Basic Energy Sciences

Funding Profile by Subprogram (Non-Comparable, or as Appropriated, Structure)

(dollars in thousands)

	FY 2008 Current Appropriation	FY 2009 Original Appropriation	FY 2009 Adjustments	FY 2009 Current Appropriation	FY 2009 Additional Appropriation[a]	FY 2010 Request
Basic Energy Sciences						
Materials Sciences and Engineering	942,744	1,129,391	+4,243[b]	1,133,634	+236,798	381,112
Chemical Sciences, Geosciences, and Energy Biosciences	216,747	297,113	-4,243[b]	292,870	+154,062	338,357
Scientific User Facilities	—	—	—	—		811,791
Subtotal, Basic Energy Sciences	1,159,491	1,426,504	—	1,426,504	+390,860	1,531,260
Construction	93,265	145,468	—	145,468	+164,546	154,240
Total, Basic Energy Sciences	1,252,756[c,d]	1,571,972	—	1,571,972	+555,406	1,685,500

Funding Profile by Subprogram (Comparable Structure to the FY 2010 Request)

(dollars in thousands)

	FY 2008 Comparable Appropriation	FY 2009 Original Appropriation	FY 2009 Adjustments	FY 2009 Comparable Appropriation	FY 2009 Additional Appropriation[a]	FY 2010 Request
Basic Energy Sciences						
Materials Sciences and Engineering	234,429	1,129,391	-787,727[b,e]	341,664	+154,062[e]	381,112
Chemical Sciences, Geosciences, and Energy Biosciences	216,747	297,113	-4,243[b]	292,870	+154,062	338,357
Scientific User Facilities	708,315	—	+791,970[b,e]	791,970	+82,736[e]	811,791
Subtotal, Basic Energy Sciences	1,159,491	1,426,504	—	1,426,504	+390,860	1,531,260
Construction	93,265	145,468	—	145,468	+164,546	154,240
Total, Basic Energy Sciences	1,252,756[c,d]	1,571,972	—	1,571,972	+555,406	1,685,500

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"

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[a] The Additional Appropriation column reflects the planned allocation of funding from the American Recovery and Reinvestment Act of 2009, P.L. 111–5. See the Department of Energy website at http://www.energy.gov/recovery for up-to-date information regarding Recovery Act funding.

[b] Reflects a reallocation of funding in accordance with the explanatory statement for the Energy and Water Development and Related Agencies Appropriations Act, 2009, P.L. 111–8.

[c] Includes $13,500,000 provided by the Supplemental Appropriations Act, 2008, P.L. 110–252.

[d] Total is reduced by $30,646,000: $27,363,000 of which was transferred to the Small Business Innovative Research (SBIR) program and $3,283,000 of which was transferred to the Small Business Technology Transfer (STTR) program.

[e] Adjustments reflect reallocation to the new subprogram, Scientific User Facilities.

Modifications were made to the budget structure to better reflect the subprograms activities in FY 2010. The two tables above show a non-comparable and comparable funding profile for the subprogram. The non-comparable table presents the FY 2010 funding in the new budget structure only and FY 2008 and FY 2009 funding is shown as appropriated. The comparable table shows the FY 2008 and FY 2009 funding in the new budget structure to assist in comparing year-to-year funding trends. A cross-walk of the new and old structure is provided at the end of this chapter, describing in detail the modification to the budget structure.

Program Overview

Mission

The mission of the Basic Energy Sciences (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 other aspects of 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 our planet’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 advances is our ability to create new materials using sophisticated synthetic and processing techniques and to precisely define the atomic arrangements in matter and control their 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.

BES and its predecessor organizations have supported a program of fundamental research focused on critical mission needs of the nation for over five decades. The federal program that became BES began with a research effort initiated to help defend our nation during World War II. The diversified program was organized into the Division of Research with the establishment of the Atomic Energy Commission in 1946 and was later renamed Basic Energy Sciences in 1977 as it continued to evolve through legislation. The program has a rich history of high impact scientific discoveries with unparalleled contributions to mission-critical needs, from radiation-resistant materials to actinide chemistry.

