Basic Energy Sciences

Funding Profile by Subprogram

(dollars in thousands)

	FY 2009 Current Appropriation	FY 2009 Current Recovery Act Appropriation[a]	FY 2010 Current Appropriation	FY 2011 Request
Basic Energy Sciences				
Materials Sciences and Engineering	1,108,351[b]	+221,788	363,642	432,663
Chemical Sciences, Geosciences, and Energy Biosciences	281,946	+169,072	296,934	403,616
Scientific User Facilities	0[b]	0	821,684	847,121
Subtotal, Basic Energy Sciences	1,390,297	+390,860	1,482,260	1,683,400
Construction	145,468	+164,546	154,240	151,600
Total, Basic Energy Sciences	1,535,765[c]	+555,406	1,636,500	1,835,000

Public Law Authorizations:
Public Law 95–91, "Department of Energy Organization Act", 1977
Public Law 108–153, "21st Century Nanotechnology Research and Development Act 2003"
Public Law 109–58, "Energy Policy Act of 2005"
Public Law 110–69, "America COMPETES Act of 2007"

Program Overview

Mission

The mission of the BES 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.

Background

Our ability to discover and transform the material resources that nature provides has shaped history and built civilizations. From prehistoric hunters and gatherers, who utilized wood-burning fires and fashioned tools from stone, to modern nations that run on processes powered primarily by coal and oil, progress has been marked by advanced technologies designed to make better use of Earth's resources. Today, science and technology is even more at the heart of many critical societal, political, and economic issues that surround the energy security and sustainability of our nation.

Fundamentally, the energy challenges of the next century will increasingly involve scientific discovery and technological innovation. The lessons of the previous century illustrate that major breakthroughs in energy technologies are largely built on a solid foundation of research advances. At the core of these

[a] The Recovery Act Current Appropriation column reflects the allocation of funding as of September 30, 2009.
[b] FY 2009 funding of $771,198,000 for Scientific User Facilities is located within the Materials Sciences and Engineering subprogram. The Materials Sciences and Engineering subprogram FY 2009 total, excluding Scientific User Facilities funding is $337,153,000.
[c] Total is reduced by $36,207,000; $32,328,000 of which was transferred to the Small Business Innovation Research (SBIR) program and $3,879,000 of which was transferred to the Small Business Technology Transfer (STTR) program.

advances is the ability to create new materials using sophisticated synthetic and processing techniques, precisely define the atomic arrangements in matter, and control physical and chemical transformations.

The research disciplines that the BES program supports—condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—are those that discover new materials and design new chemical processes. These disciplines touch virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. BES research provides a knowledge base to help understand, predict, and ultimately control the natural world and serves as an agent of change in achieving the vision of a secure and sustainable energy future.

The BES program is one of the nation's largest sponsors of research in the natural sciences. In FY 2009, the program funded research in more than 170 academic institutions located in 50 states and in 14 DOE laboratories located in 12 states. BES supports a large extramural research program, with approximately 40% of the program's research activities sited at academic institutions. The BES program also supports world-class scientific user facilities that provide outstanding capabilities for imaging; for characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples; and for studying the chemical transformation of materials. These facilities are used to correlate the microscopic structure of materials with their macroscopic properties, which provides critical insights to their electronic, atomic, and molecular configurations, often at ultrasmall length and ultrafast time scales.

The energy systems of the future, whether they tap sunlight, store electricity, or make fuel from splitting water or reducing carbon dioxide, will revolve around materials and chemical changes that convert energy from one form to another. Such materials will need to be more functional than today's energy materials. To control chemical reactions or to convert a solar photon to an electron requires coordination of multiple steps, each carried out by customized materials with designed nanoscale structures. Such advanced materials are not found in nature; they must be designed and fabricated to exacting standards using principles revealed by basic science.

The 20th century witnessed revolutionary advances in physical sciences, bringing remarkable discoveries such as high temperature superconductors, electron microscopy with atomic resolution, and carbon nanotubes that combine the strength of steel with the mass of a feather. Observational science is now giving birth to the science of control, where accumulated knowledge derived from observations is used to design, initiate, and direct the chemical and physical behavior of materials at atomic and nanoscale. BES-supported research stands at the dawn of an age in which materials can be built with atom-by-atom precision and computational models can predict the behavior of materials before they exist. These capabilities, unthinkable only a few decades ago, create unprecedented opportunities to revolutionize the future of sustainable energy applications and beyond, from information management to national security.

Subprograms

To accomplish its mission and address the scientific challenges outlined above, the BES program is organized into three subprograms: Materials Sciences and Engineering; Chemical Sciences, Geosciences, and Energy Biosciences; and Scientific User Facilities.

The *Materials Sciences and Engineering* subprogram supports research that explores the origin of macroscopic material behaviors and their fundamental connections to atomic, molecular, and electronic structures. At the core of the subprogram is the quest for a paradigm shift for the deterministic design and discovery of new materials with novel structures, functions, and properties. To accomplish this goal, the portfolio stresses the need to probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials systems over multiple time and length scales. Such understanding and control are critical to science-guided design of highly efficient energy conversion processes, such as new electromagnetic pathways for enhanced light emission in solid-state lighting and multi-functional nanoporous structures for optimum charge transport in batteries and fuel cells. This subprogram also seeks to conceptualize, calculate, and predict processes underlying physical transformations, tackling challenging real-world systems—for example, materials with many atomic constituents, with complex architectures, or that contain defects; systems that exhibit correlated emergent behavior; and systems that are far from equilibrium. Such understanding will be critical to developing predictive capability for complex systems behavior, such as in superconductivity and magnetism. The subprogram also supports the development and advancement of the experimental and computational tools and techniques that in turn enable the understanding of the behaviors of materials, especially their reactivity under the full range of extreme conditions and the ability to predict the structure and properties of formed phases. Finally, the subprogram exploits the interfaces between physical and biological sciences to explore bio-mimetic processes as new approaches to novel materials design. This subprogram will also support an Energy Innovation Hub focused on Batteries and Energy Storage.

The *Chemical Sciences, Geosciences, and Energy Biosciences* subprogram supports research that explores fundamental aspects of chemical reactivity and energy transduction over an enormous range of scale and complexity. Phenomena are studied over spatial scales from the sub-nanometer, as defined by the structure of atoms and molecules, to kilometers, appropriate to the behavior of subsurface geological structures, and over time scales defined by the motions of electrons in atoms, attoseconds (10^{-18} seconds), to millennia over which geological change must be understood. At the heart of this research lies the quest to understand and control chemical reactions and the transformation of energy at the molecular scale in systems ranging from simple atoms and molecules, to active catalysts, to complex biochemical or geochemical moieties. At the most fundamental level, the development and understanding of the quantum mechanical behavior of electrons, atoms, and molecules in the 20th century has now evolved into the ability to control and direct such behavior to achieve desired results, such as the optimal conversion of solar energy into electronic excitation in molecular chromophores or into the creation of multiple charge carriers in nanoscale semiconductors. This subprogram also seeks to extend this era of 21st century control science to include the capability to tailor chemical transformations with atomic and molecular precision. Here, the goal is fully predictive capability for larger, more complex chemical systems, such as interfacial catalysis, at the same level of detail now known for simple molecular systems. Finally, this subprogram seeks ultimately to extend a molecular level understanding and control to the emergent and highly non-equilibrium behavior of biological and geological systems through the application of modern experimental and computational tools. This subprogram will also support an Energy Innovation Hub focused on Fuels from Sunlight.

The *Scientific User Facilities* subprogram supports the operation of a nationwide suite of major facilities that provide open access to sophisticated instrumentation needed to probe and create materials for scientists of many disciplines from academia, national laboratories, and industry. These large-scale user facilities consist of a complementary set of intense x-ray sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science. These facilities probe materials in space, time, and energy with the appropriate resolutions that can interrogate the inner workings of matter—transport, reactivity, fields, excitations, and motion—to answer some of the most challenging grand science questions. Taking advantage of the intrinsic charge, mass, and magnetic characteristics of x-rays, neutrons, and electrons, these tools offer unique capabilities to help understand the fundamental aspects of the natural world. The subprogram recognizes that at the heart of scientific discovery lies advanced tools and instruments. The continual development and renovation of the instrumental capabilities includes new x-ray and neutron experimental stations, improved core facilities, and new stand-alone instruments. The subprogram also manages a research portfolio in accelerator and detector development to explore technology options for developing the next generations of x-ray and neutron sources. Collectively, these user facilities and enabling tools produce a host of important research results that span the continuum from basic to applied research and embrace the full range of scientific and technological endeavors, including chemistry, physics, geology, materials science, environmental science, biology, and biomedical science. These capabilities offer critical scientific insights for the discovery and design of advanced materials and novel chemical processes with broad societal impacts, from energy applications to information and biomedical technologies.

Benefits

The BES program supports basic research that underpins a broad range of energy technologies. Research in materials sciences and engineering leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety of energy generation, conversion, transmission, storage, and use. For example, advances in superconductivity have been introduced commercially in a number of demonstration projects around the country. Improvements in alloy design for high temperature applications are used in commercial furnaces and in green technologies such as lead-free solder. Research in chemistry has led to advances such as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for the production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in geosciences results in advanced monitoring and measurement techniques for reservoir definition and an understanding of the fluid dynamics of complex fluids through porous and fractured subsurface rock. Research in the molecular and biochemical nature of photosynthesis aids the development of solar photo-energy conversion.

The BES program also plays a major role in enabling the nanoscale revolution. The importance of nanoscience to future energy technologies is clearly reflected by the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, and chemical reactions) take place on the nanoscale. The development of new nanoscale materials, as well as the methods to characterize, manipulate, and assemble them, create an entirely new paradigm for developing new and revolutionary energy technologies.

Program Planning and Management

Inputs to program planning and prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. Many long-range planning exercises for elements of the BES program are performed under the auspices of the Basic Energy Sciences Advisory Committee (BESAC). During the past few years, BESAC has provided advice on new directions in nanoscale science and complex systems; on the operation of the major scientific user facilities; on the need for new, next-generation facilities for x-ray, neutron, and electron-beam scattering; on performance measurement; on the quality of the BES program management and its consequent impacts on the program portfolio; on new directions in research relating to specific aspects of fundamental science such as catalysis, biomolecular materials, and computational modeling at the nanoscale; on the fundamental research challenges posed by the Department's energy missions; on a 20-year roadmap for BES facilities; and on theory and computation needs across the entire portfolio of BES research.

Of particular note is the 2003 BESAC report, *Basic Research Needs to Assure a Secure Energy Future*, which was the foundation for ten follow-on Basic Research Needs workshops supported by BES in the past six years in the areas of the hydrogen economy, solar energy utilization, superconductivity, solid-state lighting, advanced nuclear energy systems, combustion of 21^{st} century transportation fuels, electrical-energy storage, geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and carbon dioxide), materials under extreme environments, and catalysis for energy applications. Together these workshops attracted over 1,500 participants from universities, industry, and DOE laboratories. BESAC was charged with summarizing the results of these ten workshops and relating this summary to the science themes identified in the 2007 BESAC Grand Challenges study. A report, entitled *New Science for a Secure and Sustainable Energy Future*, was released in December 2008. The report highlighted the magnitude of the challenges in the realm of energy and environment facing the U.S and the importance of fundamental science to finding transformational solutions.

Together these reports describe a continuum of research spanning the most fundamental questions of how nature works to the questions that address technological show-stoppers in the applied research programs supported by the DOE technology offices. Dealing with these issues requires breakthrough advances with new understanding, new materials, and new phenomena that will come from fundamental science. The BES program portfolios have been reassessed and restructured to reflect the results of these workshops.

Planning for the facilities of the BES program is also an ongoing activity. The BES program has a long tradition of planning, constructing, and operating facilities well. During the past ten years, the BES program has delivered nearly $2 billion of facilities and upgrades on schedule and within budget. Among others, this includes the Spallation Neutron Source, the complete reconstruction of the Stanford Synchrotron Radiation Light Source, five Nanoscale Science Research Centers, the Linac Coherent Light Source, and numerous instrument fabrication projects. Recently, BESAC sponsored a workshop *Next-Generation Photon Sources for Grand Challenges in Science and Energy* to explore the scientific frontiers that could be tackled with next generation photon sources. The workshop identified new research opportunities in materials, chemistry, biology, medicine, environment, and physics for science and energy that can be addressed with diffraction, excitation, and imaging by photons. BES will build on this foundation with a workshop to assess the technical readiness of various accelerator-based techniques for 4th generation light sources and the corresponding R&D needs. It is expected that the output of these workshops will help set the course for photon science facilities for the next decade.

All research projects supported by BES undergo regular peer review and merit evaluation based on procedures set down in 10 CFR Part 605 for the extramural grant program and in an analogous process for the laboratory programs and scientific user facilities. The BES peer review process evaluates the following four criteria, in order of decreasing importance: scientific and/or technical merit of the project, appropriateness of the proposed method or approach, competency of the personnel and adequacy of proposed resources, and reasonableness and appropriateness of the proposed budget. The criteria for review may also include other appropriate factors established and announced by BES.

Facilities are reviewed using external, independent review committees operating according to the procedures established for peer review of BES laboratory programs and facilities. Important aspects of the reviews include assessments of the quality of research performed at the facility, the reliability and availability of the facility, user access policies and procedures, user satisfaction, facility staffing levels, R&D activities to advance the facility, management of the facility, and long-range goals of the facility. The outcomes of these reviews helped improve operations and develop new models of operation for existing light sources, the Spallation Neutron Source, and the National Synchrotron Light Source-II (NSLS-II), which began construction in FY 2009.

Facilities that are in design or construction are reviewed according to procedures set down in DOE Order 413.3A "Program and Project Management for Capital Assets" and in the Office of Science "Independent Review Handbook."[a] In general, once a project has entered the construction phase, it is

[a] http://www.science.doe.gov/opa/PDF/revhndbk.pdf

reviewed with external, independent committees approximately biannually. These Office of Science construction project reviews enlist experts in the technical scope of the facility under construction and its costing, scheduling, and construction management.

Information and reports for all of the above mentioned advisory and consultative activities are available on the BES website.[a] Other studies are commissioned as needed using the National Academies' National Research Council and other independent groups.

Basic and Applied R&D Coordination

As is demonstrated by the depth and scope of the Basic Research Needs workshop series, the BES program is committed to R&D integration. These workshops and the follow-on solicitations seek to partner the BES program with its counterparts in the DOE technology offices and NNSA. Many activities facilitate cooperation and coordination between BES and the applied research programs, including joint efforts in strategic planning, solicitation development, peer reviews, and program contractors meetings. For example, in hydrogen research, BES has actively engaged with the Offices of Energy Efficiency and Renewable Energy, Fossil Energy, and Nuclear Energy to coordinate activities such as budget submissions, solicitation topic selections and proposal reviews, posture plan development, and joint contractors meetings. BES also participates in interagency coordination activities, such as the Interagency Working Group on Hydrogen and Fuel Cells led by the White House Office of Science and Technology Policy; the Hydrogen Technical Advisory Committee (HTAC), a Federal Advisory Committee established by the Energy Policy Act of 2005 to advise the Secretary of Energy on issues related to hydrogen and fuel cell research, development, demonstration, and deployment; and the Hydrogen and Fuel Cell Interagency Task Force consisting of senior agency representatives across the federal government. BES also coordinates with the Office of Energy Efficiency and Renewable Energy and the Office of Electricity Delivery and Energy Reliability on electrical energy storage research for transportation and grid-level storage, respectively. BES has involved program managers in both offices in regular information exchange meetings and in developing a preliminary coordination plan in electrical energy storage. Since FY 2007, BES has worked with the Office of Electricity Delivery and Energy Reliability to initiate SBIR awards in electrical energy storage for grid applications.

At the program manager level, there have been regular intra-departmental meetings for information exchange and coordination on solicitations, program reviews and project selections in research areas such as biofuels derived from biomass; solar energy utilization; hydrogen production, storage, and use; building technologies, including solid-state lighting; advanced nuclear energy systems and advanced fuel cycle technologies; vehicle technologies; improving efficiencies in industrial processes; and superconductivity for grid applications. These activities facilitate cooperation and coordination between BES and the technology offices and defense programs. DOE program managers have also established formal technical coordinating committees (e.g., the Energy Materials Coordinating Committee) that meet on a regular basis to discuss R&D programs with wide applications for basic and applied programs. Additionally, technology offices staff participate in reviews of BES research, and BES staff participate in reviews of research funded by the technology offices.

The Department's national laboratory system plays an important role in the ability of BES to effectively integrate research and development by providing opportunities to collocate activities at the laboratories. Co-funding and co-siting of research by BES and DOE technology programs at the same institutions, such as the DOE laboratories or universities, has proven to be a valuable approach to facilitate close integration of basic and applied research. In these cases, teams of researchers benefit by sharing of resources, expertise, and knowledge of research breakthroughs and program needs.

[a] http://www.sc.doe.gov/bes/

Budget Overview

The FY 2011 budget request provides targeted increases and sets new directions in two key components in the BES program: research that advances understanding of the natural world and addresses the DOE mission and enabling tools—the operation and construction of scientific user facilities and the development of unique instruments for the nation. A significant portion of the funding increase will be devoted to expand the research program to capture new, emerging opportunities by furthering its scientific reach and potential technological impact.

BES supports three types of research rewards—core research, Energy Frontier Research Centers (EFRCs), and Energy Innovation Hubs. These funding mechanisms constitute an increasing progression of scientific scope and level of effort. The BES core research awards permit individual scientists and small groups to pursue their discovery-driven research interests with broad energy relevance. The dozens of EFRC awards bring together multiple investigators to address major scientific challenges necessary to solve complex energy research problems. The Hub awards focus multiple teams of researchers—each working in separate but collaborative research areas—on overcoming the related scientific barriers to development of a complete energy system that has potential for implementation into a transformative energy technology. The core research represents over 70% of the total BES research funding and complements larger group efforts comprised of the EFRCs and the Energy Innovation Hubs.

- *BES core research*—primarily supporting single principal investigator and small group projects—will be continued and expanded to initiate promising new activities in research areas in response to the five grand challenges identified in the BESAC Grand Challenges report: quantum control of electrons in atoms, molecules, and materials, with an emphasis on molecular science and engineering; basic architecture of matter; directed assemblies, structure, and properties; emergence of collective phenomena; energy and information on the nanoscale; and matter far beyond equilibrium. An increase in funding for ultrafast science, which deals with phenomena that occur in the range of one-trillionth of a second (one picosecond) to less than one-quadrillionth of a second (one femtosecond), is requested in FY 2011. This research has the promise of expanding our understanding of chemistry and materials sciences by allowing real-time stroboscopic investigations of the earliest stages of dynamic phenomena. Such knowledge will be critical to advancing the science frontiers in energy transduction in natural and artificial solar energy conversion systems, real-time bond breakage and formation in catalytic reactions, the dynamics of materials in extreme environments, correlation in strongly correlated electron systems, the nucleation of defects in materials that result in the degradation of their properties, and structural dynamics in complex biomolecules. Additional research will also be initiated in the area of multiscale modeling for advanced engine design.

