross-program communications and collaboration to ensure coordination of basic and applied research and effective integration of R&D results.
  - Technology Teams: working groups focused on specific technologies the meet to discuss R&D programs across the Department
  - Energy Innovation Hubs: working group to coordinate programmatic oversight and promote commonality across all the Hubs
  - ARPA-E: ad-hoc groups to identity "white space" where others are not making investments in energy technologies but that would be appropriate for ARPA-E support
  - Topical items of interest: working groups established to address current issues such as critical materials

Science-Based Engine Design

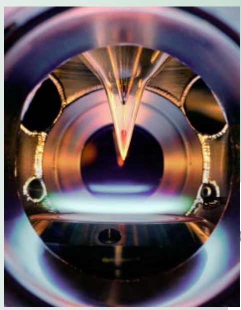
An early example

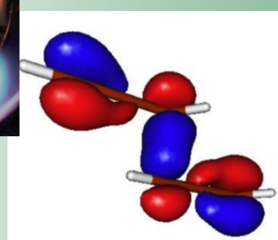
Basic Science

BES

Sustained support in 2 areas

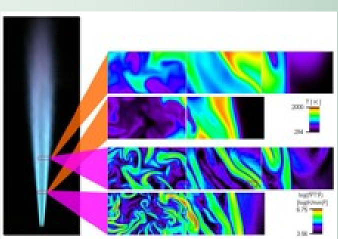
Development of predictive chemistry in model flames





Computational kinetics and experiments

Advance laser diagnostics applied to model flames

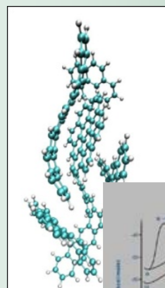


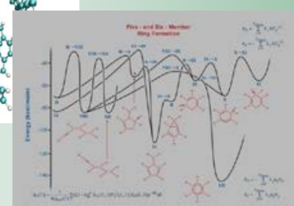
Laser-based chemical imaging

Applied R&D

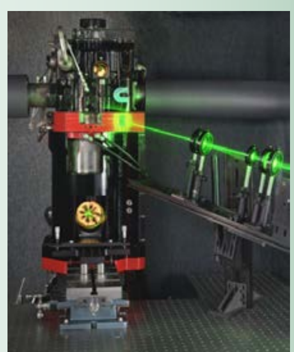
BES → EERE

Applications of chemistry and diagnostics to engines





Predictive chemical models under realistic conditions



Laser diagnostics of diesel fuel sprays in engine cylinders

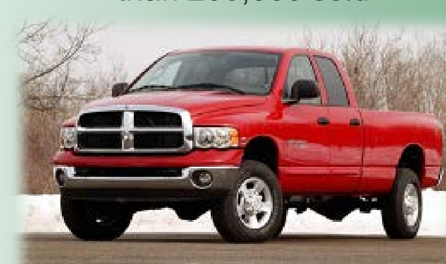
Manufacturing/ Commercialization

Cummins and Dodge

Cummins used simulation tools and improved understanding of diesel fuel sprays to design a new diesel engine with reduced development time and cost and improved fuel efficiency.

Cummins®

ISB 6.7 liter Cummins diesel engine first marketed in the 2007 Dodge Ram pickup truck; more than 200,000 sold

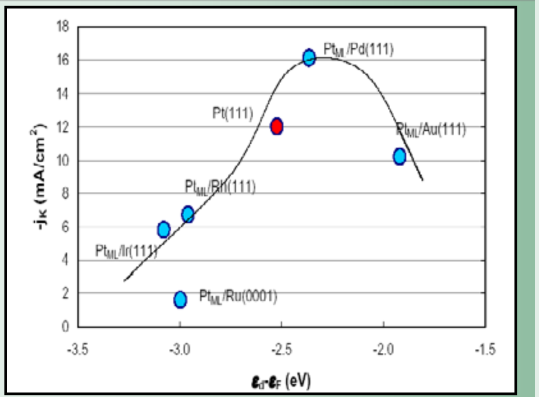


Platinum Monolayer Electro-Catalysts:
Stationary and Automotive Fuel Cells

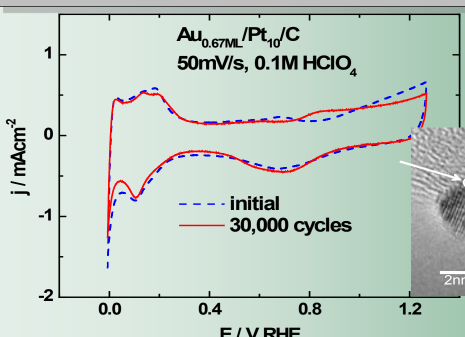
Basic Science	Applied R&D	Manufacturing/ Commercialization

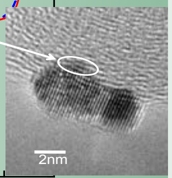
BES
Two research advances

Pt core-shell nano-catalysts: high activity with ultralow Pt mass



Pt stabilized against corrosion in voltage cycling by Au clusters



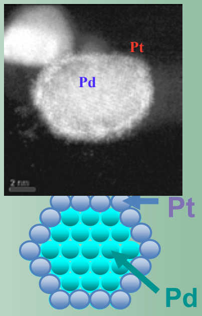


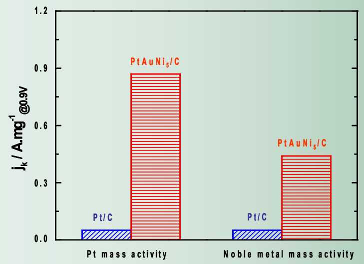
Science **315**, 220 (2007)