The BES program is one of the nation’s largest sponsors of research in the natural sciences. In FY 2008, the program funded research in more than 170 academic institutions located in 50 states and in 13 DOE laboratories located in 9 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, providing 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 were supported because of the need to correlate the microscopic structure of materials with their macroscopic properties, lending 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 much smarter and 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 like fossil fuels; they must be designed and fabricated to exacting standards using principles revealed by basic science.

The 20th century witnessed revolutionary advances in observational science, 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 nanoscales. 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 non-existing materials before they are made. 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 designing 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; 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 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

Hub will support large-scale, multidisciplinary team efforts to focus on nurturing and harnessing science to solve our most critical energy problems. The vision for a secure and sustainable energy future entails transitioning from our reliance on foreign fossil fuels to the development, deployment and export of new carbon-free energy technologies invented and manufactured in the U.S. The traditional linear model of discovery science leading to technology development and deployment will not meet the challenge of timeliness and scale. Rather, there is a need for bold and innovative approaches that better couple all of the elements of the science and technology chain and combine the talents of universities, national labs, and the private sector in concerted efforts to define and construct a sustainable energy economy. The Hub approach is designed to integrate a major national mobilization of basic energy research with appropriate investments in engineering and technology to accelerate bringing energy solutions to market.

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 our 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. This Hub will support large-scale, multidisciplinary team efforts to focus on nurturing and harnessing science to solve our most critical energy problems. The vision for a secure and sustainable energy future entails transitioning from our reliance on foreign fossil fuels to the development, deployment and export of new carbon-free energy technologies invented and manufactured in the U.S. The traditional linear model of discovery science leading to technology development and deployment will not meet the challenge of timeliness and scale. Rather, there is a need for bold and innovative approaches that better couple all of the elements of the science and technology chain and combine the talents of universities, national labs, and the private sector in concerted efforts to define and construct a sustainable energy economy. The Hub approach is designed to integrate a major national mobilization of basic energy research with appropriate investments in engineering and technology to accelerate bringing energy solutions to market.

The *Scientific User Facilities* subprogram supports the operation of a nationwide suite of major facilities that provides 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 the development of new tools and instruments. The continual advancement and renovation of the instrumental capabilities include developments of 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 to enable 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, research on toughened ceramics results in improved high-speed cutting tools, engine turbines, and a host of other applications requiring lightweight, high-temperature materials. Research in chemistry leads to the development of 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 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, creates an entirely new paradigm for developing new and revolutionary energy technologies.

Looking to the future, eliminating our half-century-long dependence on imported oil and halting our emission of carbon dioxide requires fundamental changes in the ways we produce, store, and use energy. Three strategic goals for which transformational science breakthroughs are needed have been identified in the recent BESAC report *New Science for a Secure and Sustainable Energy Future*: making fuels from sunlight, generating electricity without carbon dioxide emissions, and revolutionizing energy efficiency and use. Achieving these visionary goals will require the development of fundamentally new technologies with performance levels far beyond those that are now possible.

Future technologies based on transformational scientific discoveries may be able to convert sunlight to electricity with triple today's efficiency, store electricity in batteries or supercapacitors at ten times today's capacity, or produce electricity from coal and nuclear plants at twice today's efficiency while capturing and sequestering the carbon dioxide emissions and hazardous radioactive wastes. Accomplishing such technology breakthroughs will only be possible with fundamental understanding of new materials and chemical processes that govern the transfer of energy between light, electricity, and chemical fuels.

A working transistor was only developed after the theory of electronic behavior on semiconductor surfaces was formulated. Lasers were only developed after the quantum theory of light emission by materials was understood. Similar breakthroughs can only be achieved for sustainable energy technologies when matter and energy can be systematically controlled at the electronic, atomic and molecular level in order to design advanced materials and direct desired chemical reactions. A series of such advances—requiring a national mobilization of basic energy research endeavors—are needed for moving beyond incremental improvements to create a truly secure and sustainable energy future.

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 21st 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 recently 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’s portfolios have been reassessed and restructured as necessary to reflect the results of these workshops. In addition to the work described in these workshops, other priority areas have been identified to highlight grand science challenges, including general support for ultrafast science, chemical imaging, and mid-scale instrumentation.