  In FY 2011, approximately $24 million will be available to fund core research efforts in two additional categories: discovery and development of new materials that are critical to both science frontiers and technology innovations, and basic research for energy needs in a limited number of areas as shown below.

  - *Discovery and development of new materials*. Research in this category will focus on new synthesis capabilities, including bio-inspired approaches, to establish a strong foundation for science-driven materials discovery and synthesis in the U.S. This work will focus on materials broadly and will include crystalline materials, which have been highlighted recently as an essential component of the science grand challenges in the 2007 BESAC report Directing Matter and Energy: Five Challenges for Science and the Imagination. As described in the November 2009 NRC report Frontiers in Crystalline Matter: From Discovery to Technology, the U.S., once the world leader in the discovery and growth of crystalline materials, has fallen behind other nations. Single crystals are vital in understanding the characteristics and properties of new materials, and they also have applications in devices that involve semiconductors, lasers, precision timing devices, solar cells or high temperature operations and provide a natural platform to explore novel states of matter.

- *Basic research for energy needs.* Major areas of emphasis will be in fundamental sciences related to carbon capture and advanced nuclear energy systems. For carbon capture, focused areas include the rational design of novel materials and separation processes for post-combustion CO_2 capture, as well as catalysis and separation research for novel carbon capture schemes to aid the design of future power plants. For advanced nuclear energy systems, focused areas include radiation resistant materials in fission and fusion applications and separation science and heavy element chemistry for fuel cycles.

- *Energy Frontier Research Centers (EFRCs),* established in FY 2009, are multi-investigator and multi-disciplinary centers to engage the talents of the nation's researchers for the broad energy sciences. The EFRCs harness the most basic and advanced discovery research in a concerted effort to accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century. These centers bring together critical masses of researchers to conduct fundamental energy research in a new era of grand challenge science and use-inspired energy research. The scientific directions of the EFRCs are overseen by program staff in the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Biosciences subprogram, who are managed centrally within BES to ensure a unified management strategy and structure. In FY 2011, approximately $40 million will be available to fund additional EFRCs. New EFRCs will be competitively solicited in the two categories described above under core reserach: discovery and development of new materials that are critical to both science frontiers and technology innovations, and basic research for energy needs in a limited number of areas that are underrepresented in the 46 original EFRC awards.

- *Energy Innovation Hubs* were initiated by the Department in FY 2010. The Hubs aim to assemble multidisciplinary teams to address basic science and technology hindering the nation's secure and sustainable energy future. Because the components and processes of energy systems are highly interdependent, innovative solutions to real-world energy challenges will require concerted efforts that couple the various elements of the technology chain and combine the talents of universities, national laboratories, and the private sector. The Energy Innovation Hubs comprise a larger set of investigators spanning science, engineering, and other disciplines, but focused on a single critical national need identified by the Department. Top talent drawn from the full spectrum of R&D performers—universities, private industry, non-profits, and government laboratories—drive each Hub to become a world leading R&D center in its topical area. With robust links to industry, the highly integrated Hubs can bridge the gap between basic scientific breakthroughs and industrial commercialization. In FY 2011, BES will support the continuation of the Fuels from Sunlight Hub and will initiate a new Hub on Batteries and Energy Storage.

The FY 2011 budget request provides continued support for the operations of the suite of BES scientific user facilities, including four x-ray synchrotron sources, three neutron sources, and five nanoscale science research centers. The total request represents an average of 3.5% increase over the FY 2010 funding level and provides near optimal support for the user operations. Funding is also provided for instrumentation to upgrade BES beamlines at the light source facilities. The Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory provides laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source, with pulse lengths of femtoseconds—the timescale of atomic motion. The LCLS will begin the first full year of operations in FY 2011. These facilities provide key capabilities for the fabrication of novel materials, for the examination of materials and their transformations at the atomic scale, and to enable scientists to correlate microscopic structures to macroscopic properties.

Recognizing that at the heart of discovery often lies with the development of new tools and instruments; BES continues to support the planning, R&D, and construction of new scientific user facilities and the associated enabling tools. The new generations of instruments will naturally bring forth devices to direct matter at the levels of electrons, atoms, or molecules, as highlighted in the BESAC Grand Challenges report.

The construction of the National Synchrotron Light Source II (NSLS-II) will continue at Brookhaven National Laboratory, including the largest component of the project—the building that will house the accelerator ring. The Spallation Neutron Source Instruments-Next Generation (SING-I, funding to be completed in FY 2011, and SING-II) and the Power Upgrade Project (PUP), as part of the planned upgrades to the Spallation Neutron Source at Oak Ridge National Laboratory, will be supported according to planned schedules and funding profiles.

Annual Performance Results and Targets

Secretarial Priority: Innovation: Lead the world in science, technology, and engineering

GPRA Unit Program Goal: Basic Energy Sciences Program Goal: Advance the Basic Science for Energy Independence – Provide the scientific knowledge and tools to achieve energy independence, securing U.S. leadership and essential breakthroughs in basic energy sciences.

Annual Performance Measure: Annual Performance Measure: Temporal resolution; maintain x-ray pulse of less than 100 femtoseconds in duration and containing more than 100 million (108) photons per pulse.[a]

FY 2006	T: Demonstrate an X-ray pulse of less than 100 femtoseconds in duration and containing more than 100 million photons per pulse. A: Goal met
FY 2007	T: Demonstrate an X-ray pulse of less than 100 femtoseconds in duration and containing more than 100 million photons per pulse. A: Goal met
FY 2008	T: Maintain x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million (10^8) photons per pulse. A: Goal met
FY 2009	T: Maintain x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million (10^8) photons per pulse. A: Goal met

[a] No further improvement is expected beyond 2008 for these measures since the current suite of instruments has met their maximum performance level. This target is a measure of SC's intent to maintain the maximum level of performance for users of the current SC facilities until the next generation of instruments and facilities becomes available.

FY 2010–FY 2015	T: Maintain x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million (10^8) photons per pulse. A: TBD

Annual Performance Measure: Spatial Resolution; maintain spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm.[a]

FY 2006	T: Demonstrate spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm. A: Goal met
FY 2007	T: Demonstrate spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm. A: Goal met
FY 2008	T: Maintain spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm. A: Goal met
FY 2009	T: Maintain spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm. A: Goal met
FY 2010–FY 2015	T: Maintain spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm. A: TBD

Annual Performance Measure: Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects.

FY 2006	T: Cost and schedule variance are both less than 10% A: Goal met
FY 2007	T: Cost and schedule variance are both less than 10% A: Goal not met

[a] No further improvement is expected beyond 2008 for these measures since the current suite of instruments has met their maximum performance level. This target is a measure of SC's intent to maintain the maximum level of performance for users of the current SC facilities until the next generation of instruments and facilities becomes available.

FY 2008	T: Cost and schedule variance are both less than 10% A: Goal met
FY 2009	T: Cost and schedule variance are both less than 10% A: Goal met
FY 2010–FY 2015	T: Cost and schedule variance are both less than 10% A: TBD

Annual Performance Measure: Achieve an average operation time of the scientific user facilities as a percentage of the total scheduled annual operating time of greater than 90%.

FY 2006	T: 90% of scheduled operating time A: Goal met
FY 2007	T: 90% of scheduled operating time A: Goal met
FY 2008	T: 90% of scheduled operating time A: Goal met
FY 2009	T: 90% of scheduled operating time A: Goal met
FY 2010–FY 2015	T: 90% of scheduled operating time A: TBD

Materials Sciences and Engineering

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Materials Sciences and Engineering			
Materials Sciences and Engineering Research	392,260[a]	354,104	421,427
Facilities Operations	689,047[a]	0	0
Other Project Costs	27,044[a]	0	0
SBIR/STTR	0	9,538	11,236
Total, Materials Sciences and Engineering	1,108,351[a]	363,642	432,663

Description

This subprogram supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties.

In condensed matter and materials physics—including activities in experimental condensed matter physics, theoretical condensed matter physics, materials behavior and radiation effects, and physical behavior of materials—research is supported to understand, design, and control materials properties and function. These goals are accomplished through studies of the relationship of materials structures to their electrical, optical, magnetic, surface reactivity, and mechanical properties and of the way in which materials respond to external forces such as stress, chemical and electrochemical environments, radiation, and the proximity of materials to surfaces and interfaces.

In scattering and instrumentation sciences—including activities in neutron and x-ray scattering and electron and scanning microscopies—research is supported on the fundamental interactions of photons, neutrons, and electrons with matter to understand the atomic, electronic, and magnetic structures and excitations of materials and the relationship of these structures and excitations to materials properties and behavior.

In materials discovery, design, and synthesis—including activities in synthesis and processing science, materials chemistry, and biomolecular materials—research is supported in the discovery and design of novel materials and the development of innovative materials synthesis and processing methods. This research is guided by applications of concepts learned from the interface between physics and biology and from nano-scale understanding of synthesis and structures.

The Energy Innovation Hub focused on Batteries and Energy Storage will consist of multidisciplinary teams of experts that blend basic scientific research with technology development, engineering design, and energy policy. They will bridge the gap between basic scientific breakthroughs and industrial commercialization through proof-of-concept prototyping, modeling, measurement, and verification of the potential for major impacts.

[a] FY 2009 funding of $771,198,000 for Scientific User Facilities is located within the Materials Sciences and Engineering Research activity ($82,151,000) and the Facility Operations activity ($689,047,000). In FY 2010 and beyond, this funding is shown in the Scientific User Facilities subprogram.

Selected FY 2009 Accomplishments

- *Encoding Information at Sub-Atomic Scales.* Using state-of-the-art nanoscience instruments and novel techniques, scientists have set a record for the smallest writing, forming letters with features that are one third of a billionth of a meter or 0.3 nanometers. This sub-atomic writing was achieved by using a scanning tunnelling microscope (STM) to precisely position carbon monoxide molecules into a desired pattern on a copper surface. The electrons that move around on the copper surface act as waves that interfere with the carbon monoxide molecules and with each other, forming an interference pattern that depends on the positions of the molecules. By altering the arrangement of the molecules, specific electron interference patterns are created, thereby encoding information for later retrieval. In addition, several data sets can be stored in a single molecular arrangement by using multiple electron energies, one of the variables possible with the STM. The same STM technology can then be used to read the data that has been stored. Because the information is stored in the electron interference pattern, rather than in the individual carbon monoxide molecules or surface copper atoms, the storage density is not limited by the size of an atom. These results demonstrate the feasibility of a new approach capable of achieving sub-atomic data storage.
- *Electronic Liquid Crystal States Discovered in Parent of Iron-Based Superconductor*. In one of the first results from an Energy Frontier Research Center, new insights were gained concerning the electronic structure of iron-based, high-temperature (high-T_c) superconductors. Using a newly developed, highly sensitive scanning tunneling microscope, static nanoscale electronic structures at about eight times the distance between individual iron atoms were observed in a parent material of the iron-based superconductors. These structures were aligned along one crystal axis, reminiscent of the way molecules spatially order in a liquid crystal display. In addition, free electrons were found to move in a direction perpendicular to these aligned 'electronic liquid crystal' states. These findings are similar to observations in cuprate superconductors, a surprise because many theorists had expected the iron-based materials to act more like conventional metal superconductors. This new understanding of electronic structure provides insights to revise theories for the mechanism of high temperature superconductivity.
- *Learning from Nature to Make Tough Ceramics*. Nature generates strong materials, such as mother-of-pearl, with orders of magnitude more fracture resistance than any man-made materials, by forming hybrid composites in which a hard, brittle mineral is combined with soft, organic molecules. Recently, researchers have used sophisticated material control techniques to create a new fabrication process that mimics Nature. The results are hybrid materials composed of aluminum oxide (strong, but brittle) and polymers (soft, organic materials) with toughness 300 times higher than either component alone. To achieve this new material, researchers oriented ceramic layers and interconnected them with bridges to impose molecular control on the bonding between the polymer and ceramics. The processing involved controlled freezing of a suspension of aluminum oxide ceramic particles in water (which drives the particles into layered structures), sublimating the ice, and then infiltrating the remaining ceramic framework with a polymer. The layer orientation and spacing were designed to ensure that a crack that forms in the brittle mineral is shielded from stress and actually stops growing, thereby resulting in the combined high strength and facture resistance.
- *Real-time Observation of Graphene Reconstruction Confirms Predicted Structure.* The world's most powerful transmission electron microscope, developed in the Transmission Electron Aberration-Corrected Microscope (TEAM) project, was used to make the first-ever real-time recordings of the movements of individual carbon atoms in a graphene sheet, providing critical insights on the properties of these unique materials. Graphene is a single atomic layer of graphite that is attracting

significant attention for its unique electronic properties. For example, theory predicts that narrow strips of graphene known as nanoribbons could conduct a current in which all the electrons have the same spin and might therefore serve as the basis for nanosized spintronic devices, electronics based on spin rather than charge. However, this conduction phenomenon is predicted to occur only if the nanoribbons are oriented along a particular direction in the graphene sheet, forming so-called zig-zag edges. The advanced capabilities of the new microscope yielded unprecedented images of individual carbon atoms around the edges of a hole in a suspended graphene sheet and allowed for the real-time observation of edge reconstruction and whole growth. Careful analysis of the time-evolution of the atomic positions and edge structures confirmed that the zig-zag configuration appeared to be the most stable, bolstering optimism for development of graphene-based spintronic devices.

- *Flexible, transparent, and cheaper silicon solar cells.* A novel fabrication strategy has been developed for thin, semi-transparent, lightweight, and flexible solar cells with one-tenth the silicon in current devices and applicable to a variety of substrates including flexible polymer and glass sheets. The process involves fabrication of micron-sized cells on single-crystal silicon wafers and lifting them off using a block of rubbery polymer. These are then printed, or transferred, to the desired substrate; a process that can be repeated many times to build a macro-scale cell. The technique has been used to print cells on flexible, rollable plastic sheets. Respectable solar energy conversion efficiencies of about 12% have been achieved for silicon with thicknesses of 15 microns, thinner than a human hair and less than a tenth the thickness of wafers used in current-generation solar cells. In addition to lower potential cost, this novel solar cell allows unprecedented design characteristics including bendability, lighter weight, and partial transparency, none of which are possible with today’s silicon devices.
- *Efficient Solar Hydrogen Production by a Hybrid Photo-Catalyst System.* Inorganic catalyst systems have been used to generate hydrogen from water by use of sunlight, but the efficiency is low because they can only use the UV portion of the solar radiation. Natural photosynthetic systems such as photosystem I (PS-I) can absorb about 45% of the solar spectrum, but are indirectly and inefficiently coupled to a non-robust, oxygen-sensitive hydrogenase enzyme to generate hydrogen. A novel bio-inspired hybrid system for faster and efficient generation of hydrogen from sunlight was developed. The new hybrid system uses a cleverly designed synthetic molecular wire to covalently link PS-I with gold or platinum nanocatalysts. The molecular wire provides a rapid, efficient pathway for shuttling photo-generated electrons to the inorganic nanocatalyst, with electron-transfer rates approaching 75% of the rates in plants. When exposed to sunlight, this new hybrid system generates hydrogen at up to 1,700 times the current benchmark.
- *Large Area, High Density Arrays of Nanopillars Achieved.* Control of the chemical interactions during the self-assembly of arrays of polymer nanopillars has resulted in perfectly ordered arrays over extremely large areas. Researchers controlled the formation of the polymer nano-cylinders, each with unprecedentedly small about 3 nm diameter normal to the substrate during synthesis, the attraction and repulsion between the segments in a block copolymer are balanced against their interaction with the zigzagged surface of the patterned substrate. The new insight was to control the features and the relationships among the substrate pattern, film thickness, and polymer nanopillars. By controlling these relationships, an ordered array of polymer nanopillars was produced with densities in excess of 10^{12} per square inch, more than an order of magnitude greater than previously possible. In a novel application of synchrotron x-ray scattering, the ordering and orientation of the pillars were confirmed to be maintained over the entire surface. This guided synthesis should be applicable to different substrates and block copolymers with built-in electron and optical properties,

opening a versatile route toward ultrahigh density arrays that could be used in photovoltaics, electronics, and information storage applications.

Detailed Justification

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Materials Sciences and Engineering Research	**392,260**	**354,104**	**421,427**
▪ **Experimental Condensed Matter Physics**	**43,584**	**48,264**	**45,966**

This activity supports experimental condensed matter physics emphasizing the relationship between the electronic structure and the properties of complex materials, often at the nanoscale. The focus is on systems whose behavior derives from strong correlation effects of electrons as manifested in superconducting, semi-conducting, magnetic, thermoelectric, and optical properties. Also supported is the development of new techniques and instruments for characterizing the electronic states and properties of materials under extreme conditions, such as in ultra low temperatures (millikelvin), in ultra high magnetic fields (100 Tesla), and at ultrafast time scales (femtosecond). Capital equipment is provided for scanning tunneling microscopes, electron detectors, superconducting magnets, and physical property measurement instruments.

Improving the understanding of the electronic behavior of materials on the atomistic scale is relevant to the DOE mission, as these structures offer enhanced properties and could lead to dramatic improvements in technologies for energy generation, conversion, storage, delivery, and use. Specifically, research efforts in understanding the fundamental mechanisms of superconductivity, the elementary energy conversion steps in photovoltaics, and the energetics of hydrogen storage provide the major scientific underpinnings for the respective energy technologies. This activity also supports basic research in semiconductor and spin-based electronics of interest for the next generation information technology and electronics industries.

In FY 2011, funding will be provided for research in the area of complex and emergent behavior. The research activities will emphasize investigations of emergent behaviors that arise from the collective, cooperative behavior of individual components of a system such as atoms or electrons that lead to physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magnetoresistance, random field magnets, and spin liquids and glasses. Additional investments will be made for the study of ultracold, atomic Fermi gasses as a means to study interaction effects that are relevant to the understanding of correlation effects in the condensed phase. These phenomena are expected to impact a wide range of energy relevant technologies.

