Basic Energy Sciences
Research Priorities and Strategic Planning

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Basic Energy Sciences Overview
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
Three Major Types of Funding Modality

- **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

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

http://science.energy.gov/bes/efrc/
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
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 nanoscale tools and theoretical approaches to enable new generation energy storage.
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
“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.”
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.

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.

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.

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.

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.
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
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
From Basic Energy Science to Technology
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 that 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 identify "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

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.
  - 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

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

Applied R&D

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

Manufacturing/Commercialization

CRADA with Industry
Scale-up synthesis: Pt-ML/Pd₉Au₁/C
Excellent fuel Cell durability 200,000 cycles

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

Commercial license signed Dec. 2011

Science 315, 220 (2007)
• 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
Thank You!