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, and numerous instrument fabrication projects. The 2003 Office of Science report, *Facilities for the Future of Science: A Twenty-Year Outlook*, and the 2007 updated interim report, described the long-range plan for the Office of Science facilities.

Recently, BESAC has been charged to sponsor a Photon Workshop to explore the scientific frontiers that could be tackled with next generation photon sources. The workshop will identify new energy and scientific opportunities in materials, chemistry, biology, medicine, environment, and physics that can be addressed with diffraction, excitation, and imaging by photons. It is expected that this workshop 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 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 BESAC website[b]. 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 the defense program. Many activities facilitate cooperation and coordination between BES and the applied research programs,

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

[b] http://www.science.doe.gov/bes/BESAC/BESAC.htm

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 Office 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 the defense program. 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.

Budget Overview

The FY 2010 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.

BES research is broadly supported via three main types of awards—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 thousands of BES core research awards permit individual scientists and small groups to pursue to their specific energy-related research interests. The dozens of EFRC awards bring together multiple investigators to address major scientific challenges necessary to solve complex energy research problems. The two Hub awards will 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.

- *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; basic architecture of matter; directed assemblies, structure, and properties; emergence of collective phenomena; energy and information on the nanoscale; and matter far beyond equilibrium.
- *Energy Frontier Research Centers (EFRCs)*, were established in FY 2009 to integrate the talents and expertise of leading scientists in a setting designed to accelerate research toward meeting our critical energy challenges. The EFRCs harness the most basic and advanced discovery research in a concerted effort to establish the scientific foundation for a fundamentally new U.S. energy economy. EFRCs 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 Division and the Chemical Sciences, Geosciences, and Biosciences Division, who will be managed centrally within BES to ensure a unified management strategy and structure. In FY 2010, no funding increases are requested for the EFRCs. Instead, emphasis is being placed on ensuring that the EFRCs established late in FY 2009 are progressing toward their full collaborative and scientific potential.
- *Energy Innovation Hubs* are part of a set of Hubs that will be initiated by the Department in FY 2010. The set of Hubs aim at assembling multidisciplinary teams to address the basic science, technology, economic, and policy issues 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. Two Hubs are proposed in BES in FY 2010: Fuels from Sunlight and Batteries and Energy Storage.

The FY 2010 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% increase over the FY 2009 funding level, and provides optimal support for the user operations, accounting for cost of living increases. FY 2010 continues the commissioning of the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory, which 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. 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 activities include the Linac Coherent Light Source (LCLS) at SLAC National Acceleratory Laboratory and the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory. NSLS-II will continue its construction phase, including the largest component of the project—the building that will house the accelerator ring.

The Spallation Neutron Source Instruments-Next Generation (SING-I and SING-II) will be fully funded according to planned schedules and funding profiles. The Power Upgrade Project, as part of the planned upgrades to the Spallation Neutron Source at Oak Ridge National Laboratory, will be initiated.

Significant Program Shifts

Two Energy Innovation Hubs are initiated in FY 2010 in the topical areas of Fuels from Sunlight and Batteries and Energy Storage. Each Hub will be funded at $25,000,000 per year for an initial period of 5 years. One-time funding of $10,000,000 will be provided for Hub start-up needs, excluding any new construction

Strategic and GPRA Unit Program Goals

The BES program has one Government Performance and Results Act (GPRA) Unit Program goal which contributes to Strategic Goal 3.1 and 3.2 in the “goal cascade”:

- GPRA Unit Program Goal 3.1/2.50.00: 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.

Contribution to GPRA Unit Program Goal 3.1/2.50.00, Advance the Basic Science for Energy Independence

Within the Basic Energy Sciences program, the Materials Science and Engineering subprogram, the Chemical Sciences, Geosciences, and Energy Biosciences subprogram, and the Scientific User Facilities subprogram contribute to this goal by producing seminal advances in the core disciplines of the basic energy sciences. These subprograms build leading research programs that provide world-class, peer-reviewed research results cognizant of both DOE mission needs and new scientific opportunities. The following indicators establish specific long-term (ten-year) goals in scientific advancement that the BES program is committed to and against which progress can be measured.