BES → EERE
Core-Shell Nanocatalysts

Active Pt ML shell – Metal/alloy core
Core tunes activity & durability of shell

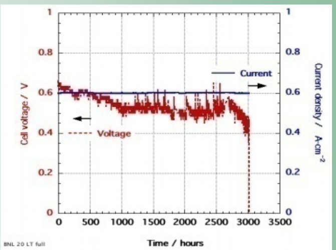
Model and actual image of a Pt Monolayer on Pd nanoparticle





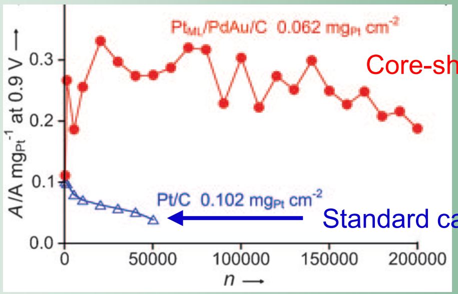
Pt-mass weighted activity enhanced 20x

3000 hr Fuel Cell Durability Performance

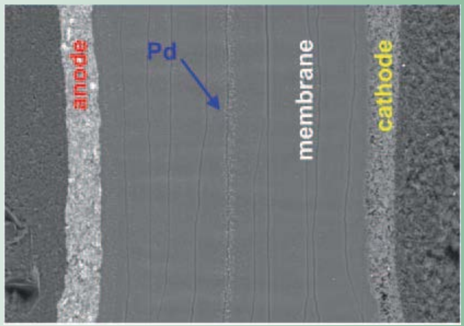


CRADA with Industry

Scale-up synthesis: **Pt-ML/Pd_9Au_1/C**
Excellent fuel Cell durability 200,000 cycles



Membrane Electrode Assembly >200K cycles
Very small Pt diffusion & small Pd diffusion



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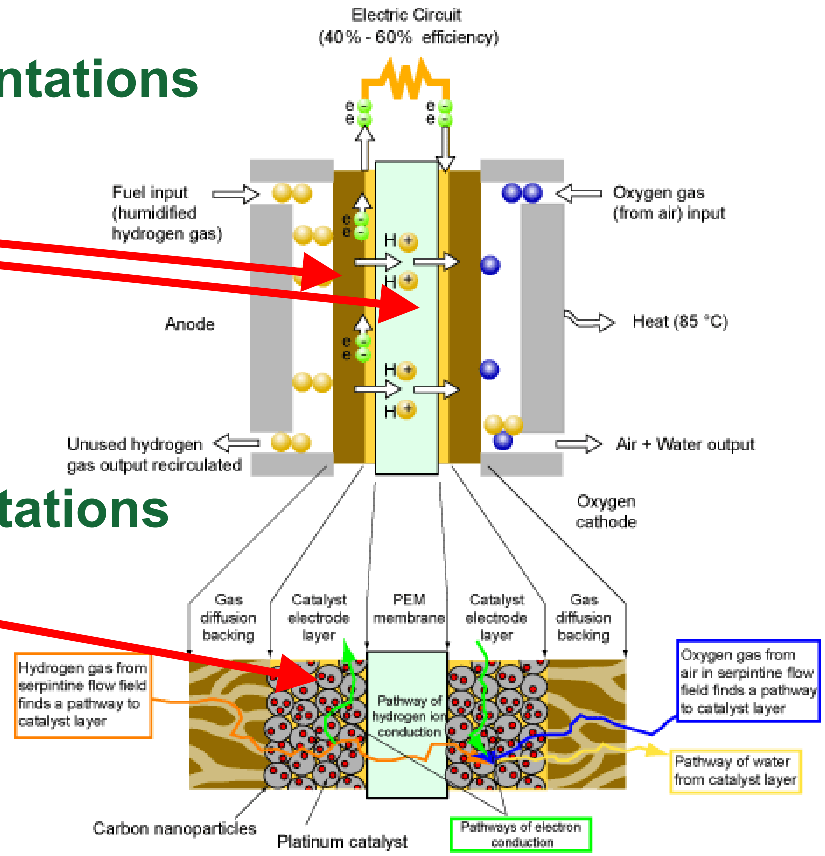
N.E. CHEMCAT
Lead The Catalyst Innovations

BES PI Participation in 2013 AMR Meeting

- **Relevant research in Basic Energy Sciences is found in the Catalysis Sciences and Separations and Analysis Programs**

- **Membranes: 3 Oral, 3 Poster Presentations**
  - Chemical functionalization
  - Simulation
  - Gas separations
  - Oral 4:15 Wed., Posters Thurs. PM



- **Catalysts: 3 Oral, 21 Poster Presentations**
  - Mesostructures
  - Catalyst interactions
  - Simulation
  - Oral 4:15 Thur., Posters Thurs. PM

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Thank You!