Department of Energy

Basic Energy Sciences: New Research Initiatives and Funding

University Materials Council

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The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things.
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales.
- Explore materials and chemical functionalities and their connections to atomic, molecular, and electronic structures.
- Explore basic research to achieve transformational discoveries for energy technologies.

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies.

Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies.

Supporting:
- 46 Energy Frontier Research Centers
- Solar Fuels and Batteries and Energy Storage Hubs
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world.

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels.
Recurring Themes - BES Strategic Planning

>>1,500 participants from academia, industry, and federal labs

Disruptive, Transformational Advances Require “Control”
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
- Designed catalysts
- Designed 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

http://science.energy.gov/bes/news-and-resources/reports/
Three Major Types of Research Thrusts

- **Core Research (many)**
  Support single investigator and small group projects to pursue their specific research interests

- **Energy Frontier Research Centers (46)**
  $2-5 million-per-year research centers, established in 2009, focus on fundamental research related to energy

- **Energy Innovation Hubs (1 in BES)**
  $20 million+ -per-year research centers focus on integrating basic & applied research with technology development to enable transformational energy applications
Hubs funded in FY 2010:
- Fuels from Sunlight (SC lead) – Joint Center for Artificial Photosynthesis (JCAP) – Caltech and LBNL
- Energy Efficient Building Systems Design (EERE) – Penn State
- Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE) – ORNL

Coming in FY 2012:
- Batteries and Energy Storage
- Critical Materials

Each Hub has a world-class, multi-disciplinary, and highly collaborative research, development and deployment team

Strong scientific leadership is located at the primary location of the Hub.
- Clear organization and management plan for achieving the HUB goal
- “Infuses” a culture of empowered central research management
46 EFRCs in 35 States were Launched in Fall 2009

- ~860 senior investigators and
  ~2,000 students, postdoctoral fellows, and technical staff at ~115 institutions
- > 250 scientific advisory board members from 12 countries and > 35 companies

Impact to date:

- >1,000 peer-reviewed papers including more than 30 publications in Science and Nature.
- > 40 patents applications and nearly 50 additional patent/invention disclosures by 28 of the EFRCs.
- at least 3 start-up companies with EFRC contributions

Assessment of Progress:

- All EFRCs have undergone mid-term peer review to assess progress towards goals and plans for the next 2 years of R&D

http://science.energy.gov/bes/efrc/
FY 2012 BES Budget Appropriation

- **Research programs**
  - Energy Innovation Hubs
    - Battery and Energy Storage Hub (+$20M)
  - Energy Frontier Research Centers
  - Core Research
    - Plan to initiate new projects in materials and chemistry by design

- **Scientific user facilities operations**
  - All facilities operate below optimum level
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers

- **Construction and instrumentation**
  - National Synchrotron Light Source-II ($159M) and NEXT instrumentation ($12M)
  - Spallation Neutron Source instruments ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($30M)
BES Strategic Planning Activities

- **Science for Discovery**

- **Science for National Needs**

- **National Scientific User Facilities, the 21st century tools of science**
FY 2013 BES Budget Request

### Research programs
- Energy Innovation Hubs (+$5M)
- Energy Frontier Research Centers
  - Joint EERE R&D (+$20M)
- Core Research
  - Materials and Chemistry by Design (+$20M)
  - Science for Clean Energy (+$42M)

### Scientific user facilities operations
- Near optimum operations of all facilities (+$42M)
  - Synchrotron light sources
  - Neutron scattering facilities
  - Nanoscale Science Research Centers
- Instrumentation for clean energy, joint with EERE (+$15M)
- NSLS-II Early Operations (+$22M)

### Construction and instrumentation
- National Synchrotron Light Source-II
- NSLS-II instrumentation (NEXT) ($12M)

Advanced Photon Source upgrade ($20M)
Linac Coherent Light Source-II ($64M)
Research to establish design rules to launch an era of predictive modeling, changing the paradigm of materials discovery to rational design (+$20M).

- 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

End Use: Software on-line for general community use

http://materialsproject.org/
Science for Clean Energy: Nanoscale to Mesoscale Sciences

- Developing the next generation of materials, chemicals, and game-changing processes - understanding structure, properties, and function from atoms and molecules, through the nanoscale, and to the mesoscale (+$42M).

- Research will enable science-based chemical and materials design and manufacturing in, for example:
  - direct conversion of solar energy to fuels
  - generation of electricity from clean energy sources
  - storage and transmission of electrical energy
  - carbon capture, utilization, and sequestration
  - the efficient use of energy

First determination of the structure of the high Tc superconductor YBa$_2$Cu$_3$O$_{7-x}$ determined using neutron scattering.