▪ **Theoretical Condensed Matter Physics**	**27,498**	**28,932**	**29,641**

This activity supports theoretical condensed matter physics with emphasis on the theory, modeling, and simulation of electronic correlations. A major thrust is nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other major research areas include strongly correlated electron systems, quantum transport, superconductivity, magnetism, and optics. Development of theory targeted at aiding experimental technique design and interpretation of experimental results is also emphasized. This activity supports the Computational Materials Science Network, which forms collaborating teams from diverse disciplines to address the increasing complexity of many current research issues. The activity also supports large-scale computation to perform complex calculations dictated by fundamental theory or to perform complex system simulations with joint funding from the Advanced Scientific Computing Research program. Capital equipment funding will be provided for items such as computer workstations and clusters.

This activity provides the fundamental knowledge for predicting the reliability and lifetime of energy use and conversion approaches and develops opportunities for next generation energy technology. Specific examples include inverse design of compound semiconductors for unprecedented solar photovoltaic conversion efficiency, solid-state approaches to improving capacity and kinetics of hydrogen storage, and ion transport mechanisms for fuel cell applications.

In FY 2011, this activity will increase the support of collaborative research activities focused on enhancing the understanding of the nature and origin of highly correlated states in strongly interacting systems that have spin, charge, lattice, and orbital degrees of freedom and that are often intrinsically inhomogeneous on nanometer length scales. Research will include both theoretical and computational approaches capable of interrogating systems to gain direct insight on the mechanisms that lead to cooperative behavior.

	FY 2009	FY 2010	FY 2011
▪ **Mechanical Behavior and Radiation Effects**	**17,830**	**20,666**	**25,172**

This activity supports basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include deformation of ultra-fine scale materials, radiation-resistant material fundamentals, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop predictive models for the design of materials having superior mechanical properties and radiation resistance. Capital equipment funding is provided for microstructural analysis, nanoscale mechanical property measurement tools, and ion-beam processing instrumentation.

The ability to predict materials performance and reliability and to address service life extension issues is important to the DOE mission areas of robust energy storage systems; fossil, fusion, and nuclear energy conversion; radioactive waste storage; environmental cleanup; and defense. Among the key materials performance goals for these technologies are good load-bearing capacity, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility and deformability, and radiation tolerance. Since materials from large-scale nuclear reactor components to nanoscale electronic switches undergo mechanical stress and may be subjected to ionizing radiation, this activity provides the fundamental scientific underpinning to enable the advancement of high-efficiency and safe energy generation, use, and storage as well as transportation systems.

In FY 2011, this activity will support research on the properties of materials in extreme environments such as the exposure to an energetic flux, chemical reactive stimulants, high temperature and pressure, and high magnetic and electric fields. The primary emphasis will be on discovering novel phenomena and materials for improved performance with superior functionality and to establish unified models to predict the mechanical and degradation behavior of solids over multiple length and time scales. Additional research will be initiated to focus on understanding the complex interactions of radiation-induced defects with microstructure, and their effects on the

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

functionalities of materials under extreme conditions, including those that exist in nuclear reactor environments. The research will focus on understanding, modeling, and designing radiation-resistant materials that maintain all of the required physical properties after prolonged exposure. In situ experiments will be closely integrated with theoretical/computational efforts to develop a fundamental understanding of degradation mechanisms and kinetics over multiple length and time scales, from atomistic to micron and nanoseconds to decades.

	FY 2009	FY 2010	FY 2011
▪ **Physical Behavior of Materials**	**30,579**	**32,888**	**34,034**

This activity supports basic research on the behavior of materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. Emphasis is on the relationships between performance (such as electrical, magnetic, optical, electrochemical, and thermal performance) and the microstructure and defects in the material. Included within the activity are research to establish the relationship of crystal defects to semiconducting, superconducting, and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments; and diffusion and transport phenomena. Basic research is also supported to develop new instrumentation, including *in situ* experimental tools, and to probe the physical behavior in real environments encountered in energy applications. Capital equipment funding is provided for items such as physical property measurement tools that include spectroscopic and analytical instruments for chemical and electrochemical analysis.

The research supported by this activity is necessary for improving materials reliability in chemical, electrical, and electrochemical applications and for improving the ability to generate and store energy in materials. Materials in energy-relevant environments are increasingly being exposed to extreme temperatures, strong magnetic fields, and hostile chemical conditions. A detailed understanding of how materials behavior is linked to the surroundings and treatment history is critical to the understanding of corrosion, photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, novel magnetic materials for low magnetic loss power generation, magnetocaloric materials for high-efficiency refrigeration, and new materials for high-temperature gasification.

In FY 2011, this activity will support research on the fundamental science of photon-matter interactions, which is likely to play a significant role in the development of metamaterials and nano-plasmonics—materials that are expected to be extremely important for the development of technologies that enable low cost power conversion. The research will also include the search for photoconversion materials, such as polycrystalline, nanocrystalline, and organic materials to replace expensive single crystals; innovative design of interpenetrating photoconversion materials networks to improve charge separation and collection efficiency; and the development of novel processes to obtain extremely high photo-conversion efficiencies. This activity also includes funding for the U.S.-India Clean Energy Research Center.

	FY 2009	FY 2010	FY 2011
▪ **Neutron and X-ray Scattering**	**44,619**	**38,678**	**42,266**

This activity supports basic research on the fundamental interactions of photons and neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and the relationships of these structures and excitations to materials properties. The main emphasis is on x-ray and neutron scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. The development and improvement of next-generation

	(dollars in thousands)	
FY 2009	FY 2010	FY 2011

instrumentation, novel detectors, sample environments, data analysis, tools, and technology for producing polarized neutrons are key aspects of this activity. Instrumentation development and experimental research in ultrafast materials science, including research aimed at generating, manipulating, and detecting ultrashort and ultrahigh-peak-power electron, x-ray, and laser pulses to study ultrafast physical phenomena in materials, is an integral part of the portfolio. Capital equipment funding is provided for items such as detectors, monochromators, focusing mirrors, and beamline instrumentation at the facilities.

The increasing complexity of DOE mission-relevant materials such as superconductors, semiconductors, and magnets requires ever more sophisticated scattering techniques to extract useful knowledge and to develop new theories for the behavior of these materials. X-ray and neutron scattering probes are some of the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. Additionally, neutrons play a key role in hydrogen research as they provide atomic- and molecular-level information on structure, diffusion, and interatomic interactions for hydrogen. They also allow access to the morphologies that govern useful properties in catalysts, membranes, proton conductors, and hydrogen storage materials. The activity is relevant to the behavior of matter in extreme environments, especially at high pressure.

In FY 2011, scattering research will take advantage of increased neutron and x-ray fluxes and optimized beamline optics at BES user facilities, combined with specialized instrumentation, to investigate electrochemical processes in real time. Emphasis will be on using elastic and inelastic neutron scattering to determine structure and local dynamics and on neutron reflectivity to examine electrode/electrolyte interfaces. Time-resolved measurements will be used to study phase transformation kinetics in both amorphous and crystalline phases. The new capabilities will be used to study materials under ultrahigh pressure and to identify novel phase and phenomena not accessible via ambient conditions. Increased emphasis will be placed on expansion of ultrafast materials science research to take advantage of new x-ray and neutron sources to perform research designed to understand dynamic phenomena in real-time, including the physics of strongly correlated systems, such as high temperature superconductors and magnetic materials with colossal magnetoresistance.

	FY 2009	FY 2010	FY 2011
▪ **Electron and Scanning Probe Microscopies**	**22,199**	**26,811**	**27,468**

This activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. This activity also supports the development and improvement of electron scattering and scanning probe instrumentation and techniques, including ultrafast diffraction and imaging techniques. Capital equipment funding is provided for items such as new scanning probes and electron microscopes as well as ancillary equipment including high resolution detectors.

Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend on a detailed understanding of the structural characteristics of advanced materials. Electron and scanning probe microscopies are some of the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. The

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

activity is relevant to hydrogen research through the structural determination of nanostructured materials for hydrogen storage and solar hydrogen generation.

In FY 2011, research will emphasize the development of tools that will dramatically improve spatial, time, and energy resolution to provide fundamental understanding of the electron and charge transfer processes and mechanisms by which ions interact with electrode materials. The effort will focus studies of transient non-equilibrium nanoscale structures, including adsorbed species in both vacuum and electrochemical environments, with near-atomic spatial resolution and at the femtosecond time scale. Ultrafast electron scattering will be developed as a companion tool to ultrafast photon probes.

	FY 2009	FY 2010	FY 2011
▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	**16,755**	**21,623**	**8,635**

This activity supports basic research spanning the broad range of science and technology programs at DOE in states that have historically received relatively less Federal research funding. The EPSCoR states are shown in the table below. The research supported by EPSCoR includes materials sciences, chemical sciences, physics, energy-relevant biological sciences, geological and environmental sciences, high energy physics, nuclear physics, fusion energy sciences, advanced computing, and the basic sciences underpinning fossil energy, nuclear energy and energy efficiency and renewable energy.

The core activity interfaces with all other core activities within the Office of Science. It is also responsive and supports the DOE mission in the areas of energy and national security and in mitigating their associated environmental impacts.

In FY 2011 efforts will continue spanning DOE missions in the Office of Science and science underpinning a number of technology programs including Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy and enhancing collaboration between programs and collaboration with DOE user facilities. The FY 2011 request will continue basic research related to DOE mission areas and will enhance collaborative efforts with DOE user facilities. The FY 2011 request reflects a decrease due to the additional funding provided by Congress in FY 2010 (-$13,103,000), and provides a funding increase for EPSCoR base amount at the same rate as BES core research (+$115,000). Additional funds provided in FY 2010 were used, to the extent possible, to fully fund grants and minimize outyear mortgages.

The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

	FY 2009	FY 2010	FY 2011
Alabama	1,305	0	585
Alaska	810	0	0
Arkansas	0	0	0
Delaware	1,861	0	0
Hawaii	0	0	0
Idaho	1,445	0	0

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Iowa[a]	0	0	0
Kansas	0	0	0
Kentucky	700	650	0
Louisiana	490	300	0
Maine	700	0	0
Mississippi	0	0	0
Montana	410	450	0
Nebraska	825	0	0
Nevada	0	0	0
New Hampshire	646	0	0
New Mexico	272	750	0
North Dakota	1,200	0	0
Oklahoma	1,175	0	0
Puerto Rico	400	450	0
Rhode Island	0	0	0
South Carolina	1,670	0	0
South Dakota	0	0	0
Tennessee	204	314	0
U.S. Virgin Islands	0	0	0
Utah[b]	0	0	0
Vermont	0	0	0
West Virginia	1,605	0	600
Wyoming	405	0	0
Technical Support	632	250	400
Other[c]	0	18,459	7,050

[a] Iowa became eligible in FY 2009.
[b] Utah became eligible in FY 2009.
[c] Uncommitted funds in FY 2010 and FY 2011 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
▪ **Synthesis and Processing Science**	**19,473**	**22,220**	**32,764**

This activity supports basic research for developing new techniques to synthesize materials with desired structure, properties, or behavior; to understand the physical phenomena that underpin materials synthesis such as diffusion, nucleation, and phase transitions; and to develop *in situ* monitoring and diagnostic capabilities. The emphasis is on the synthesis of complex thin films and nanoscale materials with atomic layer-by-layer control; preparation techniques for pristine single crystal and bulk materials with novel physical properties; understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and low energy processing techniques for large scale nanostructured materials. The focus of this activity on bulk synthesis and crystal and thin films growth via physical means is complementary to the Materials Chemistry and Biomolecular Materials activity, which emphasizes chemical and biomimetic routes to new materials synthesis and design. Capital equipment funding is provided for crystal growth apparatus, heat treatment furnaces, lasers, chemical vapor deposition and molecular beam epitaxial processing equipment, plasma and ion sources, and deposition instruments.

Synthesis and processing science is a key component in the discovery and design of a wide variety of energy relevant materials. In this regard, the activity supports DOE's mission in the synthesis of wide bandgap semiconductors for solid state lighting; light-weight metallic alloys for efficient transportation; novel materials such as metal organic frameworks for hydrogen storage; and structural ceramics and the processing of high temperature superconductors for near zero-loss electricity transmission. The research activity aims at providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations in ways to probe the atomistic basis for materials properties.

In FY 2011, research will seek to develop novel design rules for synthesizing nanostructured materials and assemblies for applications including solid-state lighting, solar energy conversion, hydrogen storage and electrical energy storage. Research on advanced materials for electrical energy storage will include studies on the fundamental electrochemical characteristics of nanoscale building blocks with varying size and shape and in confined geometry. The development of new capabilities for synthesis will be emphasized including novel crystal growth techniques that will expand our ability to discover needed materials for advanced energy technologies, as well as to facilitate our understanding of new phenomena in energy generation and transport, including superconductivity, photovoltaics, and energy storage.

▪ **Materials Chemistry and Biomolecular Materials**	**52,373**	**52,265**	**63,461**

This activity supports basic research in chemical and bio-inspired synthesis and discovery of new materials. In the materials chemistry area, discovery, design, and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties are supported. Major thrust areas include nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials; surface and interfacial chemistry including electrochemistry; and the development of new, science-driven, laboratory-based analytical tools and techniques. In the biomolecular materials area, research supported includes biomimetic and bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. The focus on exploratory chemical and biomolecular formation of new materials is complementary to the emphasis on bulk synthesis, crystal growth, and thin films in the Synthesis and Processing Science activity. Capital equipment funding is provided for items such as advanced nuclear magnetic resonance and magnetic resonance imaging instruments and novel scanning probe microscopes.

Research supported in this activity underpins many energy-related technological areas such as batteries and fuel cells, catalysis, energy conversion and storage, friction and lubrication, high-efficiency electronic devices, hydrogen generation and storage, light-emitting materials, light-weight high-strength materials, and membranes for advanced separations.

In FY 2011, emphasis will be on developing a predictive understanding of the role of interfaces in the electrochemical processes underpinning energy storage technologies, devising experimental strategies for atom-by-atom synthesis or molecular assembly of structures for new storage materials, and exploring novel concepts for electrical and electrochemical energy storage. The research will seek to advance the ability for materials to self-repair, regulate, clean, sequester impurities, and tolerate abuse which will ultimately improve their performance. Expanded research to understand carbon capture phenomena will be initiated, including investigation of novel chemical and biomimetic approaches for efficient carbon capture and release. Kinetics for both carbon capture and release will be investigated in environments that include the contaminants found in flue gases. Nanoscale hybrid materials and advances in the understanding of photosynthetic and catalytic systems will be used to study inorganic/organic components in engineered assemblies to produce new materials for the conversion of solar photons to fuels and chemicals. In addition, an increased emphasis will be on bio-inspired materials discovery—linking physical and chemical synthesis with the synthesis strategies of biology, which can be extended to create new materials *in vitro* with altered morphologies and desired materials properties. Biological self-assembly occurs on both spatial and temporal scales, controlled to provide function that can change dynamically. In addition, biological self-assembly can be reversible and result in complex structures that are far from equilibrium, opening new avenues to materials with emergent behaviors. The challenge is to understand the biological self-assembly and translate these into new methods for physical and chemical growth of materials.

	FY 2009	FY 2010	FY 2011
▪ **Energy Frontier Research Centers (EFRCs)[a]**	**58,000**	**58,000**	**78,000**

The 46 EFRCs established in late FY 2009 are multi-investigator and multi-disciplinary centers that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future.[b] The EFRCs represent an important new research modality for BES, bringing together the skills and talents of a critical mass of investigators to enable energy relevant, basic research of a scope and complexity that would not be possible with the standard single-investigator or small-group award. The scope and unique nature of the EFRC program requires special oversight, which is accomplished through a BES-wide, dedicated EFRC management team.

[a] A complimentary set of EFRCs is also included in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. This set includes ongoing EFRCs as well as new awards to be initiated in FY 2011.
[b] 16 of the 46 EFRCs were forward funded for the five-year initial award period under the American Recovery and Reinvestment Act of 2009.

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

This team has the direct management responsibility over all EFRCs and also coordinates EFRC research with the complementary research conducted within the BES core research areas.

This activity supports those EFRCs that are best coordinated with and most suitably complement the ongoing core research activities within the Materials Science and Engineering subprogram. In general terms, these EFRCs are focused on the design, discovery, synthesis, and characterization of novel, solid-state materials that improve the conversion of solar energy and heat into electricity; that improve the conversion of electricity to light; that can be used to improve electrical energy storage; that are resistant to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures; that take advantage of emergent phenomena, such as superconductivity, to improve energy transmission; that optimize energy flow to improve energy efficiency; and that are tailored at the atomic level for catalytic activity.

In FY 2011, new EFRCs will be solicited in two categories: discovery and development of new materials that are critical to both science frontiers and technology innovations, and basic research for energy needs in a limited number of areas that are underrepresented in the 46 original EFRC awards.

For the discovery and development of new materials, the emphasis will be on new synthesis capabilities, including advanced crystal growth techniques that will expand our ability to discover new materials for advanced energy technologies, as well as to drive our understanding of new phenomena in energy generation and transport, including superconductivity, photovoltaics, and energy storage. The expansion of synthesis capabilities in the EFRC modality will enable the development of a stronger culture of discovery-based research, and enhance the scientific and intellectual manpower in this critical area for science and technology. BES will foster this community to link the synthesis of materials with experimental research to discover new phenomena and to solve energy-related challenges, as well as integrating materials synthesis with advanced theoretical research to model and predict materials behavior, accelerating the rate of materials discovery.

For research for energy applications, areas of emphasis include: fundamental science of carbon capture, including the rational design of novel materials and separation processes for post-combustion CO_2 capture and fundamental science for advanced nuclear energy systems, e.g., radiation resistant materials in fission and fusion applications. EFRC research will focus on interdisciplinary team approaches to develop the scientific understanding to enable new, low energy routes to carbon capture/release including the discovery of new chemical, bioinspired, and materials approaches. For nuclear energy systems, EFRC research will couple understanding of radiation effects with other extreme conditions and will establish a greater breadth in multiscale modeling of physical behavior at a systems level.

▪ **Energy Innovation Hub—Batteries and Energy Storage**	**0**	**0**	**34,020**

As an energy carrier, electricity has no rival with regard to its environmental cleanliness, flexibility in interfacing with multiple production sources and end uses, and efficiency of delivery. Electrical energy storage offers one of the most significant solutions to the effective use of electricity in energy management. Improved energy storage is critical for load-leveling and peak-shaving for more efficient and reliable smart electric grid technologies; plug-in hybrid or all-electric vehicles in the transportation sector; and the deployment of intermittent renewable energy power sources such as solar, wind, and wave energy into the utility sector. Today's electrical energy storage approaches, such as batteries and electrochemical devices, suffer from limited energy and power capacities, lower-than-desired rates of charge and discharge, calendar and cycle life limitations, low abuse tolerance, high cost, and poor performance at high or low temperatures. These performance deficiencies adversely affect the successful use and integration of renewable, intermittent power sources such as solar, wind, and wave energy into the utility sector. These same fundamental problems have also limited broad consumer acceptance and market adaptation of hybrid and all-electric vehicles.