- Design, model, fabricate, characterize, analyze, assemble, and use a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more—particularly at the nanoscale—for energy-related applications.
- Understand, model, and control chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.
- Develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.
- Conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials.

Annual Performance Results and Targets

FY 2005 Results	FY 2006 Results	FY 2007 Results	FY 2008 Results	FY 2009 Targets	FY 2010 Targets
GPRA Unit Program Goal 3.1/2.50.00 (Advance the Basic Science for Energy Independence)					
Scientific User Facilities					
Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 90 nm and in the soft x-ray region was measured at 15 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal]	Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 90 nm and in the soft x-ray region was measured at 15 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal]	Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 90 nm and in the soft x-ray region was measured at 15 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal].	Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 90 nm and in the soft x-ray region was measured at 15 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal].	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]	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]
Improve temporal resolution: X-ray pulses were measured at 70 femtoseconds in duration with an intensity of 100 million photons per pulse. [Met Goal]	Improve temporal resolution: X-ray pulses were measured at 70 femtoseconds in duration with an intensity of 100 million photons per pulse. [Met Goal]	Improve temporal resolution: X-ray pulses were measured at 70 femtoseconds in duration with an intensity of 100 million photons per pulse. [Met Goal]	Improve temporal resolution: X-ray pulses were measured at 70 femtoseconds in duration with an intensity of 100 million photons per pulse. [Met Goal]	Maintain x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse ($>10^8$ photons/pulse).[a]	Maintain x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse ($>10^8$ photons/pulse).[a]
Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 97.7%). [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 96.7%). [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 102.1%). [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 101.9%). [Met Goal]	Achieve an average operation time of the scientific user facilities as a percentage of the total scheduled annual operating time of greater than 90%.	Achieve an average operation time of the scientific user facilities as a percentage of the total scheduled annual operating time of greater than 90%.
Chemical Sciences, Geosciences, and Energy Biosciences					
As a part of the Scientific Discovery through Advanced Computing (SciDAC) program, a three-dimensional combustion reacting flow simulation was performed involving 11 reacting species and 0.5 billion grid points. [Met Goal]	As a part of the Scientific Discovery through Advanced Computing (SciDAC) program, a three-dimensional combustion reacting flow simulation was performed involving 33 reacting species and 21.2 million grid points. [Met Goal]	Improve Simulation: Beginning in FY 2007, increasing the size of the simulation will no longer provide useful new information. Thus, this measure was discontinued.			

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[a] No further improvement is expected in FY 2008-FY 2013 for these measures, because the current suite of instruments has met the 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 2005 Results	FY 2006 Results	FY 2007 Results	FY 2008 Results	FY 2009 Targets	FY 2010 Targets
Construction					
Cost and timetables were maintained within 10% of the baselines given in the construction project datasheets for all construction projects ongoing during the year (Results: +0.2% cost variance and -2.5% schedule variance). [Met Goal]	Cost and timetables were maintained within 10% of the baselines given in the construction project datasheets for all construction projects ongoing during the year (Results: -1.7% cost variance and -3.2% schedule variance). [Met Goal]	Cost and timetables were not maintained within 10% of the baselines given in the construction project datasheets for all construction projects ongoing during the year (Results: -2.7% cost variance and -10.4% schedule variance). [Goal of <10% Variance Not Met]	Cost and timetables were maintained within 10% of the baselines given in the construction project datasheets for all construction projects ongoing during the year (Results: 1.0% cost variance and -1.4% schedule variance). [Goal Met]	Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects. In FY 2009, it is less than 10% and 10%, respectively.	Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects. In FY 2010, it is less than 10% and 10%, respectively.

Materials Sciences and Engineering

Funding Schedule by Activity[a]

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Materials Sciences and Engineering			
Materials Sciences and Engineering Research	234,429	332,833	371,190
SBIR/STTR	—	8,831	9,922
Total, Materials Sciences and Engineering	234,429	341,664	381,112

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 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. The activity emphasizes correlation effects, which can lead to the formation of new particles, new phases of matter, and unexpected phenomena. The theoretical efforts include research on the development of advanced computer algorithms and codes to treat large or complex systems.