Magneto-optical images of superconducting films

Fabricated industrial wires of MgB$_2$ superconductors used in MRIs and commercial magnets.
Visionary Outcomes:

- Complexity and functionality of biology with inorganic earth abundant materials
- Systems with many degrees of freedom; new organization principles
- Paradigm shift from top down design with classical building blocks to bottom up design with atomic, molecular and nano components
The Basic Energy Sciences Advisory Committee will carry out a study of mesoscale materials and chemistry, the regime where classical, microscale and nanoscale science meet. The study will address two areas: (i) new mesoscale phenomena and functionality, and (ii) facilities and tools needed to make, characterize and describe mesoscale materials, phenomena and functionality.

The mesoscale materials and chemistry report draws its motivation from three themes developed in earlier BESAC and BES reports:

- The need for innovation, articulated in the Science for Energy Technology Report
- The insights and tools we have gained and are still gaining from nano, articulated in the New Science for a Secure and Sustainable Energy Future Report
- The grand challenges of materials and chemistry, articulated in the Grand Science Challenges Report
Office of Science Early Career Research Program

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

Award Size: University grants $150,000 per year for 5 years to cover summer salary and expenses; Lab Awards cover ~ annual research costs for 5 years

About 70 awards per year since FY 2010

FY 2012 Process:

- Funding Opportunity Announcement issued in July 2011
  - Pre-applications deadline Sept. 1, 2011
  - Full proposals due November 29, 2011
- Awards to be announced in the Spring of 2012
BES 2011 Summary Report
http://science.energy.gov/bes/research/
- Overview of BES
- How BES does business
- Descriptions and representative research highlights for 3 BES divisions, EFRCs, and Energy Innovation Hubs

BES FY 2011 Research Summaries
http://science.energy.gov/bes/research/
- Summaries of more than 1300 research projects across 3 BES divisions, including senior investigators, postdocs, graduate and undergraduate students, and a brief project description

Science Serving the Nation
http://science.energy.gov/bes/benefits-of-bes/
- Brief vignettes describing the impact of BES funded research on scientific innovation and its impact on end-use technology
Questions?
**Materials Discovery, Design, and Synthesis**

Rational design and synthesis of materials via physical, chemical, and bio-molecular routes

- **Synthesis and Processing Science**
  - Learn to control synthesis and processing by developing scientific foundations, *in situ* studies, and for a wide range of materials

- **Biomolecular Materials**
  - Discovery, design and synthesis of biomimetic and bioinspired functional materials and energy conversion processes based on principles and concepts of biology

- **Materials Chemistry**
  - Nanoscale chemical synthesis and assembly; solid state chemistry; novel polymeric materials and complex fluids; surface and interfacial chemistry

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A bionanoelectronic system that integrates membrane proteins and nanowire electronics. It uses electric field to open and close the pores and to detect ions.

The 3D bicontinuous battery cathode provides both high power and energy density.
Control and understanding of materials behavior and discovery of new emergent phenomena

- **Experimental Condensed Matter Physics**
  - Fundamental understanding of the relationships between intrinsic electronic structure and the properties of complex materials

- **Theoretical Condensed Matter Physics**
  - Theory, modeling, and simulation of electronic correlations, with a particular emphasis on nanoscale science

- **Mechanical Behavior and Radiation Effects**
  - Experimental and modeling studies of defects in materials and their effects on the properties of strength, structure, deformation, and failure.

- **Physical Behavior of Materials**
  - Behavior of materials in response to temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces.

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Voltage versus theoretical capacity for thousands of compounds. (G. Ceder. MRS Bulletin 35, 693, 2010)
Scattering and Instrumentation Sciences

Study of photon, neutron, and electron interactions with matter for characterization of materials structures and excitation

- Elucidate the mechanisms that control superconductivity and other phenomena in correlated electron systems
  - Use scattering probes to determine important correlations (spin, lattice, charge, orbital) that govern superconductivity, magnetism, and other phenomena.

- Develop a structural and dynamical understanding of nanostructured materials
  - Understand the interplay between properties and structure at the nanometer length scale and develop new nanoscience tools

- Understand the behavior of materials using Ultrafast Diffraction, Spectroscopy and Imaging Techniques
  - Understand how entities form, grow, and move under the influence of external fields, and understand functionality.

- Unify the complementary information obtained through multiple techniques
  - Develop the capability to analyze, visualize, and understand data from different experimental probes.