Recent developments in nanoscience and nanotechnology offer tantalizing clues on promising scientific directions that may enable conceptual breakthroughs. They include the abilities to synthesize novel nanoscale materials with architectures tailored for specific electrochemical performance, to characterize materials and dynamic chemical processes at the atomic and molecular level, and to simulate and predict structural and functional relationships using modern computational tools. Based on this, radically new concepts in materials design can be developed for producing storage devices with materials that are abundant and low in manufacturing cost, are capable of storing higher energy densities, have long cycle lifetimes, and have high safety and abuse tolerance.

Together, these new capabilities provide the potential for addressing the gaps in cost and performance separating the current electrical energy storage technologies and those required for sustainable utility and transportation needs.

Fundamental performance limitations of energy storage systems are rooted in the constituent materials making up an electrical energy storage device, and novel approaches are needed to develop multifunctional electrical energy storage materials that offer new self-healing, self-regulating, failure-tolerant, impurity-sequestering, and sustainable characteristics. The Hub would address a number of specific areas of research for both batteries and electrochemical capacitors that have been identified in the BES workshop report *Basic Research Needs for Electrical Energy Storage*. These include:

- Efficacy of structure in energy storage—new approaches combining theory and synthesis for the design and optimization of materials architectures including self-healing, self-regulation, failure-tolerance, and impurity sequestration.
- Charge transfer and transport—molecular scale understanding of interfacial electron transfer.
- Electrolytes—electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity.
- Probes of energy storage chemistry and physics at all time and length scales—analytical tools capable of monitoring changes in structure and composition at interfaces and in bulk phases with spatial resolution from atomic to mesoscopic levels and temporal resolution down to femtoseconds.
- Multi-scale modeling—computational tools with improved integration of length and time scales to understand the complex physical and chemical processes that occur in electrical energy storage processes from the molecular to system scales.

	FY 2009	FY 2010	FY 2011

(dollars in thousands)

One-time funding of $10,000,000 will be provided for Hub start-up needs, excluding new construction.

▪ **General Plant Projects (GPP)**	**4,243**	**3,757**	**0**

GPP funding is provided for the Stanford Institute for Materials and Energy Sciences (SIMES) project. This GPP project will renovate space for SIMES. Phase I prepares currently vacant space in Building 40 for build-out by upgrading the area to current ADA compliance and construction of common space. Phase II builds out the SIMES laboratories and renovates SIMES office and interaction space in Building 40. The TEC for this project is $8,000,000. No funds are requested in FY 2011.

▪ **Electron-beam Microcharacterization**	**11,313**	**0**	**0**

This activity supports three electron-beam microcharacterization centers, which operate as user facilities, work to develop next-generation electron-beam instrumentation, and conduct corresponding research. These centers are the Electron Microscopy Center for Materials Research at Argonne National Laboratory (ANL), the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory (LBNL), and the Shared Research Equipment program at Oak Ridge National Laboratory (ORNL).

Beginning in FY 2010, this research is budgeted for in a separate subprogram, within the Basic Energy Sciences program, entitled “Scientific User Facilities.”

▪ **Accelerator and Detector Research**	**9,794**	**0**	**0**

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Accelerator research is the corner stone for the development of new technologies that will improve performance of our light sources and neutron spallation facilities. This research will explore new areas of science and technologies that will facilitate the construction of our next generation accelerator-based user facilities. Detector research is a crucial, but often overlooked, component in the optimal utilization of our user facilities. This research program is investing aggressively in research leading to a new and more efficient generation of photon and neutron detectors.

Beginning in FY 2010, this research is budgeted for in a separate subprogram, within the Basic Energy Sciences program, entitled “Scientific User Facilities.”

▪ **Spallation Neutron Source Instrumentation I (SING I)**	**12,000**	**0**	**0**

Funds support a Major Item of Equipment to fabricate five instruments for the Spallation Neutron Source (SNS).

Beginning in FY 2010, this research is budgeted for in a separate subprogram, within the Basic Energy Sciences program, entitled “Scientific User Facilities.”

▪ **Spallation Neutron Source Instrumentation II (SING II)**	**7,000**	**0**	**0**

Funds support a Major Item of Equipment to fabricate four instruments to be installed at the SNS.

Beginning in FY 2010, this research is budgeted for in a separate subprogram, within the Basic Energy Sciences program, entitled “Scientific User Facilities.”

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)**	**15,000**	**0**	**0**

Funds support a Major Item of Equipment for three instruments for the Linac Coherent Light Source (LCLS) that will be installed after the LCLS line item project is completed in FY 2010. The technical concepts for the three instruments have been developed in consultation with the scientific community through a series of workshops, conferences, and focused review committees. Instrument designs for the LUSI project have been competitively selected using a peer review process. The project is managed by the SLAC National Accelerator Laboratory. It is anticipated that these three instruments will be installed at the LCLS on a phased schedule between FY 2010–2012. The baseline TPC was approved at Approve Performance Baseline, CD-2. The project is fully funded as of FY 2009.

Facilities Operations	**689,047**	**0**	**0**

This activity supports the operation of the BES scientific user facilities, which consist of light sources, neutron sources, nanoscience centers, and the Linac Coherent Light Source Free Electron Laser at SLAC.

Beginning in FY 2010, Facilities Operations is budgeted for in a separate subprogram, within the Basic Energy Sciences program, entitled "Scientific User Facilities." The number of users and operating hours for the synchrotron radiation sources and neutron scattering facilities are shown in the Scientific User Facilities subprogram.

▪ **Synchrotron Radiation Light Sources**	**338,755**	**0**	**0**
Advanced Light Source, LBNL	55,728	0	0
Advanced Photon Source, ANL	116,440	0	0
National Synchrotron Light Source, BNL	40,154	0	0
Stanford Synchrotron Radiation Light Source, SLAC	33,412	0	0
Linac Coherent Light Source (LCLS), SLAC	3,000	0	0
Linac for LCLS, SLAC	90,021	0	0
▪ **High-Flux Neutron Sources**	**249,802**	**0**	**0**
High Flux Isotope Reactor, ORNL	58,000	0	0
Intense Pulsed Neutron Source, ANL	4,000	0	0
Manuel Lujan, Jr. Neutron Scattering Center, LANL	11,302	0	0
Spallation Neutron Source, ORNL	176,500	0	0
▪ **Nanoscale Science Research Centers (NSRCs)**	**100,490**	**0**	**0**
Center for Nanophase Materials Sciences, ORNL	19,900	0	0
Center for Integrated Nanotechnologies, SNL/LANL	19,950	0	0

	FY 2009	FY 2010	FY 2011
	(dollars in thousands)		
Molecular Foundry, LBNL	20,000	0	0
Center for Nanoscale Materials, ANL	20,640	0	0
Center for Functional Nanomaterials, BNL	20,000	0	0
Other Project Costs	**27,044**	**0**	**0**

Other Project Costs (OPC) are associated with line-item construction or major item of equipment projects and include all project costs that are not identified as Total Estimated Cost costs. Total Estimated Cost includes project costs incurred after Critical Decision-1 such as costs associated with the acquisition of land and land rights; engineering, design, and inspection; direct and indirect construction/fabrication; and the initial equipment necessary to place the plant or installation in operation. Generally, OPC are costs incurred during the project's initiation and definition phase for planning, conceptual design, research and development, and during the execution phase for research and development, startup and operation. Other Project Costs are always operating funds.

	FY 2009	FY 2010	FY 2011
▪ Advanced Light Source User Support Building, LBNL	4	0	0
▪ Linac Coherent Light Source, SLAC	17,000	0	0
▪ National Synchrotron Light Source-II, BNL	10,000	0	0
▪ Photon Ultrafast Laser and Science and Engineering Building Renovation, SLAC	40	0	0
SBIR/STTR	**0**	**9,538**	**11,236**

In FY 2009, $25,592,000 and $3,071,000 were transferred to the SBIR and STTR programs, respectively. The FY 2010 and FY 2011 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR program.

	FY 2009	FY 2010	FY 2011
Total, Materials Sciences and Engineering	**1,108,351**	**363,642**	**432,663**

Explanation of Funding Changes

	FY 2011 vs. FY 2010 ($000)
Materials Sciences and Engineering Research	
▪ **Experimental Condensed Matter Physics**	
Increased funding is provided for enhanced research in the area of complex and emergent behavior (+$1,104,000). No direct funding is planned in FY 2011 for pension payments at ORNL and LBNL (-$3,402,000).	-2,298
▪ **Theoretical Condensed Matter Physics**	
Increased funding is provided for enhanced research to support multi-investigator projects in theory and modeling and simulation.	+709

	FY 2011 vs. FY 2010 ($000)
▪ **Mechanical Behavior and Radiation Effects**	
Increased funding is provided for enhanced research on the properties of materials in extreme environments such as the exposure to an energetic flux, chemical reactive stimulants, high temperature and pressure, and high magnetic and electric fields.	+4,506
▪ **Physical Behavior of Materials**	
Increased funding is provided for enhanced research on the fundamental science of photon-matter interactions.	+1,146
▪ **Neutron and X-ray Scattering**	
Increased funding is provided for scattering research to take advantage of increased neutron and x-ray fluxes and optimized beamline optics at BES user facilities, combined with specialized instruments, to investigate electrochemical processes in real time (+$1,088,000). Increased emphasis will be placed on expansion of ultrafast materials science research to take advantage of new x-ray and neutron sources to perform research on dynamic phenomena in real-time (+$2,500,000).	+3,588
▪ **Electron and Scanning Probe Microscopies**	
Increased funding is provided to emphasize the development of tools that will dramatically improve spatial, time, and energy resolution to provide fundamental understanding of the electron and charge transfer processes and mechanisms by which ions interact with electrode materials.	+657
▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	
The FY 2011 decrease is a result of the additional funding provided by Congress in FY 2010 (-$13,103,000); EPSCoR, funding increases at the same rate as BES core research (+$115,000). Additional funds provided in FY 2010 were used, to the extent possible, to fully fund grants and minimize outyear mortgages.	-12,988
▪ **Synthesis and Processing Science**	
Increased funding is provided to develop novel design rules for synthesizing nanostructured materials and assemblies for use-inspired technologies including solid state lighting, solar energy conversion, hydrogen storage, and electrical energy storage.	+10,544
▪ **Materials Chemistry and Biomolecular Materials**	
Increased funding is provided for research on the design and synthesis of new energy relevant materials and processes which includes those inspired by biology for new three-dimensional nanostructured architectures that can be precisely tailored for advanced energy storage and novel chemistries and materials for carbon capture.	+11,196

	FY 2011 vs. FY 2010 ($000)
▪ **Energy Frontier Research Centers**	
Increased funding is provided for research in discovery and development of new materials and energy related research topics.	+20,000
▪ **Energy Innovation Hub – Batteries and Energy Storage**	
Funds are provided for an Energy Innovation Hub focused on developing radically new concepts in materials design for producing storage devices with materials that are abundant and low in manufacturing cost, are capable of storing higher energy densities, have long cycle lifetimes, and have safety and abuse tolerance.	+34,020
▪ **General Plant Projects (GPP)**	
No GPP funding is requested in FY 2011. The SIMES project is complete in FY 2010.	-3,757
Total, Materials Sciences and Engineering Research	**+67,323**
SBIR/STTR	
Increased funding in SBIR/STTR funding because of an increase in total operating expenses.	+1,698
Total Funding Change, Materials Sciences and Engineering	**+69,021**

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Chemical Sciences, Geosciences, and Energy Biosciences			
Chemical Sciences, Geosciences, and Energy Biosciences Research	281,946	288,978	393,131
SBIR/STTR	0	7,956	10,485
Total, Chemical Sciences, Geosciences, and Energy Biosciences	281,946	296,934	403,616

Description

This subprogram supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use.

In fundamental interactions, basic research is supported in atomic, molecular, and optical sciences; gas-phase chemical physics; ultrafast chemical science; theoretical and computational chemistry; and condensed phase and interfacial molecular science. Emphasis is placed on structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail, with the aim of providing a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. Novel sources of photons, electrons, and ions are used to probe and control atomic, molecular, and nanoscale matter. Ultrafast optical and x-ray techniques are developed and used to study and direct molecular, dynamics, and chemical reactions.

In photochemistry and biochemistry, including solar photochemistry, photosynthetic systems, and physical biosciences, research is supported on the molecular mechanisms involved in the capture of light energy and its conversion into chemical and electrical energy through biological and chemical pathways. Natural photosynthetic systems are studied to create robust artificial and bio-hybrid systems that exhibit the biological traits of self assembly, regulation, and self repair. Complementary research encompasses organic and inorganic photochemistry, photo-induced electron and energy transfer, photo-electrochemistry, and molecular assemblies for artificial photosynthesis.

In chemical transformations, research themes include the characterization, control, and optimization of chemistry in many forms, including catalysis; separations and analysis; actinide chemistry; and geosciences. Catalysis science underpins the design of new catalytic methods for the clean and efficient production of fuels and chemicals and emphasizes inorganic and organic complexes; interfacial chemistry, nanostructured and supramolecular catalysts, photocatalysis and electrochemistry, and bio-inspired catalytic processes. Heavy element chemistry focuses on the spectroscopy, bonding, and reactivity of actinides and fission products. Complementary research on chemical separations focuses on the use of nanoscale membranes and the development of novel metal-adduct complexes. Chemical analysis research emphasizes laser-based and ionization techniques for molecular detection, particularly the development of chemical imaging techniques. Geosciences research covers analytical and physical geochemistry, rock-fluid interactions, and flow/transport phenomena.

The Energy Innovation Hub focused on Fuels from Sunlight will consist of multidisciplinary teams of experts that blend basic scientific research with technology development, engineering design, and energy policy. They will bridge the gap between basic scientific breakthroughs and industrial commercialization through proof-of-concept prototyping, modeling, measurement, and verification of the potential for major impacts.

Selected FY 2009 Accomplishments

- *Controlling x-rays with light.* The advent of x-ray free electron lasers and laser-based x-ray sources is enabling a rapidly expanding frontier of ultrafast x-ray science. A central application of these new sources is the visualization of atomic, molecular, and electronic dynamics, as triggered by an ultrafast light pulse, on atomic time and length scales. In such studies, visible light is used to modify the target and x-rays are used to monitor the response. Researchers have demonstrated for the first time that visible light pulses can also be used for a fundamentally different purpose—to control x-ray interactions with matter. Through an effect known as electromagnetically induced transparency, intense visible light can be used to induce transparency in a material that normally is opaque to x-ray radiation due to resonant x-ray absorption. The induced transparency is ultrafast and reversible and functions as an ultrafast x-ray switch. The ability to control x-ray/matter interactions with visible light will create new research opportunities at current and next-generation x-ray light sources. These results will also form a foundation for planned experiments at the Linac Coherent Light Source, in which intense x-rays will be used to both control and probe matter.
- *New tools for understanding interfacial chemistry*. The interactions of atoms and molecules at gas-solid and liquid-solid interfaces are critical in areas including heterogeneous catalysis, electrical energy storage, and solar energy conversion. The study of chemical interactions at surfaces at the molecular level is profoundly difficult because of the small amount of material available for study, the small spatial scales in which the interactions occur, and the ultrafast time scales over which they take place. Recent advances in low-temperature scanning tunneling microscopy (STM) have been combined with temporally and spatially resolved spectroscopic tools such as ultrafast, two-photon photoemission, to enable important new discoveries. New, long-lived electronic surface states have been discovered that could lead to new ways to induce and control electronic excitation at surfaces. Positioning the tip during STM measurements of light emission from single molecules with sub-nanometer resolution yields an unprecedented view of the coupling of electronic and vibrational motion within a single molecule. These new experimental tools are being combined with modern theoretical and computational methods to provide unprecedented capability to predict, monitor, and control the flow of energy and chemical reactivity at interfaces.
- *Understanding the Earth's geochemistry at the nanoscale.* Minerals and mineral composites coexist in the environment with a variety of inorganic and organic molecules, naturally buffering the chemistry of the natural environment. The behavior of water molecules surrounding nanoparticles in subsurface environments is thought to be an important influence on their growth and may account for the strong variation in surface chemistry with particle size. New research demonstrates that the size and shape of mineral particles controls the structure of the first few layers of water on their surfaces, profoundly influencing geochemical reactivity. The residence time of water molecules near the surface is shorter for smaller, less-crystalline nanoparticles than for larger nanoparticles or for the bulk mineral surface. Particles with facets or low curvature tend to preferentially stabilize the water network and in some cases cause faceting within the water layer itself. Molecular dynamics simulations of iron-oxide (hematite) particles show that water ordering around the particle decreases with decreasing particle size. These results show that nanophase structures formed by geochemical reactions can modify the interfacial forces present in aqueous solution near a surface. By mapping these interfacial forces, more sophisticated and accurate models can be developed to understand and

predict processes affecting contaminant immobilization and bacterial attachment on mineral surfaces under natural conditions.

