The Role of Advanced Computing in Basic Energy Sciences

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The mission of the Basic Energy Sciences program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

Priorities:

• To discover and design new materials and molecular assemblies with novel structures, functions, and properties.
• To conceptualize, calculate, and predict processes underlying physical and chemical transformations.
• To 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 conceive, plan, design, construct, and operate scientific user facilities to probe the most fundamental electronic and atomic properties of materials at extreme limits of time, space, and energy resolution through x-ray, neutron, and electron beam scattering.
• To foster integration of the basic research conducted in the program with research in NNSA and the DOE technology programs.
Control and understanding of materials behavior and discovery of new emergent phenomena

Condensed Matter and Materials Physics

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

Materials Discovery Design and Synthesis

Scattering & Instrumentation Sciences

Rational design and synthesis of new materials via physical, chemical, and biomolecular routes

Teams have unique focus but some common, synergistic scientific themes:
- Correlation phenomena
Key Areas of Research in Materials Discovery, Design, and Synthesis

- Develop scientific strategies to fabricate macroscopic materials with nanometer scale precision
- Establish fundamental understanding of thermodynamics, kinetics and dynamics of self-assembly
- Understand fundamental principles to produce materials with precisely controlled defects
- Develop multi-component, multi-functional materials
- Develop new classes of materials and innovative architectures that can revolutionize energy conversion, storage and transfer

PS-I covalently attached to nanoparticle catalysts via a molecular wire yields 75% of plant electron transfer rates resulting in photo-generated hydrogen at ~1700 X current benchmarks
Key Areas of Research in Condensed Matter and Materials Physics

- Develop a detailed understanding of the phenomena of superconductivity and magnetism
- Understand the influence of defects on materials at the atomic scale
- Investigate the properties of materials under extreme environments
- Understand and control the structure and properties of materials at the nanoscale
- Design, fabrication and characterization of metamaterials

Two-Dimensional Electrons in Gallium Arsenide Semiconductors

Electronic Structure in Graphene

Tetragonal structure with square nets of Fe$^{2+}$ in BaFe$_{1.84}$Co$_{0.16}$As$_2$
Key Areas of Research in Scattering and Instrumentation Sciences

- Utilize scanning probes to elucidate mechanisms that control phenomena in correlated electron systems
- Develop a structural and dynamical understanding of nanostructured materials
- Understand dynamics and materials functionality using ultrafast diffraction, spectroscopy and imaging techniques
- Unify the complementary information obtained through multiple techniques

Magnetic Fluctuations in Superconductors

LBCO

YBCO

Neutron scattering studies demonstrate universal magnetic excitation spectrum
Chemical Sciences, Geosciences and Biosciences

Molecular mechanisms of light capture and its conversion to chemical and electrical energy via chemical and biochemical pathways

Application of physical science tools to biochemical systems

Structural and dynamical studies of atoms, molecules, and nanostructures; description of their interactions with external stimuli (photons, electrons) at full quantum detail

Photo- and Biochemistry

Biomimetic catalytic systems

Characterization, control, and optimization of chemical transformations, from catalysis to geochemistry

Fundamental Interactions

Chemical Transformations

Interfacial nanoscale chemistry

Division-wide themes: chemical imaging; ultrafast chemical sciences; nanoscale science; catalytic science; theory, modeling, & simulation; synthesis
Key Areas of Research in Fundamental Interactions

- Discover, understand, and exploit fundamental phenomena associated with interactions of intense electromagnetic fields and matter on ultrashort time scales.

- Develop a fundamental understanding of chemical reactivity, validated theories, models, and computational tools to predict rates, products, and dynamics of chemical processes in the gas phase.

- Develop a molecular-level understanding of chemical, physical, and electron driven processes in aqueous media and at interfaces.

- Theory and computational methods to advance research goals across the Division.
Key Areas of Research in Photo- and Bio-Chemistry

- Learning from natural photosynthesis to improve the biological process and to provide a roadmap for robust artificial systems.

- Chlorophyll monomer and trimer building block for supramolecular charge transport systems. (Tiede et al, ANL)

- Basic research in solar photochemistry with the goal of creating viable and efficient artificial photosynthetic systems.