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. Major research areas include fundamental dynamics in complex materials, correlated electron systems, nanostructures, and the characterization of novel systems. The development of next-generation neutron, x-ray, and electron microscopy instrumentation is a key element of this portfolio.

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. Major research thrust areas include nanoscale synthesis, organization of nanostructures into macroscopic structures, solid state chemistry, polymers and polymer composites, surface and interfacial chemistry including electrochemistry and electro-catalysis, synthesis, and processing science including biomimetic and bioinspired routes to functional materials and complex structures.

The proposed Energy Innovation Hub focused on Batteries and Energy Storage will consist of multidisciplinary teams of experts that blend basic scientific research with technology development,

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[a] This table shows the FY 2008 and FY 2009 funding in the new (comparable) budget structure to assist in comparing year-to-year funding trends. A crosswalk of the new and old structure is provided at the end of this chapter, describing in detail the modification to the budget structure.

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 2008 Research Accomplishments

- *DNA directed fabrication of 3-D nanomaterials*. DNA has been used for the first time to create three-dimensional, ordered, crystalline structures of nanoparticles, which could not be fabricated using conventional techniques. The ability to engineer 3-D structures from nanoscale building blocks is essential to producing practical functional materials that take advantage of the unique properties of nano-objects, e.g., enhanced magnetism, improved catalytic activity, or new optical properties, but the nano-scale precision required makes them difficult to produce. This strategy utilizes nature-derived bio-molecules and takes advantage of their highly specific and well controlled recognitions to precisely direct the organization of inorganic nano-objects. It is particularly attractive as an inexpensive, scalable, and precise method for material fabrication and can provide a powerful means for assembly of individual nanoscale objects into designed architectures with unique physical properties. The research demonstrated the role of DNA design in the formation of such ordered nano-structures, thus providing the way for creation of new classes of novel nanomaterials by design.
- *Breakthrough in solar cell power output via organic solar concentrators***.** A tenfold increase in the amount of power converted by solar cells has been demonstrated via the use of organic solar concentrators. The increase in efficiency is achieved through the novel use of organic dyes and optical wave guides to efficiently absorb and trap the incident solar radiation until it can reach a solar cell. The new organic solar concentrators consist of a layer of transparent glass onto which multiple thin layers of organic dye molecules are deposited. Typically only part of the light spectrum can be utilized by solar cells to create electricity but these dyes act to absorb light across a broader spectrum of wavelengths, thereby increasing efficiency. Specific tailoring of these dyes allows light to be absorbed across the face of the glass, and then re-emitted by the dye molecules at a specific wavelength so that most of the energy stays in the pane of the glass (like a waveguide) and is emitted only at the edge. Small solar cells are then attached along the edges of the glass panel enabling the collection of a large portion of the solar spectrum over full surface of the glass panel yet only requiring small solar collectors, resulting in a further increase in geometric efficiency.
- *Ultrafast x-ray study enables real-time measurement and control of materials in extreme environments.* Using femtosecond x-ray probe pulses, atomic-scale resolution snapshots of complex nanocrystal nucleation processes in materials have been recorded. Researchers used ultrashort laser pulses to rapidly heat a material, ultimately causing melting and vaporization. Application of synchronous femtosecond x-ray probe pulses are used as a stroboscopic probe to observe ultrafast atomic and molecular motions. The images provide new insight into the steps accompanying disordering, melting and refreezing, which is required to model, predict, and enhance a material’s performance at extreme conditions.
- *Tuning a crystal for coherence.* Terahertz (THz) imaging and sensing can reveal depth and detail that other techniques cannot, and because terahertz radiation is non-ionizing it does not cause damage like x-rays can. While terahertz radiation is all around us in nature, it has been difficult to produce in a lab because it falls between the capabilities of electronic devices and lasers. By clever use of the inherent internal structure of a high-temperature superconducting material coupled with a special crystal geometry a new source of coherent radiation at THz frequencies has been developed. Researchers found that by using the edges of the crystal to create a resonating cavity, similar to the

mechanism for generating lasers, the switching of hundreds of naturally occurring nanoscale electronic circuits in the material (called Josephson junctions) could be synchronized. This synchronized switching emits powerful, coherent radiation in the THz frequency. In this discovery, the emitted power is proportional to the height of the crystal, and the frequency may be controlled by the width of the crystal. This new approach generates a power density several orders of magnitude greater than other methods, with the added benefit that the radiation is coherent and tunable.