- *Sub-nanometer catalysts are remarkably effective.* Heterogeneous catalysts are central to the conversion of natural resources into about 80% of all chemicals used by humankind. The scarcer and more expensive resources demand attainment of ever higher selectivity and energy efficiency in chemical catalysis, which imposes strict requirements for the control of catalyst structure. A new frontier has recently been achieved through the synthesis of sub-nanometer metal particles (clusters) containing only a few atoms that maintain their size throughout the stages of a chemical reaction, which is critical to attaining high activity and selectivity. Cluster size stability was achieved through delicate control over the structure of and reaction with the catalyst support, typically a mixed metal oxide. Clusters containing only 8–10 atoms of platinum bound to aluminum oxide films display 40–100 times higher catalytic activity and thousands time more chemical selectivity than conventional catalysts. Achieving this feat required synergistic efforts in the synthesis of atomically-layered, ordered oxides, leaving reaction sites open to bind certain metal clusters; soft landing and reaction of metal clusters of the selected size; synchrotron x-ray diagnostics to demonstrate cluster stability; and quantum chemical calculations for the prediction of catalytic activity as a function of cluster size.
- *New promise for plastic solar cells*. Plastic solar cells hold great promise for the conversion of solar energy into electricity because they are flexible, lightweight, inexpensive, and made from abundant organic materials. But current plastic solar cells have poor conversion efficiencies. New research on the polymers in plastic solar cells has revealed that the speed of electron transport and excitation diffusion through the polymer is much faster than was previously assumed. The new experiments used pulsed radiolysis to place electrons at the end of polymer chain tens of nanometers in length and then monitored the time it took for the electron or excitation to fall into a trap at the end of the chain. The results showed that electrons and optical excitations created in the polymers can wend their way through the chains in a matter of 10^{-10} seconds. Current, low-efficiency plastic solar cells are designed and engineered with the assumption that this transport of charge and energy down the polymer is intrinsically much slower. The discovery of more rapid transport paves the way toward more efficient plastic solar cells.
- *Nature's most efficient light harvesting system revealed.* Certain photosynthetic bacteria have evolved a sophisticated antenna complex, called the chlorosome, which allows them to thrive in an extremely light-limited environment. Unlike other natural antenna systems, chlorosomes lack a protein matrix supporting the photosynthetic pigments of up to 250,000 individual chlorophyll molecules. Structural analysis shows that the chlorophyll molecules inside the chlorosome are arranged as densely packed nanotubes in helical spirals. A recent study of the antenna protein that transfers energy absorbed by the chlorosome to the main photosynthetic reaction center determined that the protein is oriented so that the side containing the pigment with the lowest potential energy is nearest to the reaction center, consistent with theoretical predictions. These studies have begun to reveal how chlorophyll organization and chlorosome structure can increase the efficiency of photosynthesis. The relatively simple interactions between chlorophylls in the chlorosome provide promising new leads for the rational design of artificial photosynthetic systems. Similarly, the increased understanding of how energy transfer occurs through the relay protein from the antenna to the reaction centers may lead to new approaches for funneling energy through artificial photosynthetic systems.

Detailed Program Justification

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Chemical Sciences, Geosciences, and Energy Biosciences Research	**281,946**	**288,978**	**393,131**
▪ **Atomic, Molecular, and Optical Science**	**25,129**	**22,717**	**26,118**

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. The research emphasizes the fundamental interactions of these systems with photons and electrons to characterize and control their behavior. These efforts aim to develop accurate quantum mechanical descriptions of properties and dynamical processes of atoms, molecules, and nanoscale matter. The study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer to ultimately make and break chemical bonds. Topics include the development and application of novel, ultrafast optical probes of matter, particularly x-ray sources; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems, including ultracold atomic and molecular gases. Capital equipment funding is provided for items such as lasers and optical equipment, unique ion sources or traps, position-sensitive and solid-state detectors, control and data processing electronics, and computational resources.

The knowledge and techniques produced by this activity form a science base that underpins several aspects of the DOE mission. New methods for using photons, electrons, and ions to probe matter lead to more effective use of BES synchrotron, nanoscience, and microcharacterization facilities. Similarly, the study of formation and evolution of energized states in atoms, molecules, and nanostructures provides a fundamental basis for understanding elementary processes in solar energy conversion and radiation-induced chemistry.

In FY 2011, there is an increase for the development and application of new ultrafast x-ray and optical probes of matter, including the first experiments to be performed on the Linac Coherent Light Source; on theoretical and computational methods for the interpretation of ultrafast measurements; and on the use of optical fields to control and manipulate quantum mechanical systems.

▪ **Chemical Physics Research**	**47,658**	**53,509**	**75,632**

This activity supports experimental and theoretical investigations in the gas phase, in condensed phases, and at interfaces aimed at elucidating the chemical transformations and physical interactions that govern combustion; surface reactivity; and solute/solvent structure, reactivity, and transport. The gas-phase chemical physics portion emphasizes studies of the dynamics and rates of chemical reactions at energies characteristic of combustion and the chemical and physical properties of key combustion intermediates. The goal is development of validated theories and computational tools for predicting chemical reaction rates for use in combustion models and experimental tools for validating these models. Combustion models using this input are developed that incorporate complex chemistry with the turbulent flow and energy transport characteristics of real combustion processes. This activity includes support for the Combustion Research Facility (CRF), a multi-investigator research laboratory for the study of combustion science and technology that emphasizes experiment, theory, and computation in chemical dynamics, chemical kinetics, combustion modeling, and diagnostic development.

The condensed-phase and interfacial chemical physics portion of this activity emphasizes molecular understanding of chemical, physical, and electron-driven processes in aqueous media and at interfaces. Studies of reaction dynamics at well-characterized metal or metal-oxide surfaces lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Research confronts the transition from detailed, molecular-scale understanding to cooperative and collective phenomena in complex systems. Capital equipment funding is provided for items such as lasers and optical equipment, novel position-sensitive and temporal detectors, specialized vacuum chambers for gas-phase and surface experiments, spectrometers, and computational resources.

The gas-phase portion of this activity contributes strongly to the DOE mission in the area of the efficient and clean combustion of fuels. The coupling of complex chemistry and turbulent flow has long challenged predictive combustion modeling. Truly predictive combustion models enable the design of new combustion devices (such as internal combustion engines, burners, and turbines) with maximum energy efficiency and minimal environmental consequences. In transportation, the changing composition of fuels, from those derived from light, sweet crude oil to biofuels and fuels from alternative fossil feedstocks, puts increasing emphasis on the need for science-based design of modern engines. The condensed-phase and interfacial portion of this activity impacts a variety of mission areas by providing a fundamental basis for understanding chemical reactivity in complex systems, such as those encountered in catalysis and environmental processes. Surface-mediated chemistry research in this activity complements more directed efforts in heterogeneous catalysis. Condensed-phase and interfacial chemical physics research on dissolution, solvation, nucleation, separation, and reaction provides important fundamental knowledge relevant to the environmental contaminant transport in mineral and aqueous environments. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiolysis effects in nuclear fuel and waste environments.

In FY 2011, a significant effort will be initiated in the area of multiscale models for advanced engine design. High-fidelity models of combustion processes will be critical to enabling the transition from hardware-intensive, experience-based engine design to simulation-intensive, science-based design, accommodating new fuel types and engine combustion systems. Scientific challenges posed by advanced engine systems include complex interactions among multiphase fluid mechanics, thermodynamic properties, heat transfer, and chemical kinetics over a vast range of spatial and temporal scales. Numerical and algorithm advances will be required to develop new combustion models that exploit the capabilities of the most advanced large-scale computers. Successful resolution of these scientific and computational challenges would provide new fundamental understanding of, and models for, the conditions and fuels that will be relevant for next-generation engines (+$20,000,000). In FY 2011, there will also be increased emphasis for experimental, theoretical, and computational research aimed at developing predictive models for clean and efficient combustion of biofuels and alternative fossil fuels. Elucidating the reactivity of individual molecular sites in interfacial processes and the effects of cooperative phenomena on chemical reactivity in the condensed phase will also receive emphasis.

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
▪ **Solar Photochemistry**	**38,385**	**36,985**	**38,453**

This activity supports molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, electrical charge generation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Supported research areas include organic and inorganic photochemistry and photocatalysis, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. This activity, with its integration of physical and synthetic scientists devoted to solar photochemistry, is unique to DOE. Capital equipment funding is provided for items such as ultrafast laser systems, scanning tunneling microscopes, fast Fourier transform infrared and Raman spectrometers, and computational resources.

Solar photochemical energy conversion is an important option for generating electricity and chemical fuels and therefore plays a vital role in DOE's development of solar energy as a viable component of the nation's energy supply. Photoelectrochemistry provides an alternative to semiconductor photovoltaic cells for electricity generation from sunlight using closed, renewable energy cycles. Solar photocatalysis, achieved by coupling artificial photosynthetic systems for light harvesting and charge transport with the appropriate electrochemistry, provides a direct route to the generation of fuels such as hydrogen, methane, and complex hydrocarbons. Fundamental concepts derived from studying highly efficient excited-state charge separation and transport in molecular assemblies is also applicable to future molecular optoelectronic device development.

In FY 2011, continued emphasis will be placed on studies of semiconductor/polymer interfaces, multiple charge generation within semiconductor nanoparticles, dye-sensitized solar cells, inorganic/organic donor-acceptor molecular assemblies, and the use of nanoscale materials in solar photocatalytic generation of chemical fuels. This activity also includes funding for the U.S.-India Clean Energy Research Center.

▪ **Photosynthetic Systems**	**16,809**	**18,499**	**19,233**

This activity supports fundamental research on the biological conversion of solar energy to chemically stored forms of energy. Topics of study include light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation and carbon storage. Emphasized areas are those involving strong intersection between biological sciences and energy-relevant chemical sciences and physics, such as in self-assembly of nanoscale components, efficient photon capture and charge separation, predictive design of catalysts, and self-regulating/repairing systems. Capital equipment funding is provided for items such as ultrafast lasers, high-speed detectors, spectrometers, environmentally controlled chambers, high-throughput robotic systems, and computational resources.

The impact of research in this activity is to uncover the underlying structure-function relationships and to probe dynamical processes in natural photosynthetic systems to guide the development of robust artificial and bio-hybrid systems for conversion of solar energy into electricity or chemical fuels. The ultimate goal is the development of bio-hybrid systems in which the best features from nature are selectively used while the shortcomings of biology are bypassed. Achieving this goal would impact DOE's efforts to develop solar energy as an efficient, renewable energy source.

In FY 2011, research will emphasize understanding and control of the weak intermolecular forces governing molecular assembly in photosynthetic systems; understanding the biological machinery for cofactor insertion into proteins and protein subunit assemblies; adapting combinatorial, directed-evolution, and high-throughput screening methods to enhance fuel production in photosynthetic systems; characterizing the structural and mechanistic features of new photosynthetic complexes; and determining the physical and chemical rules that underlie biological mechanisms of repair and photo-protection.

	FY 2009	FY 2010	FY 2011
▪ **Physical Biosciences**	**16,148**	**17,780**	**18,486**

This activity combines experimental and computational tools from the physical sciences with biochemistry and molecular biology. A fundamental understanding of the complex processes that convert and store energy in living systems is sought. Research supported includes studies that investigate the mechanisms by which energy transduction systems are assembled and maintained, the processes that regulate energy-relevant chemical reactions within the cell, the underlying biochemical and biophysical principles determining the architecture of biopolymers and the plant cell wall, and active site protein chemistry that provides a basis for highly selective and efficient bio-inspired catalysts. Capital equipment is provided for items including advanced atomic force and optical microscopes, lasers and detectors, equipment for x-ray or neutron structure determinations, and Fourier transform infrared and nuclear magnetic resonance spectrometers.

The research provides basic structure-function information necessary to accomplish solid-phase nanoscale synthesis in a targeted manner, i.e., controlling the basic architecture of energy-transduction and storage systems. This impacts numerous DOE interests, including improved biochemical pathways for biofuel production, next generation energy conversion/storage devices, and efficient, environmentally benign, sustainable catalysts.

In FY 2011, continued emphasis will be placed on probing the organizational principles of biological energy transduction and chemical storage systems using advanced molecular imaging and x-ray or neutron methods for structural determination. Of particular interest is the molecular scale characterization of the structure and chemistry of the biopolymers of the plant cell wall, knowledge that is required for the direct catalytic conversion of biomass into chemical fuels. In FY 2011, continued emphasis will be placed on probing the organizational principles of biological energy transduction and chemical storage systems using advanced molecular imaging and x-ray or neutron methods for structural determination. Of particular interest is the molecular scale characterization of the structure and chemistry of the biopolymers of the plant cell wall, knowledge that is required for the direct catalytic conversion of biomass into chemical fuels.

	FY 2009	FY 2010	FY 2011
▪ **Catalysis Science**	**42,401**	**46,603**	**48,510**

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. Capital equipment funding is provided for items such as ultrahigh vacuum equipment with various probes of interfacial structure, spectroscopic analytical instrumentation, and specialized cells for *in situ* synchrotron-based experiments, and computational resources.

Catalytic transformations impact an enormous range of DOE mission areas. Particular emphasis is placed on catalysis relevant to the conversion and use of fossil and renewable energy resources and the creation of advanced chemicals. Catalysts are vital in the conversion of crude petroleum and biomass into clean burning fuels and materials. They control the electrocatalytic conversion of fuels into energy in fuel cells and batteries and play important roles in the photocatalytic conversion of energy into chemicals and materials. Catalysts are crucial to creating new, energy-efficient routes for the production of basic chemical feedstocks and value-added chemicals. Environmental applications of catalytic science include minimizing unwanted products and transforming toxic chemicals into benign ones, such as the transformation of chlorofluorocarbons into environmentally acceptable refrigerants.

In FY 2011, research will focus on the chemistry of inorganic, organic, and hybrid porous materials, the nanoscale self-assembly of these systems, and the integration of functional catalytic properties into nanomaterials. New strategies for design of selective catalysts for fuel production from both fossil and renewable biomass feedstocks will be explored. Increased emphasis will be placed on the use of spectroscopy and microscopy to probe both model systems in vacuum and realistic catalytic sites. Research on catalytic cycles involved in electrochemical energy storage and solar photocatalytic fuel formation will receive increased emphasis.

	FY 2009	FY 2010	FY 2011
▪ **Separations and Analysis**	**17,150**	**15,881**	**16,511**

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial resolution to achieve chemical imaging. This activity is the nation’s most significant long-term investment in the fundamental science underpinning actinide separations and mass spectrometry. The overall goal is to obtain a thorough understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that their full utility can be realized. Capital equipment funding is provided for items such as lasers for use in sample ionization and chemical imaging, advanced mass spectrometers with nanoprobes, confocal microscopes for sub-diffraction limit resolution, and computational resources.

Work is closely coupled to DOE’s stewardship responsibility for transuranic chemistry; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

components of the portfolio. Knowledge of molecular-level processes is required to characterize and treat extremely complex radioactive mixtures in, for example, new nuclear fuel systems, and to understand and predict the fate of radioactive contaminants in the environment. Separations are essential to nearly all operations in processing industries and are also necessary for many analytical procedures.

In FY 2011, separations research will focus on fluid flow in nanoscale membranes and the formation of macroscopic separation systems via self-assembly of nanoscale building blocks. Special additional emphasis will be placed on the development of new materials and methods for separation and capture of CO_2 from post-combustion gas streams and oxygen from air prior to oxy-combustion. Research will include experimental and theoretical/computational studies of how weak intermolecular forces can be understood and controlled to achieve separations with high selectivity and capture with only modest energy requirements for subsequent release. Chemical analysis research will emphasize the development of techniques with high spatial, temporal, and chemical resolution; and simultaneous application of multiple analytical techniques.

	FY 2009	FY 2010	FY 2011
▪ **Heavy Element Chemistry**	**11,033**	**11,729**	**12,195**

This activity supports research in the chemistry of the heavy elements, including actinides and fission products. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structures, bond strengths, and chemical reaction rates. Additional emphasis is placed on the chemical and physical properties of actinides to determine solution, interfacial, and solid-state bonding and reactivity; on determining chemical properties of the heaviest actinide and transactinide elements; and on bonding relationships among the actinides, lanthanides, and transition metals. Capital equipment funding is provided for items such as instruments used to characterize actinide materials (spectrometers, diffractometers, etc.) and equipment to handle the actinides safely in laboratories and at synchrotron light sources.

This activity represents the nation's only funding for basic research in actinide and fission product chemistry and is broadly relevant to the DOE mission. Knowledge of the chemical characteristics of actinide and fission-product materials under realistic conditions provides a basis for advanced fission fuel cycles. Fundamental understanding of the chemistry of these long-lived radioactive species is required to accurately predict and mitigate their transport and fate in environments associated with the storage of radioactive wastes.

In FY 2011, continued emphasis will be placed on bonding and reactivity studies in solutions, solids, nanoparticles, and interfaces, incorporating theory and modeling to understand, predict, and control the chemical bonding and reactivity of the heavy elements, especially under extreme conditions of temperature and radiation fields to be found in advanced nuclear energy systems. Increased study of organo-actinide chemistry may provide new insights into metal-carbon bonds with metals that have large ion sizes, f-orbital bonding, and multiple oxidation states.

	FY 2009	FY 2010	FY 2011
▪ **Geosciences Research**	**22,028**	**22,432**	**50,839**

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance; it seeks fundamental understanding of wave propagation physics in complex media and the fluid dynamics of complex fluids through porous and fractured subsurface rock units. Application of x-ray and neutron scattering using BES facilities plays a key role in the geochemical and geophysical studies within this activity. The activity also emphasizes incorporating physical and chemical understanding of geological processes into multiscale computational modeling. Capital equipment funding is provided for items such as x-ray and neutron scattering end stations at BES facilities for environmental samples and for augmenting experimental, field, and computational capabilities.

This activity provides the basic research in geosciences that underpins the nation's strategy for understanding and mitigating the terrestrial impacts of energy technologies and thus is relevant to the DOE mission in several ways. It develops the fundamental understanding of geological processes relevant to geological disposal options for byproducts from multiple energy technologies. Knowledge of subsurface geochemical processes is essential to determining the fate and transport properties of harmful elements from possible nuclear or other waste releases. Geophysical imaging methods are needed to measure and monitor subsurface reservoirs for hydrocarbon production or for carbon dioxide storage resulting from large-scale carbon sequestration schemes.

In FY 2011, new research will be initiated in theory, multi-scale modeling, and field/experimental investigations of the geochemistry and geophysics of CO_2—rock/mineral interactions and other related topics (+$5,000,000). Additional research will support high-resolution geophysical and geochemical investigations. The objective will be to develop robust, broadly applicable measurement approaches to verify the effectiveness of CO_2 sequestration and other geological greenhouse gas mitigation measures. Specific emphasis will be on physical and chemical approaches for measuring properties and concentrations of chemical species in large-scale systems. The research will produce new tools and techniques that derive from longstanding BES capabilities in optical and physico-chemical diagnostics related to geosciences (+$5,000,000). In FY 2011 emphasis will also be placed on geochemical studies and computational analysis of complex subsurface fluids and solids, including nanophases; understanding the dynamics of fluid flow, particulate transport and associated rock deformation in the deep subsurface; and developing the ability to integrate multiple data types in predictions of subsurface processes and properties.

In FY 2011, Basic Energy Sciences will initiate a new research program in gas hydrates (+$17,517,000). Gas hydrates are naturally occurring combinations of methane and water that form at low temperatures and high pressure. This program will study fundamental scientific questions surrounding methane hydrates: How do they form? What is their role in the global carbon cycle? What is their role in seafloor ecological systems? How extensive are they? How stable are they? For the next 24 months, the program will also study hydrates via controlled *in situ* depressurization and physical, thermal, and chemical stimulation in the Arctic with supporting laboratory and numerical modeling to enable interpretation and extrapolation of results. Existing core sample data from the Arctic hydrate formations will provide the scientific information of how the hydrate structure sits in the pore space at various depths. The planned tests in the Gulf of Mexico in FY 2011 will take *in situ* core samples at various depths and locations for evaluation. Computer simulations will be compared with data from previous *in situ* tests. This activity will also support theory, multi-scale modeling and

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

simulation, and experimental research in areas such as the intermolecular forces that govern the structure and properties of gas hydrates and studies of gas hydrates in the natural environment.