- Mechanism of plant cell wall loosening by the protein expansin, which modulates non-covalent linkages between hemi-cellulose and cellulose (Cosgrove, Penn State).
Key Areas of Research in Chemical Transformations

- Understanding the mechanisms and dynamics of catalyzed reactions leading to the deliberate design and controlled synthesis of catalysts for energy applications
- Resolving the f-electron challenge to understand the chemistry and physics of actinide compounds
- Molecular dynamics simulation of water on a mineral surface based on neutron scattering data from the SNS
- Imaging molecules in real time and space to unravel single-molecule chemistry
- Modeling the geosphere from nanometers to kilometers

Actinide elements of interest to advanced fuel cycle:
Three Major Types of Research Thrusts

- **Core Research**
  Support single investigator and small group projects to pursue their specific research interests.
  - Enable seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, and aspects of geosciences and biosciences. Accelerator and detector R&D is also supported.
  - Build research programs that provide world-class, peer-reviewed research results cognizant of both DOE mission needs and new scientific opportunities. 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, established in 2009, focused on fundamental research related to energy
  - Multi-investigator and multi-disciplinary centers to 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.
  - EFRCs are overseen by program staff, who are managed centrally within BES to ensure a unified management strategy and structure.

- **Energy Innovation Hubs**
  $20$ million+ -per-year research centers will focus on integrating basic & applied research with technology development to enable transformational energy applications
  - Hubs comprise a larger set of investigators spanning science, engineering, and other disciplines focused on a single critical national need identified by the Department; each Hub is expected to become a world leading R&D center in its topical area to develop a complete energy system.
  - With robust links to industry, the highly integrated Hubs can bridge the gap between basic scientific breakthroughs and industrial commercialization.
BES Scientific User Facilities

**Light sources**
Stanford Synchrotron Radiation Laboratory (SLAC)
National Synchrotron Light Source (BNL)
National Synchrotron Light Source II (BNL)  
(start construction FY 2010)
Advanced Light Source (LBNL)
Advanced Photon Source (ANL)
Linac Coherent Light Source (SLAC)

**Neutron sources**
Manuel Lujan, Jr. Neutron Scattering Center (LANL)
High Flux Isotope Reactor (ORNL)
Spallation Neutron Source (ORNL)

**Electron beam sources**
Electron Microscopy Center for Materials Research (ANL)
National Center for Electron Microscopy (LBNL)
Shared Research Equipment Program (ORNL)

**Nanoscale Science Research Centers**
Center for Nanophase Materials Sciences (ORNL)
Molecular Foundry (LBNL)
Center for Integrated Nanotechnologies (SNL/A & LANL)
Center for Functional Nanomaterials (BNL)
Center for Nanoscale Materials (ANL)
Nanoscale Science Research Centers

Center for Nanoscale Materials (Argonne National Laboratory)

Molecular Foundry (Lawrence Berkeley National Laboratory)

Center for Functional Nanomaterials (Brookhaven National Laboratory)

Center for Integrated Nanotechnologies (Sandia & Los Alamos National Labs)
Ultra-small and Ultra-fast: A Unified Theme for Research and Facilities

[Diagram showing ultra-small and ultra-fast examples, including molecular structures and technological applications.]
BESAC & BES Strategic Planning Activities

- **Science for Discovery**

- **Science for National Needs**

- **National Scientific User Facilities, the 21st century tools of science**
Science for Discovery -
Directing and Controlling Matter and Energy

Control the quantum behavior of electrons in materials
Direct manipulation of the charge, spin, and dynamics of electrons to control and imitate the behavior of physical, chemical and biological systems, such as digital memory and logic using a single electron spin, the pathways of chemical reactions and the strength of chemical bonds, and efficient conversion of the Sun’s energy into fuel through artificial photosynthesis.

Synthesize, atom by atom, new forms of matter with tailored properties
Create and manipulate natural and synthetic systems that will enable catalysts that are specific and produce no unwanted byproducts, or materials that operate at the theoretical limits of strength and fracture resistance, or that respond to their environment and repair themselves like those in living systems.