▪ **Energy Frontier Research Centers (EFRCs)[a]**	**42,000**	**42,000**	**62,000**

The 46 EFRCs established in late FY 2009 are multi-investigator and multi-disciplinary centers that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future.[b] The EFRCs represent an important new research modality for BES, bringing together the skills and talents of a critical mass of investigators to enable energy relevant, basic research of a scope and complexity that would not be possible with the standard single-investigator or small-group award. The scope and unique nature of the EFRC program requires special oversight, which is accomplished through a BES-wide, dedicated EFRC management team. This team has the direct management responsibility over all EFRCs and also coordinates EFRC research with the complementary research conducted within the BES core research areas.

This activity supports those EFRCs that are best coordinated with and most suitably complement the ongoing core research activities within the Chemical Sciences, Geosciences and Energy Biosciences subprogram. In general terms, these EFRCs are focused on the design, discovery, synthesis, and characterization of novel, solid-state materials that improve the conversion of solar energy and heat into electricity; that improve the conversion of electricity to light; that can be used to improve electrical energy storage; that are resistant to corrosion, decay, or failure in extreme conditions of temperature, pressure, radiation, or chemical exposures; that take advantage of emergent phenomena, such as superconductivity, to improve energy transmission; that optimize energy flow to improve energy efficiency; and that are tailored at the atomic level for catalytic activity.

In FY 2011, new EFRCs will be solicited in two categories: discovery and development of new materials that are critical to both science frontiers and technology innovations and basic research for energy needs in a limited number of areas that are underrepresented in the 46 original EFRC awards.

For the discovery and development of new materials, the emphasis will be on new synthesis capabilities, particularly bio-inspired approaches, to establish a strong foundation for science-driven materials discovery and synthesis in the U.S. Emphasis will be placed on understanding the mechanisms by which biological systems manipulate and exchange energy and information on the nanoscale. Such information can then be used as the basis for the design and synthesis of purely artificial or bio-hybrid materials with functionalities that rival their biological counterparts. One critical application area is the development of bio-inspired catalytic materials. Lessons learned from biological catalysts, including their ability to fine tune catalytic function based on subtle, dynamic changes in the structural and electronic properties of the catalytic site, will be used to design and synthesize purely artificial or bio-hybrid catalytic materials.

For research for energy applications, areas of emphasis include fundamental science of carbon capture, including the rational design of novel materials and separation processes for post-combustion CO_2 capture and catalysis and separation research for advanced carbon capture schemes

[a] A complimentary set of EFRCs is also included in the Materials Sciences and Engineering subprogram. This set includes ongoing EFRCs as well as new awards to be initiated in FY 2011.
[b] 16 of the 46 EFRCs were forward funded for the five-year initial award period under the American Recovery and Reinvestment Act of 2009.

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

in new power plants, and fundamental science for advanced nuclear energy systems, e.g., separation science and heavy element chemistry for fuel cycles. Advances in post-combustion CO_2 capture require experimental and theoretical/computational studies of how weak intermolecular forces can be understood and controlled to enable the design of capture materials and methods that are highly selective to CO_2 versus nitrogen but that release the captured CO_2 with minimum energy penalty. Carbon capture schemes for new power plants require research into efficient and cheaper ways of separating oxygen from air for oxy-combustion and new catalytic routes for the conversion of fossil feedstocks and biomass into cleaner burning fuels. Fundamental science for advanced nuclear fuel cycles includes bonding and reactivity studies in solutions, solids, nanoparticles, and interfaces, incorporating theory and modeling to understand, predict, and control the chemical bonding and reactivity of the heavy elements, especially under extreme conditions of temperature and radiation fields. Complementary emphasis will be placed on the separation and analysis of molecular species containing transuranic isotopes and their radioactive decay products, which is required to characterize and treat extremely complex radioactive mixtures in new nuclear fuel systems.

	FY 2009	FY 2010	FY 2011
▪ **Energy Innovation Hub—Fuels from Sunlight**	**0**	**0**	**24,300**

After nearly 3 billion years of evolution, nature can effectively convert sunlight into energy-rich chemical fuels using the abundant feedstocks of water and carbon dioxide. All fuels used today to power vehicles and create electricity, whether from fossil or biomass resources, are ultimately derived from photosynthesis. While biofuels are renewable resources that avoid the environmental consequences of burning the sequestered carbon of fossil fuels, their scalability and sustainability are ongoing issues. Furthermore, the overall energy efficiency of converting sunlight to plant material and then converting biomass into fuels is low. The natural photosynthetic apparatus is a remarkable machine, but plants and photosynthetic microbes were not designed to meet human energy needs—much of the energy captured from the sun is necessarily devoted to the life processes of the plants. Imagine the potential energy benefits if we could generate fuels directly from sunlight, carbon dioxide, and water in a manner analogous to the natural system, but without the need to maintain life processes. The impact of replacing fossil fuels with fuels generated directly by sunlight would be immediate and revolutionary. Recognizing this, the BESAC report, *New Science for Secure and Sustainable Energy Future*, the production of fuels directly from sunlight as one its three strategic goals for which transformational science breakthroughs are urgently needed.

Basic research has already provided enormous advances in our understanding of the subtle and complex photochemistry associated with the natural photosynthetic system. Similar advances have occurred using inorganic photo-catalytic methods to split water or reduce carbon dioxide. Yet, we still lack sufficient knowledge to design solar fuel generation systems with the required efficiency, scalability, and sustainability for economic viability. The Fuels from Sunlight Hub will develop an effective solar energy to chemical fuel conversion system. The system should operate at an overall efficiency and produce fuel of sufficient energy content to enable transition from bench-top discovery to proof-of-concept prototyping. The magnitude of this challenge is daunting, but not insurmountable, and will require that this Hub draw expertise and premier scientific talent from the disciplines of chemistry, physics, materials sciences, biology, and engineering. Critical issues to be addressed include: understanding and designing catalytic complexes or solids that generate

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

chemical fuel from carbon dioxide and/or water; integration of all essential elements from light capture to fuel formation into an effective solar fuel generation system; and pragmatic evaluation of the solar fuel system under development.

The Fuels from Sunlight Hub was initiated in FY 2010 with $22,000,000 provided through the Office of Energy Efficiency and Renewable Energy. SC/BES provides programmatic oversight for the Fuels from Sunlight Hub, including management of the solicitation and its merit review process, and coordination with the two other Energy Innovation Hubs initiated in FY 2010 – Modeling and Simulation for Nuclear Reactors in the Office of Nuclear Energy and Energy Efficient Building Systems Design in the Office of Energy Efficiency and Renewable Energy. In FY 2011, BES will provide funding for the continuation of the Fuels from Sunlight Hub.

	FY 2009	FY 2010	FY 2011
▪ **General Plant Projects (GPP)**	**3,205**	**843**	**854**

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems principally at the Ames Laboratory and the Combustion Research Facility at Sandia National Laboratories. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Materials Sciences and Engineering subprogram and the Scientific User Facilities subprogram. The total estimated cost of each GPP project will not exceed $5,000,000 in FY 2011.

In FY 2009, non-programmatic GPP funding for ORNL and ANL was transferred to the Science Laboratories Infrastructure program to support the SC Infrastructure Modernization Initiative.

	FY 2009	FY 2010	FY 2011
SBIR/STTR	**0**	**7,956**	**10,485**

In FY 2009, $6,736,000 and $808,000 were transferred to the SBIR and STTR programs, respectively. The FY 2010 and FY 2011 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR programs.

	FY 2009	FY 2010	FY 2011
Total, Chemical Sciences, Geosciences, and Energy Biosciences	**281,946**	**296,934**	**403,616**

Explanation of Funding Changes

	FY 2011 vs. FY 2010 ($000)
Chemical Sciences, Geosciences, and Biosciences Research	
▪ **Atomic, Molecular and Optical Science**	
Increased funding is provided for the development and application of new ultrafast x-ray and optical probes of matter (+$2,500,000), and on theoretical and computation methods for interpretation of ultrafast measurements and on the use of optical fields to control and manipulate quantum mechanical systems (+$901,000).	+3,401

	FY 2011 vs. FY 2010 ($000)
▪ **Chemical Physics Research**	
Increased funding is provided to initiate a significant effort in the area of multiscale models for advanced engine design (+$20,000,000). Increased funding is also provided for additional emphasis on experimental, theoretical, and computational research aimed at developing predictive models for clean and efficient combustion of biofuels and alternative fossil fuels (+$2,123,000).	+22,123
▪ **Solar Photochemistry**	
Increased funding is provided for research on inorganic/organic donor-acceptor molecular assemblies and in the use of nanoscale materials in solar photocatalytic generation of chemical fuels.	+1,468
▪ **Photosynthetic Systems**	
Increased funding is provided for solar energy conversion in biological and bio-hybrid systems and enhanced efforts in understanding defect tolerance and self-repair in natural photosynthetic systems.	+734
▪ **Physical Biosciences**	
Increased funding is provided for probing the organizational principles of biological energy transduction and chemical storage systems using advanced molecular imagining and x-ray or neutron methods for structural determination.	+706
▪ **Catalysis Science**	
Increased funding is provided for focus on the chemistry of inorganic, organic, and hybrid porous materials, the nanoscale self-assembly of these systems, and the integration of functional catalytic properties into nanomaterials.	+1,907
▪ **Separations and Analysis**	
Increased funding is provided for advanced chemical separations, particularly separation techniques relevant to capture of carbon dioxide and for analytical chemical imaging.	+630
▪ **Heavy Element Chemistry**	
Increased funding is provided for enhanced efforts on actinide chemistry and separations science related to advanced nuclear energy systems.	+466
▪ **Geosciences Research**	
Increased funding is provided for new research to improve understanding of the chemistry and physics of potential geophysical controls that could be used to modify effects induced by greenhouse gases (+$5,000,000) and for additional research to support high-resolution geophysical and geochemical investigations (+$5,000,000). Increased funding is also provided for continuing research in solid earth geophysics and geochemistry ($+890,000). In addition, funding is provided for the new gas hydrates research program (+$17,517,000).	+28,407

	FY 2011 vs. FY 2010 ($000)
▪ **Energy Frontier Research Centers**	
Increased funding is provided for research in discovery and development of new materials and energy related research topics.	+20,000
▪ **Energy Innovation Hub—Fuels from Sunlight**	
Funds are provided for an Energy innovation Hub focused on making fuels from sunlight. The Hub will develop a solar fuel conversion system that completely bypasses plants as the medium, drawing from the disciplines of chemistry physics, materials sciences, biology, and engineering.	+24,300
▪ **General Plant Projects (GPP)**	
Small increase for general plant projects.	+11
Total, Chemical Sciences, Geosciences and Energy Biosciences Research	**+104,153**
SBIR/STTR	
Increased funding for SBIR/STTR because of increase in operating expenses.	+2,529
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	**+106,682**

Scientific User Facilities

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Scientific User Facilities			
Research	0	32,525	27,339
Major Items of Equipment	0	25,000	22,400
Facilities Operations	0	730,621	775,823
Other Project Costs	0	13,500	1,500
SBIR/STTR	0	20,038	20,059
Total, Scientific User Facilities	0[a]	821,684	847,121

Description

This subprogram supports the R&D, planning, and operation of scientific user facilities for the development of novel nano-materials and for materials characterization through x-ray, neutron, and electron beam scattering; the former is accomplished through five Nanoscale Science Research Centers and the latter is accomplished through the world's largest suite of synchrotron radiation light source facilities, neutron scattering facilities, and electron-beam microcharacterization centers.

The BES-supported suite of facilities and research centers provides a unique set of analytical tools for studying the atomic structure and functions of complex materials. These facilities provide key capabilities to correlate the microscopic structure of materials with their macroscopic properties. The synchrotron light sources, producing photons largely over a very wide range of photon energies (from the infrared to hard x-rays), shed light on fundamental aspects of the physical world, investigating energy, momentum, and position using the techniques of spectroscopy, scattering, and imaging applied over various time scales. Neutron sources take advantage of the electrical neutrality and special magnetic properties of the neutron to probe atoms and molecules and their assembly into materials. Electron beam instruments provide the spatial resolution needed to observe individual nanostructures and even single atoms by exploiting the strong interactions of electrons with matter and the ability to readily focus beams of charged particles. The Nanoscale Science Research Centers provide the ability to fabricate complex nanostructures using chemical, biological, and other synthesis techniques, and to characterize, assemble, and integrate them into devices.

Annually, the BES user facilities are visited by more than 10,000 scientists and engineers in many fields of science and technology. These facilities provide unique capabilities to the scientific community and are a critical component of maintaining U.S. leadership in the physical sciences. The light sources are an outstanding example of serving users from a diverse range of disciplines, including physical and life sciences. For example, the life sciences sector of the light sources users increased from less than 10% in the 1990s to over 40% in 2009. Also supported are research activities leading to the improvement of today's facilities and better detectors, paving the foundation for the development of next generation facilities.

[a] FY 2009 funding of $771,198,000 for Scientific User Facilities is located within the Materials Sciences and Engineering subprogram.

Selected FY 2009 Accomplishments

- *Advanced Photon Source Develops Non-Destructive Tool for Tomography.* The research technique known as synchrotron-radiation computed laminography (SRCL) has been developed at the Advanced Photon Source for surface tomography characterization. The SRCL overcomes the limitation of standard synchrotron-radiation computed tomography, which restricts the lateral dimension of an object to be studied or requires that a sample be cut from the subject. It allows high-resolution, non-destructive three-dimensional imaging of objects, such as imaging fossil specimens for paleontological studies. Due to the complex geological and environmental processes involved, many fossils exhibit laterally-extended structures. Traditionally, this type of fossil is sectioned and imaged utilizing scanning electron microscopy or visible-light microscopes. The specimens are, however, unavoidably destroyed after inspection. The successful application of this technique opens the door to the non-destructive study of laterally-extended fossils. SRCL also finds application in imaging dimensionally long objects, including printed circuit boards, a wide range of microelectronics, and the efficacy of industrial welds and solders.
- *Top-off Operation at Advanced Light Source Achieves High Current and Stable Beam.* The Advanced Light Source has recently completed a successful upgrade, making top-off operation available to user service. The top-off operational mode allows frequent injection of electron beam into the storage ring, resulting in an almost constant current while keeping the beam accessible to users at all times. This mode presents several important advantages for users. Instead of having multiple injections of a large number of electrons in a short time period followed by uninterrupted beam decay over the course of 8 hours, a small number of electrons are added to the storage ring approximately every 30–60 seconds. The near-constant beam current enhances the flux and brightness of the radiation while simultaneously improving the thermal stability of the machine and its beamlines. Compared with pre-top-off operation, top-off mode achieves a current level of 500 mA, which doubles the time-averaged current and increases the photon flux by a factor of two.
- *Nanoparticle Research at Molecular Foundry Yields Promising Results for Energy Applications.* Researchers at the Molecular Foundry have produced for the first time non-toxic magnesium oxide nanocrystals that efficiently emit blue light and could also play a role in long-term storage of carbon dioxide, a potential means of tempering the effects of global warming. This bright blue luminescence upon exposure to ultraviolet light could be an inexpensive, attractive alternative in applications such as bio-imaging or solid-state lighting. Efficient blue light emitters are difficult to produce, suggesting these magnesium oxide nanocrystals could be a bright candidate for lighting that consumes less energy and has a longer lifespan. Along with their promising optical behavior, these nanocrystals will allow researchers to probe a key pathway in carbon dioxide capture and storage. If properly stored, captured carbon dioxide pumped underground forms carbonate minerals with the surrounding rock by reacting with nanoparticles of magnesium oxide and other mineral oxides; these nanocrystals will provide a model system to mimic this process.
- *New Technique Developed at Center for Functional Nanomaterials (CFN) for Nanostructure Fabrication.* The unique phenomena that emerge when nanoscale objects, such as gold nanoparticles or quantum dots, are arranged in small clusters offer great opportunities for energy-related applications. Unfortunately, conventional solution-based reaction methods are quite limited and inefficient, e.g., producing clusters with a broad distribution of sizes and compositions. CFN researchers have developed a novel method for producing dimmers of DNA-encoded nanoparticles with remarkably high yields. The method, which incorporates two different DNA strands on a single nanoparticle, was employed to assemble both homogenous (gold-gold) and heterogeneous (gold-

silver) nanoparticle dimmers with novel nanoscale optical properties. Because this method is scalable to large quantities with more complex cluster arrangements, it may become a practical way of inexpensively fabricating predictable and reliable nanostructures with customized properties.

- *Spallation Neutron Source Set Another World Record*. On July 11, 2009, SNS researchers set a new world record by creating 155 trillion protons in a single pulse and delivering that pulse to the SNS mercury target. This test exceeds the SNS design intensity of 150 trillion protons in a pulse. If pulses of this intensity were delivered to the SNS target at the design repetition rate of 60 pulses per second, it would provide a beam power of 1.5 megawatts—0.1 megawatts more than the design beam power of 1.4 megawatts. The SNS facility has already been operated at close to the megawatt level. The test, performed at a rate of less than one pulse per second, confirms that the SNS linear accelerator and accumulator ring—two vital components that supply the proton beam pulses—will meet and exceed the 1.4 megawatt design criteria.
- *New Technique Developed at Electron Microscopy Center.* Magnetic structure in discrete particles and complex assemblages is important in a variety of fields, particularly information storage technologies. A new approach to characterize such structures has been developed, based on the energy losses of high-energy electrons when they traverse a material and interact with spin-charge structures. The technique, electron magnetic linear dichroism, has been demonstrated by mapping the temperature and angular dependence of the signal in hematite, a form of iron oxide. The approach complements similar linear dichroism approaches that have been developed and utilized at synchrotron x-ray facilities; data quality is comparable, and the new technique extends the spatial resolution of the information into the nanoscale.

Detailed Program Justification

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Research	**0**	**32,525**	**27,339**
▪ **Electron-beam Microcharacterization**	**0**	**11,571**	**11,809**

This activity supports three electron-beam microcharacterization centers, which operate as user facilities, work to develop next-generation electron-beam instrumentation, and conduct corresponding research. These centers are the Electron Microscopy Center for Materials Research at Argonne National Laboratory (ANL), the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory (LBNL), and the Shared Research Equipment program at Oak Ridge National Laboratory (ORNL). Operating funds are provided to enable expert scientific interaction and technical support and to administer a robust user program at these facilities, which are made available to all researchers with access determined via peer review of brief proposals. Capital equipment funding is provided for instruments such as scanning, transmission, and scanning transmission electron microscopes; atom probes and related field ion instruments; related surface characterization apparatus and scanning probe microscopes; and/or ancillary tools such as spectrometers, detectors, and advanced sample preparation equipment.

Electron scattering has key attributes that give such approaches unique advantages and make them complementary to x-ray and neutron beam techniques. These characteristics include strong interactions with matter (allowing the capture of meaningful signals from very small amounts of material, including single atoms under some circumstances) and the ability to readily focus the

	(dollars in thousands)	
FY 2009	FY 2010	FY 2011

charged electron beams using electromagnetic lenses. The net result is unsurpassed spatial resolution and the ability to simultaneously get structural, chemical, and other types of information from subnanometer regions, allowing study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. All of these are fundamental to understanding and improving materials for energy applications and the associated physical characteristics and changes that govern performance.

In FY 2011, full user operations continue at all three of these facilities, which are routinely available to users during normal working hours. The Transmission Electron Aberration Corrected Microscope (TEAM) instrument at the National Center for Electron Microscopy at LBNL will, in addition, be available to the research community 24 hours a day. This instrument was developed as a DOE Major Item of Equipment project and completed in FY 2009. It leads the world in spatial resolution and embodies the first chromatic aberration corrector in an instrument of this kind, and thus its availability opens new frontiers in imaging of materials on the nanoscale for the broad scientific community. Further research and technique development proceeds using this and other instruments at the Electron Beam Microcharacterization Centers on high-resolution imaging, atomic scale tomography, *in situ* experimentation within electron microscopes, strain and segregation in individual nanostructures, and many other related topics.

In FY 2009, $11,313,000 was provided for this activity in the Materials Sciences and Engineering Research Subprogram.

	FY 2009	FY 2010	FY 2011
▪ **Accelerator and Detector Research**	**0**	**13,061**	**15,530**

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Accelerator research is the corner stone for the development of new technologies that will improve performance of light sources and neutron spallation facilities. This research will explore new areas of science and technologies that will facilitate the construction of next generation accelerator-based user facilities. Detector research is a crucial, but often overlooked, component in the optimal utilization of user facilities. This research program is investing aggressively in research leading to a new and more efficient generation of photon and neutron detectors. Research includes studies on creating, manipulating, transporting, and diagnosing ultra-high brightness beam behavior from its origin at a photocathode to its travel through undulators. Studies on achieving sub-femtosecond (hundreds of attoseconds) free electron laser (FEL) pulses will also be underway. Demonstration experiments will take place in advanced FEL seeding techniques, such as echo-enhanced harmonic generation and other optical manipulation to reduce the cost and complexity of seeding harmonic generation FELs. A very high frequency laser photocathode radio frequency (RF) gun using a room temperature cavity will be developed which can influence the design of linac-based FELs with megahertz rates. Research will also occur on construction and beam testing of a high current, high gradient compact superconducting linac which can serve as a prototype for future light sources. Studies will continue on collective electron effects, such as micro-bunch instabilities from coherent synchrotron and edge radiation; beam bunching techniques, such as magnetic compression or velocity bunching; fast instruments to determine the structure of femtosecond electron bunches; and detectors capable of acquiring x-ray and neutron scattering data at very high collection rates.

This activity interacts with BES scientific research that employs synchrotron and neutron sources. It also coordinates with other DOE offices, especially in the funding of capabilities whose cost and

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

complexity require shared support. Research at the Accelerator Test Facility at Brookhaven National Laboratory is jointly funded by the High Energy Physics and BES programs. There is also planned collaboration with the National Science Foundation (NSF) on energy recovery linac (ERL) research. There is a coordinated effort between DOE and NSF to facilitate x-ray detector development. There are ongoing industrial interactions through the DOE Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) programs for the development of x-ray detectors and advanced accelerator technology.

Additional funds provided in FY 2011 will increase selected R&D activities related to light sources. These include the physics of gain mechanisms in FELs, rapid electron bunch diagnostics, advanced x-ray and neutron detectors, H^- high intensity sources, and accelerator modeling. These projects are essential to the efficient operation and use of present BES x-ray and neutron scattering facilities and to the design of future facilities.

In FY 2009, $9,794,000 was provided for this activity in the Materials Sciences and Engineering Research Subprogram.

▪ **General Plant Projects (GPP)**	**0**	**7,893**	**0**

GPP funding is provided in FY 2010 for the ORNL Guest House. The Guest House is designed to meet the needs of the guest users coming to perform research at ORNL's world class DOE scientific user facilities (SNS, CNMS, HFIR, SHaRE, etc.). No funds are requested in FY 2011.

Major Items of Equipment	**0**	**25,000**	**22,400**
▪ **Spallation Neutron Source Instrumentation I (SING I)**	**0**	**5,000**	**400**

Funds are provided to complete a Major Item of Equipment with a total estimated cost and total project cost of $68,500,000 for five instruments for the Spallation Neutron Source (SNS). The instrument concepts for the project were competitively selected using a peer review process, and the instruments are being installed at the SNS on a phased schedule between FY 2008–2011.

In FY 2009, $12,000,000 was provided for this activity in the Materials Sciences and Engineering Research Subprogram.

▪ **Spallation Neutron Source Instrumentation II (SING II)**	**0**	**18,000**	**17,000**

Funds are provided to continue a Major Item of Equipment with a total estimated cost and total project cost of $60,000,000 to fabricate four instruments to be installed at the SNS. The instrument concepts for the project have been competitively selected using a peer review process. The project is managed by Oak Ridge National Laboratory. It is anticipated that these instruments will be installed at the SNS on a phased schedule beginning in about FY 2012. The SING II instruments are in addition to the five instruments to be provided by the SING I MIE. The TPC is now approved at the Approve Performance Baseline, CD-2, for three of the four instruments. The FY 2011 request is to complete engineering design of the final instrument and to continue fabrication of the others.

In FY 2009, $7,000,000 was provided for this activity in the Materials Sciences and Engineering Research Subprogram.

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
▪ **SNS Power Upgrade Project (PUP)**	**0**	**2,000**	**5,000**

Funds are provided for a Major Item of Equipment with a preliminary Total Project Cost range of $89,600,000–$96,100,000 for activities to design, build, install, and test the equipment necessary to increase the Spallation Neutron Source (SNS) proton beam energy. CD-1 was approved on January 16, 2009. In addition to the improvements in performance of instruments at the existing high power target station, this power upgrade will enable the eventual construction of a second target station. The existing facility layout and much of the existing SNS equipment was designed and built to meet the requirements of this upgrade.

The power upgrade project increases the linac beam energy from 1 GeV to 1.3 GeV. This will be accomplished by adding nine additional high beta cryomodules into the remaining nine open slots in the east end of the superconducting section of the linac. These additional cryomodule units will increase the number of high beta units from twelve to twenty one, allowing the energy to increase. The accelerator tunnel structure and cryogenic system were constructed to allow this upgrade.

FY 2010 is the first year of funding for this project. The FY 2011 request supports engineering design of the accelerator sub-systems and project management.

Facilities Operations	**0**	**730,621**	**775,823**

This activity supports the operation of the BES scientific user facilities, which consist of light sources, neutron sources, nanoscience centers, and the Linac Coherent Light Source free electron laser at SLAC. These forefront research facilities require resource commitments well beyond the scope of any non-government institution and open up otherwise inaccessible facets of Nature to scientific inquiry. The BES user facilities provide open access to specialized instrumentation and expertise that enable scientific users from universities, national laboratories, and industry to carry out experiments and develop theories that could not be done at their home institutions. For approved, peer-reviewed projects, operating time is available without charge to researchers who intend to publish their results in the open literature. These large-scale user facilities—many of which were justified and built to serve a specific discipline of the physical sciences—have made significant contributions to many other fields of importance, including biology and medicine. The number of users for the synchrotron radiation sources and neutron scattering facilities are shown at the end of this subprogram description, and the number of users for all BES facilities, FY 2000–2009, is provided at http://www.sc.doe.gov/bes/users.htm. The web sites for all of the BES user facilities are available at http://www.sc.doe.gov/bes/BESfacilities.htm.

In FY 2011, operation of these scientific user facilities is funded at a level that will permit near optimal service to users. Additional funds are provided in FY 2011 for the first year of full operation of the LCLS at SLAC and for enhanced capabilities and user support at the new SNS and HFIR neutron beamlines. The light source budget increases reflect the increase in the number of operating beamlines, user support and instrumentation to upgrade beamlines at these facilities. Increases in the NSRC budgets reflect full functionality and staffing of the five NSRCs. Other project costs are provided for the National Synchrotron Light Source II at BNL. The Intense Pulsed Neutron Source is closed as a result of competing priorities, and funds are provided to begin the decommissioning of the target assembly.

In FY 2009, $689,047,000 was provided for this activity in the Materials Sciences and Engineering Research Subprogram.

	FY 2009	FY 2010	FY 2011
(dollars in thousands)			

The facility operations budget request includes operating funds, capital equipment, and accelerator and reactor improvement project (AIP) funding under $5,000,000. AIP funding will support additions and modifications to accelerator and reactor facilities. General plant project (GPP) funding is also required for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed $10,000,000. Capital equipment is needed to maintain optimal operation at the facilities. Items include beam monitors, interlock systems, vacuum systems, beam line front end components, optical components, and new equipment at the NSRCs. A summary of the funding for the facilities is provided below.

	FY 2009	FY 2010	FY 2011
All Facilities			
Achieved Operating Hours	30,995	N/A	N/A
Planned Operating Hours	31,800	34,000	38,000
Optimal Hours	34,000	34,000	39,000
Percent of Optimal Hours	91%	100%	97%
Unscheduled Downtime	6%	<10%	<10%
Number of Users	11,509	12,780	13,560

	FY 2009	FY 2010	FY 2011
▪ **Synchrotron Radiation Light Sources**	**0**	**366,974**	**403,613**
Advanced Light Source, LBNL	0	58,000	62,716
Advanced Photon Source, ANL	0	129,500	139,651
National Synchrotron Light Source, BNL	0	40,200	41,170
Stanford Synchrotron Radiation Light Source, SLAC	0	34,774	37,076
Linac Coherent Light Source (LCLS), SLAC	0	10,500	123,000
Linac for LCLS, SLAC	0	94,000	0

The unique properties of synchrotron radiation include its continuous spectrum, high flux and brightness, and in the case of the Linac Coherent Light Source, high coherence, which makes it an indispensable tool in the exploration of matter. The wavelengths of the emitted photons span a range of dimensions from the atom to biological cells, thereby providing incisive probes for advanced research in a wide range of areas, including materials science, physical and chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences.

Researchers use a variety of experimental techniques when applying synchrotron radiation to their own problems. The fundamental parameters that we use to perceive the physical world (energy, momentum, position, and time) correspond to three broad categories of synchrotron experimental measurement techniques: spectroscopy, scattering, and imaging. By exploiting the short pulse lengths of synchrotron radiation, each technique can also be performed in a timing fashion.

	(dollars in thousands)	
FY 2009	FY 2010	FY 2011

In FY 2011 funds are provided to continue operations of the synchrotron radiation light sources. Additional funding is provided in FY 2011 for research and development associated with improvements in the Advanced Photon Source storage ring for future performance enhancement. In addition, funds are provided for research and development, leading to new and improved scattering beam lines for the 3rd generation light sources. The budget also reflects a significant increase in the beam line and accelerator operations hours as well as user support at the LCLS as it ramps up its user program in its first full year of operations. Increased funding is also provided for instrumentation to upgrade BES beamlines at the light source facilities. Capital equipment is needed at the facilities for items such as beam monitors, interlock systems, vacuum transport systems, beamline front ends, optical components and detectors.

In FY 2009, $338,755,000 was funded in the Materials Sciences and Engineering Research subprogram as follows: $55,728,000 at the Advanced Light Source, LBNL; $116,440,000 at the Advanced Photon Source, ANL; $40,154,000 at the National Synchrotron Light Source, BNL; $33,412,000 at the Stanford Synchrotron Radiation Light Source, SLAC; $3,000,000 at the Linac Coherent Light Source (LCLS), SLAC; and $90,021,000 at the Linac for LCLS, SLAC.

	FY 2009	FY 2010	FY 2011
Advanced Light Source			
Achieved Operating Hours	5,278	N/A	N/A
Planned Operating Hours	5,400	5,600	5,600
Optimal Hours	5,600	5,600	5,600
Percent of Optimal Hours	94%	100%	100%
Unscheduled Downtime	3.5%	<10%	<10%
Number of Users	1,918	2,200	2,300
Advanced Photon Source			
Achieved Operating Hours	4,883	N/A	N/A
Planned Operating Hours	4,800	5,000	5,000
Optimal Hours	5,000	5,000	5,000
Percent of Optimal Hours	98%	100%	100%
Unscheduled Downtime	2.3%	<10%	<10%
Number of Users	3,537	3,700	3,800

		(dollars in thousands)	
	FY 2009	FY 2010	FY 2011

	FY 2009	FY 2010	FY 2011
National Synchrotron Light Source			
Achieved Operating Hours	5,499	N/A	N/A
Planned Operating Hours	5,200	5,400	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	102%	100%	100%
Unscheduled Downtime	2.6%	<10%	<10%
Number of Users	2,214	2,200	2,200
Stanford Synchrotron Radiation Light Source			
Achieved Operating Hours	5,050	N/A	N/A
Planned Operating Hours	5,000	5,400	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	94%	100%	100%
Unscheduled Downtime	1%	<10%	<10%
Number of Users	1,361	1,400	1,400
Linac Coherent Light Source			
Achieved Operating Hours	0	0	N/A
Planned Operating Hours	0	0	4,000
Optimal Hours	0	0	5,000
Percent of Optimal Hours	0	0	80%
Unscheduled Downtime	0	0	<10%
Number of Users	0	0	250

	FY 2009	FY 2010	FY 2011
▪ **High-Flux Neutron Sources**	**0**	**258,980**	**262,736**
High Flux Isotope Reactor, ORNL	0	60,700	61,390
Intense Pulsed Neutron Source, ANL	0	4,000	3,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	0	11,350	11,821
Spallation Neutron Source, ORNL	0	182,930	186,525

Neutrons are a unique and effective tool for probing the structure of matter. Beams of neutrons are particularly well-suited for measurement of the positions as well as the fluctuations in the positions of atomis (phonons), and the structure (position and direction) of atomic magnetic moments in solids and the excitations in their magnetic structure (spin waves). Such studies allow physicists to

	FY 2009	FY 2010	FY 2011

(dollars in thousands)

take measurements leading to an understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of materials.

In FY 2011 funds are provided to continue operations of the neutron sources. Additional funds are provided in FY 2011 for new operating beamlines at the Spallation Neutron Source and the High Flux Isotope Reactor at ORNL. The Intense Pulsed Neutron Source is closed and funds are provided to continue decommissioning of the target assembly.

In FY 2009, $249,802,000 was funded in the Materials Sciences and Engineering Research subprogram as follows: $58,000,000 at the High Flux Isotope Reactor, ORNL; $4,000,000 at the Intense Pulsed Neutron Source, ANL; $11,302,000 at the Manuel Lujan, Jr. Neutron Scattering Center, LANL; and $176,500,000 at the Spallation Neutron Source, ORNL.

	FY 2009	FY 2010	FY 2011
High Flux Isotope Reactor			
Achieved Operating Hours	3,892	N/A	N/A
Planned Operating Hours	3,900	4,500	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	86%	100%	100%
Unscheduled Downtime	0%	<10%	<10%
Number of Users	358	500	600
Manuel Lujan, Jr. Neutron Scattering Center			
Achieved Operating Hours	2,840	N/A	N/A
Planned Operating Hours	3,500	3,600	3,600
Optimal Hours	3,600	3,600	3,600
Percent of Optimal Hours	79%	100%	100%
Unscheduled Downtime	18.1%	<10%	<10%
Number of Users	416	400	400
Spallation Neutron Source			
Achieved Operating Hours	3,553	N/A	N/A
Planned Operating Hours	4,000	4,500	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	79%	100%	100%
Unscheduled Downtime	19.5%	<10%	<10%
Number of Users	307	700	750

	FY 2009	FY 2010	FY 2011
	(dollars in thousands)		
▪ **Nanoscale Science Research Centers (NSRCs)**	**0**	**104,667**	**109,474**
Center for Nanophase Materials Sciences, ORNL	0	20,641	21,595
Center for Integrated Nanotechnologies, SNL/LANL	0	20,790	21,748
Molecular Foundry, LBNL	0	20,833	21,792
Center for Nanoscale Materials, ANL	0	21,570	22,547
Center for Functional Nanomaterials, BNL	0	20,833	21,792

The NSRCs are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. The centers are housed in recently-constructed and custom-designed laboratory buildings near one or more other major BES facilities for x-ray, neutron, or electron scattering, which complement and leverage the capabilities of the NSRCs.
These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. These facilities are routinely made available to the research community during normal working hours. In FY 2011 funds are provided to continue operations for all five NSRCs.

In FY 2009, $100,490,000 was funded in the Materials Sciences and Engineering Research subprogram as follows: $19,900,000 at the Center for Nanophase Materials Sciences, ORNL; $19,950,000 at the Center for Integrated Nanotechnologies, SNL/LANL; $20,000,000 at the Molecular Foundry, LBNL; $20,640,000 at the Center for Nanoscale Materials, ANL; and $20,000,000 for the Center for Functional Nanomaterials, BNL.

	FY 2009	FY 2010	FY 2011
Number of Users[a]			
Center for Nanophase Materials Sciences	317	350	380
Center for Integrated Nanotechnologies	354	380	400
Molecular Foundry	209	300	350
Center for Nanoscale Materials	305	350	380
Center for Functional Nanomaterials	213	300	350

[a] Facility operating hours are not measured at user facilities that do not rely on one central machine.

	FY 2009	FY 2010	FY 2011
Other Project Costs	**0**	**13,500**	**1,500**
National Synchrotron Light Source-II, BNL	0	2,000	1,500
Linac Coherent Light Source (LCLS), SLAC	0	11,500	0

(dollars in thousands)

Other Project Costs (OPC) are associated with line-item construction or major item of equipment projects and include all project costs that are not identified in the Total Estimated Cost. Total Estimated Cost includes project costs incurred after Critical Decision-1 such as costs associated with the acquisition of land and land rights; engineering, design, and inspection; direct and indirect construction/fabrication; and the initial equipment necessary to place the plant or installation in operation. Generally, OPC are costs incurred during the project's initiation and definition phase for planning, conceptual design, research and development, and during the execution phase for research and development, startup, and operation. Other Project Costs are always operating funds.