Control emergent properties that arise from the complex correlations of atomic and electronic constituents
Orchestrate the behavior of billions of electrons and atoms to create new phenomena, like superconductivity at room temperature, or new states of matter, like quantum spin liquids, or new functionality combining contradictory properties like super-strong yet highly flexible polymers, or optically transparent yet highly electrically conducting glasses, or membranes that separate CO₂ from atmospheric gases yet maintain high throughput.

Synthesize man-made nanoscale objects with capabilities rivaling those of living things
Master energy and information on the nanoscale, leading to the development of new metabolic and self-replicating pathways in living and non-living systems, self-repairing artificial photosynthetic machinery, precision measurement tools as in molecular rulers, and defect-tolerant electronic circuits.

Control matter very far away from equilibrium
Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically-inspired molecular machines, long-term storage of spent nuclear fuel through adaptive earth chemistry, and achieving environmental sustainability by understanding and utilizing the chemistry and fluid dynamics of the atmosphere.
Science for National Need

Bringing forefront scientific knowledge and state-of-the-art tools to solving grand energy challenges

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

10 workshops; 5 years; more than 1,500 participants from academia, industry, and DOE labs
BES Strategic Priorities

Energy Sustainability and Control Science

**Traditional Energy Materials**

- Fuels: coal, oil, gas
  - $CH_{0.8}$, $CH_2$, $CH_4$

  **Passive Function:** Combustion

  **Value:** Commodities
  - High Energy Content

**Sustainable Energy Materials**

- Diverse Functions
  - PV, Superconductors
  - Photocatalysts
  - Battery Electrodes
  - Electrolytic Membranes

  **Active Function:** Converting Energy

  **Value:** Functionality
  - 30 year Lifetime

**Greater Sustainability = Greater Complexity**, higher functional materials
Basic and Applied R&D Coordination
How Nature Works … to … Design and Control … to … Technologies for the 21st Century

**Grand Challenges**
- How nature works
- Use-Inspired Basic Research
- Materials properties and chemical functionalities by design
- Applied Research
- Technology Maturation & Deployment

**Discovery and Use-Inspired Basic Research**
- Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies
- Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation
- Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies

**Technology Maturation & Deployment**
- Research with the goal of meeting technical milestones, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Proof of technology concepts
- Scale-up research
- At-scale demonstration
- Cost reduction
- Prototyping
- Manufacturing R&D
- Deployment support

**BESAC & BES Basic Research Needs Workshops**

**BESAC Grand Challenges Panel**

**DOE Technology Office/Industry Roadmaps**
**EFRC awards** provide the recipients with $2-5 million/year over a five-year award period to pursue collaborative basic research that addresses both energy challenges and science grand challenges in areas including:

- Solar Energy Utilization
- Bio-Fuels
- Catalysis
- Energy Storage
- Geosciences for Waste and CO₂ Storage
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen
- Combustion
- Superconductivity
- Solid State Lighting
- Bio-Fuels
- Advanced Nuclear Energy Systems
- Materials Under Extreme Environments
- Hydrogen
- Combustion
- Superconductivity
- Solid State Lighting

As stated in the Funding Opportunity Announcement for the EFRCs:

“... the research proposed in the EFRC application must:

1) address one or more of the challenges described in the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination* ([http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf](http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf), and

2) address one or more of the energy challenges described in the 10 BES workshop reports in the *Basic Research Needs* series ([http://www.sc.doe.gov/bes/reports/list.html](http://www.sc.doe.gov/bes/reports/list.html))”

**FY 2009 EFRCs Funding:**

<table>
<thead>
<tr>
<th>Recovery Act (Stimulus Bill)</th>
<th>Omnibus Appropriations</th>
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<td>$277M</td>
<td>$100M</td>
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Total EFRCs = $777M over 5 years
The Status of the SC/BES Energy Frontier Research Centers

46 EFRCs were launched in late FY 2009 using FY 2009 Appropriations and Recovery Act Funds

46 centers awarded, representing 103 participating institutions in 36 states plus D.C.

By Lead Institution:
- Universities: 31
- DOE Labs: 12
- Industry/Nonprofit: 12

By Topical Category:
- Energy Efficiency: 6
- Crosscutting Sciences: 14
- Energy Supply: 20
- Energy Storage: 6

Energy Frontier Research Center Locations (Leads; Participants)
EFRC Highlight: Understanding Radiation Resistance in Materials
Energy Frontier Research Center for Materials at Irradiation and Mechanical Extremes

- Key to radiation resistance is efficient recombination of vacancies and interstitials (point defects) created by damage cascades formed when neutrons collide with atoms in materials. In this early EFRC result, grain boundaries were found to enable a surprising mechanism for increasing point-defect recombination and potentially imparting greater radiation resistance to materials.

- After a simulated collision cascade (at right, showing displaced atoms 0.5 ps after the cascade initiation), fast-moving interstitials move quickly to a nearby boundary (below, at left). Slower-moving vacancies remain in the bulk material.

- This research showed that a grain boundary loaded with interstitials emits these interstitials (below, center) via a newly-discovered low-energy mechanism to annihilate nearby vacancies much faster than other mechanisms (below, at right).

- This new mechanism may explain the enhanced radiation resistance observed in nanocrystalline materials with large numbers of grain boundaries.

Simulations predict that light absorption and charge collection are optimal when the diameter of wires is on the order of the minority-carrier diffusion length, ca. 2 to 10 microns in low-purity silicon.

Based on this prediction, silicon solar cells were fabricated as follows:

- Si wire arrays with these diameters and SiN$_x$ antireflective coating
- Arrays embedded in PDMS with 0.9 micron Al$_2$O$_3$ which redirect light towards micropillars
  Arrays can be peeled off and put on flexible substrate

Absorb up to 85% of the sunlight but fills as little as 1% of the cell’s volume and uses only 1/100th of the Si in a conventional cell.

Potential for increased photovoltaic efficiency owing to an effective optical concentration of up to 20 times.
The Science Base for Multi-Scale Simulation of Internal Combustion Engines-

A New Initiative in FY 2011
Transportation Combustion Challenge: How to get “clean” and “efficient”? 

- Transportation accounts for 60% of oil consumption 
- Combustion engine viable for decades to come, but efficiency & cleanliness difficult to achieve together 
- Fuel streams are rapidly evolving 
  - Heavy hydrocarbons: oil sands, oil shale, coal 
  - New renewable fuel sources: ethanol, biodiesel 
- New engine technologies 
  - Direct Injection (DI) 
  - Homogeneous Charge Compression Ignition (HCCI) 
  - Low-temperature combustion 
- Hybrid vehicle technologies
Multi-scale Simulation of Internal Combustion Engines
A new initiative to develop the science base for computational design of advanced engines

Predictive simulation of combustion in an evolving fuel environment is essential for developing more efficient and cleaner engines.

The scientific community has provided a roadmap via:

- BES workshop: Basic Research Needs for Clean and Efficient Combustion, October 2006
- ASCR/BES workshop: Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, August 2009
- SC ongoing collaboration with EERE’s Vehicle Technology Program

The new BES activity (+$20,000K) will provide:

- Models that span vast scale ranges: coupling of combustion chemistry with turbulent flow requiring simulation over 9 orders of magnitude in space and time.
- Improved understanding of fundamental physical and chemical properties: multi-phase fluid dynamics, thermodynamic properties, heat transfer, and chemical reactivity.
- Engine simulation: science-based predictive simulation and modeling design
Establishing the science base for multi-scale simulation of advanced engines

- Computational chemistry and benchmark combustion simulations (in collaboration with ASCR).
  - Numerical investigations of canonical flame behavior
  - Automated discovery of chemical reaction mechanisms and kinetics
- Experimental validation, verification, and discovery.
  - Cinematic imaging of canonical flames
  - Multiplex investigation of chemical reactions
- To set the stage for subsequent development of new, science-based engineering tools for advanced engine design (in collaboration with EERE Vehicle Technologies Program).

Top: Direct numerical simulation of a CO/H2 slot flame
Bottom: Imaging of a model flame jet flame