Funds are provided in FY 2011 for other project costs associated with the National Synchrotron Light Source-II, BNL.

In FY 2009, $27,044,000 was funded in the Materials Sciences and Engineering Research subprogram as follows: $17,000,000 for the Linac Coherent Light Source, SLAC, $40,000 for the Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC, $4,000 for the Advanced Light Source User Support Building, LBNL and $10,000,000 for the National Synchrotron Light Source–II, BNL.

	FY 2009	FY 2010	FY 2011
SBIR/STTR	**0**	**20,038**	**20,059**

The FY 2010 and FY 2011 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR programs.

	FY 2009	FY 2010	FY 2011
Total, Scientific User Facilities	**0**	**821,684**	**847,121**

Explanation of Funding Changes

	FY 2011 vs. FY 2010 ($000)
Research	
▪ **Electron-beam Microcharacterization**	
Increase is provided for enhanced user operations within the current operating schedules of the facilities, scientific research of facility staff, and development of new instruments or techniques at the facilities.	+238
▪ **Accelerator and Detector Research**	
Increase is provided to expand the portfolio of accelerator and detector research projects, including the physics of gain mechanisms in free electron lasers (FELs), rapid electron bunch diagnostics, advanced x-ray and neutron detectors, H^- high intensity sources, and accelerator modeling.	+2,469

	FY 2011 vs. FY 2010 ($000)
▪ **General Plant Project**	
No GPP is requested in FY 2011. Funding for the ORNL Guest House project is completed in FY 2010.	-7,893
Total Research	**-5,186**
Major Items of Equipment	
▪ **Spallation Neutron Source Instrumentation I**	
Scheduled decrease for the Major Item of Equipment for the Spallation Neutron Source Instrumentation I.	-4,600
▪ **Spallation Neutron Source Instrumentation II**	
Scheduled decrease for the Major Item of Equipment for the Spallation Neutron Source Instrumentation II.	-1,000
▪ **SNS Power Upgrade Project**	
Scheduled increase for the Major Item of Equipment for the SNS Power Upgrade Project	+3,000
Total, Major Items of Equipment	**-2,600**
Facilities Operations	
▪ **Synchrotron Radiation Light Sources**	
• Increase for the Advanced Light Source to support accelerator operations and users and to provide instrumentation to upgrade BES beamlines.	+4,716
• Increase for Advanced Photon Source to support accelerator operations and users, for research and development associated with improvements in the APS storage ring for future performance enhancement, and to provide instrumentation to upgrade BES beamlines.	+10,151
• Increase for National Synchrotron Light Source to support accelerator operations and users, for research and development leading to new and improved scattering beam lines for the 3rd generation light sources, and to provide instrumentation to upgrade BES beamlines.	+970
• Increase for the Stanford Synchrotron Radiation Light Source to support accelerator operations and users and to provide instrumentation to upgrade BES beamlines.	+2,302
• Increase for the Linac Coherent Light Source to begin the first full year of operations in FY 2011.	+18,500
Total, Synchrotron Radiation Light Sources	**+36,639**

	FY 2011 vs. FY 2010 ($000)
▪ **High-Flux Neutron Sources**	
• Increase for High Flux Isotope Reactor for new operating beamlines and to support reactor operations.	+690
• Decrease for the Intense Pulsed Neutron Source to continue decommissioning of the target assembly.	-1,000
• Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and users.	+471
• Increase for Spallation Neutron Source for new operating beamlines and to support operations and users.	+3,595
Total, High-Flux Neutron Sources	**+3,756**
▪ **Nanoscale Science Research Centers**	
• Increase for the Center for Nanophase Materials to support operations and users.	+954
• Increase for the Center for Integrated Nanotechnologies to support operations and users.	+958
• Increase for the Molecular Foundry to support operations and users.	+959
• Increase for the Center to Nanoscale Materials to support operations and users.	+977
• Increase for the Center for Functional Nanomaterials to support operations and users.	+959
Total, Nanoscale Science Research Centers	**+4,807**
Total, Facilities Operations	**+45,202**
Other Project Costs	
▪ Decrease for National Synchrotron Light Source-II per the project schedule.	-500
▪ Decrease for Linac Coherent Light Source per the project schedule.	-11,500
Total, Other Project Costs	**-12,000**
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expenses.	+21
Total Funding Change, Scientific User Facilities	**+25,437**

Construction

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Construction			
Advanced Light Source User Support Building, LBNL	11,500	0	0
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	3,728	0	0
National Synchrotron Light Source-II, BNL	93,273	139,000	151,600
Linac Coherent Light Source, SLAC	36,967	15,240	0
Total, Construction	145,468	154,240	151,600

Description

Experiments in support of basic research require construction of state-of-the-art facilities and/or that existing facilities be modified to meet unique research requirements. Reactors, x-ray light sources, and pulsed neutron sources are among the expensive, but necessary, facilities used. The budget for the BES program includes funding for the construction and modification of these facilities.

The new facilities that are in design or under construction—the Linac Coherent Light Source and the National Synchrotron Light Source-II—continue the tradition of BES and SC providing the most advanced scientific user facilities for the nation's research community in the most cost effective way. All of the BES construction projects are conceived and planned with the broad user community and, during construction, are maintained on schedule and within cost. Furthermore, the construction projects all adhere to the highest standards of safety. These facilities will provide the research community with the tools to fabricate, characterize, and develop new materials and chemical processes to advance basic and applied research across the full range of scientific and technological endeavor, including chemistry, physics, earth science, materials science, environmental science, biology, and biomedical science.

Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet.

Detailed Justification

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Advanced Light Source (ALS) User Support Building, LBNL	**11,500**	**0**	**0**

The ALS User Support Building (USB) will provide high-quality user support space in sufficient quantity to accommodate the significant growth during the past decade in both the number of beamlines and the number of ALS users and to accommodate projected future expansion. The USB will provide staging areas for ALS experiments, including valuable high-bay space, wet laboratories, and temporary office space for visiting users.

The FY 2009 construction funding was used to award contract(s) as appropriate and continue the design-build construction project efforts. In addition, the project will remediate contaminated soils discovered on the project site during foundation activities. FY 2009 Recovery Act funding is used to remobilize the

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011

design-build construction contractor, erect the steel, complete exterior cladding, and commence interior construction project efforts. The combination of the FY 2009 Appropriations and the Recovery Act funds fully funds this project.

Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	**3,728**	**0**	**0**

Photon Ultrafast Laser Science and Engineering (PULSE) is the new center for ultrafast science at the SLAC National Accelerator Laboratory. PULSE represents a major research activity at SLAC that is a key component of the shift in the emphasis of the laboratory from high energy physics to a multi-program laboratory with significant activities in photon science. The PULSE Center is located in the Central Laboratory building (B040), a mixed use building of laboratories, offices, meeting rooms, and a library. Approximately 18,000 square feet of existing space in the two-story wing of the Central Laboratory building was renovated to meet the new PULSE programs needs for offices, laboratories, and conference rooms. FY 2009 funding was used to complete construction of PULSE.

National Synchrotron Light Source-II (NSLS-II), BNL	**93,273**	**139,000**	**151,600**

The National Synchrotron Light Source-II (NSLS-II) will be a new synchrotron light source highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of about 1 nm, an energy resolution of about 0.1 meV, and the ultra-high sensitivity required to perform spectroscopy on a single molecule. The NSLS-II project will design, build, and install the accelerator hardware, experimental apparatus, civil construction, and central facilities, including offices and laboratories required to produce a new synchrotron light source. It includes a third generation storage ring, full energy injector, experimental areas, an initial suite of scientific instruments, and appropriate support equipment, all housed in a new building.

In FY 2009, construction funding was used to start the civil construction activities and progress on the NSLS-II systems components (e.g., magnet development, storage ring vacuum chambers, and radio frequency systems). In FY 2009, Recovery Act funds were used to accelerate the ring building civil construction contract activities and several major infrastructure improvements that support the NSLS-II project.

In FY 2010, construction funding will be used to continue civil construction activities and advance experimental and accelerator systems.

In FY 2011, construction funding will be used to continue civil construction activities and advance experimental and accelerator systems. Additional information is provided in the construction project data sheet 07-SC-06.

Beyond the scope of the NSLS-II construction project, an instrument development program will be implemented in the near future to address new advanced experimental techniques that will go beyond the six initial instruments funded by the project.

Linac Coherent Light Source, SLAC	**36,967**	**15,240**	**0**

The Linac Coherent Light Source (LCLS) Project will provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak brightness than any existing coherent x-ray light

	FY 2009	FY 2010	FY 2011

(dollars in thousands)

source. The LCLS Project will provide the first demonstration of an x-ray free electron laser (FEL) in the 1.5-15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems described below. This will be the world's first such facility. The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called table-top x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing 10^{11} x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific application in the chemical, material, and biological sciences.

In FY 2009, funding was used for installation of undulator and photon diagnostics, experimental halls, and technical hardware for x-ray transport systems. In addition, SLAC commenced a design and initiated construction of a user office builder adjacent to the near experimental hall to provide space in support of the LCLS operations in lieu of renovating of existing older buildings at SLAC. This user building adjacent to the near experimental hall provided a more cost effective and efficient solution to addressing the user office space needs than renovating old space at various buildings in SLAC. Commissioning of the facility will also continue on a phased schedule. In FY 2010, funds will complete construction and commissioning elements of the project. FY 2011 is expected to be the first full year of LCLS facility operations.

Total, Construction	**145,468**	**154,240**	**151,600**

Explanation of Funding Changes

	FY 2011 vs. FY 2010 ($000)
National Synchrotron Light Source-II (NSLS II), BNL	
Increase in funding to continue construction of the NSLS II project, as scheduled.	+12,600
Linac Coherent Light Source, SLAC	
Decrease in funding representing the completion of construction funding in FY 2010, as scheduled.	-15,240
Total Funding Change, Construction	**-2,640**

Supporting Information

Operating Expenses, Capital Equipment and Construction Summary

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Operating Expenses	1,256,023	1,334,500	1,492,137
Capital Equipment	100,916	100,068	151,637
General Plant Projects	11,848	13,992	2,364
Accelerator Improvement Projects	21,510	33,700	37,262
Construction	145,468	154,240	151,600
Total, Basic Energy Sciences	1,535,765	1,636,500	1,835,000

Funding Summary

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Research	632,758	663,114	841,006
Scientific User Facilities Operations	689,047	730,621	775,823
Major Items of Equipment	34,000	25,000	22,400
Construction Projects (includes OPC)	172,512	167,740	153,100
Other	7,448	50,025	42,671
Total, Basic Energy Sciences	1,535,765	1,636,500	1,835,000

Scientific User Facility Operations

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Light Source User Facilities			
Advanced Light Source, LBNL	55,728	58,000	62,716
Advanced Photon Source, ANL	116,440	129,500	139,651
National Synchrotron Light Source, BNL	40,154	40,200	41,170
Stanford Synchrotron Radiation Light Source, SLAC	33,412	34,774	37,076
Linac Coherent Light Source (LCLS), SLAC	3,000	10,500	123,000
Linac for LCLS, SLAC	90,021	94,000	0
Total, Light Sources User Facilities	338,755	366,974	403,613
Neutron Source User Facilities			
High Flux Isotope Reactor, ORNL	58,000	60,700	61,390
Intense Pulsed Neutron Source, ANL	4,000	4,000	3,000

	(dollars in thousands)		
	FY 2009	FY 2010	FY 2011
Manuel Lujan, Jr. Neutron Scattering Center, LANL	11,302	11,350	11,821
Spallation Neutron Source, ORNL	176,500	182,930	186,525
Total, Neutron Source User Facilities	249,802	258,980	262,736
Nanoscale Science Research Center User Facilities			
Center for Nanophase Materials Sciences, ORNL	19,900	20,641	21,595
Center for Integrated Nanotechnologies, SNL/LANL	19,950	20,790	21,748
Molecular Foundry, LBNL	20,000	20,833	21,792
Center for Nanoscale Materials, ANL	20,640	21,570	22,547
Center for Functional Nanomaterials, BNL	20,000	20,833	21,792
Total, Nanoscale Science Research Center User Facilities	100,490	104,667	109,474
Total, Scientific User Facility Operations	689,047	730,621	775,823

Facilities Users and Hours

	FY 2009	FY 2010	FY 2011
Advanced Light Source			
Achieved Operating Hours	5,278	N/A	N/A
Planned Operating Hours	5,400	5,600	5,600
Optimal Hours	5,600	5,600	5,600
Percent of Optimal Hours	94%	100%	100%
Unscheduled Downtime	3.5%	<10%	<10%
Number of Users	1,918	2,200	2,300
Advanced Photon Source			
Achieved Operating Hours	4,883	N/A	N/A
Planned Operating Hours	4,800	5,000	5,000
Optimal Hours	5,000	5,000	5,000
Percent of Optimal Hours	98%	100%	100%
Unscheduled Downtime	2.3%	<10%	<10%
Number of Users	3,537	3,700	3,800

	FY 2009	FY 2010	FY 2011
National Synchrotron Light Source			
Achieved Operating Hours	5,499	N/A	N/A
Planned Operating Hours	5,200	5,400	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	102%	100%	100%
Unscheduled Downtime	2.6%	<10%	<10%
Number of Users	2,214	2,200	2,200
Stanford Synchrotron Radiation Light Source			
Achieved Operating Hours	5,050	N/A	N/A
Planned Operating Hours	5,000	5,400	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	94%	100%	100%
Unscheduled Downtime	1%	<10%	<10%
Number of Users	1,361	1,400	1,400
Linac Coherent Light Source			
Achieved Operating Hours	0	0	N/A
Planned Operating Hours	0	0	4,000
Optimal Hours	0	0	5,000
Percent of Optimal Hours	0	0	80%
Unscheduled Downtime	0	0	<10%
Number of Users	0	0	250
High Flux Isotope Reactor			
Achieved Operating Hours	3,892	N/A	N/A
Planned Operating Hours	3,900	4,500	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	86%	100%	100%
Unscheduled Downtime	0%	<10%	<10%
Number of Users	358	500	600

	FY 2009	FY 2010	FY 2011
Manuel Lujan, Jr. Neutron Scattering Center			
Achieved Operating Hours	2,840	N/A	N/A
Planned Operating Hours	3,500	3,600	3,600
Optimal Hours	3,600	3,600	3,600
Percent of Optimal Hours	79%	100%	100%
Unscheduled Downtime	18.1%	<10%	<10%
Number of Users	416	400	400
Spallation Neutron Source			
Achieved Operating Hours	3,553	N/A	N/A
Planned Operating Hours	4,000	4,500	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	79%	100%	100%
Unscheduled Downtime	19.5%	<10%	<10%
Number of Users	307	700	750
Center for Nanophase Materials Sciences[a]			
Number of Users	317	350	380
Center for Integrated Nanotechnologies[a]			
Number of Users	354	380	400
Molecular Foundry[a]			
Number of Users	209	300	350
Center for Nanoscale Materials[a]			
Number of Users	305	350	380
Center for Functional Nanomaterials[a]			
Number of Users	213	300	350

[a] Facility operating hours are not measured at user facilities that do not rely on one central machine.

	FY 2009	FY 2010	FY 2011
Total, All Facilities			
Achieved Operating Hours	30,995	N/A	N/A
Planned Operating Hours	31,800	34,000	38,000
Optimal Hours	34,000	34,000	39,000
Percent of Optimal Hours	91%	100%	97%
Unscheduled Downtime	6%	<10%	<10%
Number of Users	11,509	12,780	13,560

Major Items of Equipment

(dollars in thousands)

	Prior Years	FY 2009	FY 2009 Recovery Act Approp.	FY 2010	FY 2011	Outyears	Total
Spallation Neutron Source Instrumentation I, ORNL							
TEC/TPC	51,100	12,000	0	5,000	400	0	68,500
Spallation Neutron Source Instrumentation II, ORNL							
TEC/TPC	6,500	7,000	0	18,000	17,000	11,500	60,000
Linac Coherent Light Source Instrumentation, SLAC							
TEC	6,500	15,000	33,600	0	0	0	55,100
OPC	4,900	0	0	0	0	0	4,900
TPC	11,400	15,000	33,600	0	0	0	60,000
SNS Power Upgrade Project (01VI), ORNL							
TEC/TPC	0	0	0	2,000	5,000	89,100	96,100
Total, Major Items of Equipment							
TEC/TPC		34,000	33,600	25,000	22,400		

Construction Projects

(dollars in thousands)

	Prior Years	FY 2009	FY 2009 Additional	FY 2010	FY 2011	Outyears	Total
08-SC-01 Advanced Light Source User Support Building, LBNL							
TEC	6,454	11,500	14,546	0	0	0	32,500[a]
OPC	2,480	4	136	0	0	0	2,620
TPC	8,934	11,504	14,682	0	0	0	35,120
08-SC-11 Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC							
TEC	7,332	3,728	0	0	0	0	11,060[b]
OPC	100	40	0	0	0	0	140
TPC	7,432	3,768	0	0	0	0	11,200
07-SC-06, National Synchrotron Light Source-II, BNL							
TEC	32,727	93,273	150,000	139,000	151,600	224,600	791,200
OPC	47,800	10,000	0	2,000	1,500	59,500	120,800
TPC	80,527	103,273	150,000	141,000	153,100	284,100	912,000
05-R-320 Linac Coherent Light Source, SLAC							
TEC	299,793	36,967	0	15,240	0	0	352,000[c]
OPC	39,500	17,000	0	11,500	0	0	68,000
TPC	339,293	53,967	0	26,740	0	0	420,000
Total, Construction							
TEC		145,468	164,546	154,240	151,600		
OPC		27,044	136	13,500	1,500		
TPC		172,512	164,682	167,740	153,100		

[a] Includes $1,500,000 of PED included in the 07-SC-12 PED, LBNL Advanced Light source User Support Building data sheet.
[b] Includes $941,000 of PED included in the 08-SC-10 PED, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC data sheet.
[c] Includes $35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source data sheet.

Scientific Employment

	FY 2009 Estimate	FY 2010 Estimate	FY 2011Estimate
# of University Grants	1,180	1,210	1,400
Average Size per year	175,000	175,000	215,000
# Permanent Ph.D's (FTEs)	4,560	4,670	5,590
# Postdoctoral Associates (FTEs)	1,270	1,300	1,620
# Graduate Students (FTEs)	2,000	2,050	2,570