- *Bringing quantum computing closer to reality.* Moore’s law has been successfully used to predict the evolutionary increase in computing power enabled over the last twenty years by chip manufacturers’ continual success at packing ever more transistors on a single chip. It also predicts the imminent finite end to what can be achieved using semiconductor-based logic—the limit when an individual component is only a handful of atoms. A promising path to extending computing power is a revolutionary approach based on the use of quantum bits (qubits) to store and manipulate information. Conventional computing represents information as a sequence of binary bits (“0” or “1”); in contrast, quantum computing represents information in quantum mechanical objects (qubits) that have the ability to exist in what is called a “superposition” of binary states; in essence, they can be “0” and “1” simultaneously. Superposition and other counter-intuitive properties of quantum mechanical objects enable certain classes of problems to be solved at a much higher speed on quantum computers. However, qubits are typically highly susceptible to environmental disturbance; to enhance their robustness solid-state qubits are typically utilized at ultra low temperatures. Recent studies have pushed back this boundary by showing that specific complexes in diamond, where a nitrogen impurity atom is linked to a vacant lattice site, can serve as reliable and robust qubits even at room temperature. Research showed that these specific qubits in diamond can be controlled with magnetic fields, allowing them to be isolated and manipulated to study how they fail. Understanding these failures may prove essential for the design and manipulation of much larger, interacting qubit systems required for practical quantum computing devices.
- *Nanoscience leads to breakthrough in efficiency of thermoelectric conversion.* Demonstrating the power of engineering materials at the nanoscale, researchers have achieved a 50-fold improvement in the ability of ordinary silicon to convert heat into electricity and vice versa. The family of materials capable of such conversion, named thermoelectrics, has been the focus of intense research because of their potential use in power generation and refrigeration. Until now useful thermoelectric properties only existed in a few rare materials, making the wide-scale deployment of this technology unfeasible. It was recently discovered that the shape of the silicon, fabricated in a very thin wire form, is key to attaining improved properties. As the wire diameter decreased to a few tens of nanometers, the thermoelectric properties unexpectedly improved to a level only seen in the best-known thermoelectric materials. This efficiency improvement in such an abundant and well-studied material such as silicon increases the potential to greatly expand the range of applications for thermoelectrics.

Detailed Justification

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Materials Sciences and Engineering Research	**234,429**	**332,833**	**371,190**
▪ **Experimental Condensed Matter Physics**	**40,628**	**46,398**	**51,387**

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 properties 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 energy generation, delivery, use, and conversion technologies. Specifically, research efforts in understanding the fundamental mechanisms in 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 2010, funding will be provided for research in the area of complex and emergent behavior. The research activities will emphasize investigations on emergent behaviors arising from the collective, cooperative behavior of individual components of a system which lead to physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magnetoresistance, random field magnets, and spin liquids and glasses. These phenomena are expected to have a wide range of impact on energy relevant technologies.

Funds are also provided in FY 2010 to cover pension payments for Oak Ridge National Laboratory (including Wackenhut) and Lawrence Berkeley National Laboratory.

	FY 2008	FY 2009	FY 2010
▪ **Theoretical Condensed Matter Physics**	**27,255**	**29,448**	**30,455**

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 2010, this activity will support multi-investigator projects in theory and modeling and simulation. The research will be focused on understanding 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 2008	FY 2009	FY 2010
▪ **Mechanical Behavior and Radiation Effects**	**13,268**	**14,336**	**14,826**

This activity supports basic research to understand defects in materials and their effects on the load-bearing 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. 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 high temperature furnaces, 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 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 are 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 2010, 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 as well as 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. In situ experiments will be closely integrated with theoretical/computational efforts to develop a fundamental understanding of degradation mechanisms and kinetics over multiple scales from atomistic to micron and nanosecond to decades.

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
▪ **Physical Behavior of Materials**	**28,226**	**30,498**	**31,541**

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 in aqueous, galvanic, and high-temperature gaseous corrosion and their mitigation; 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 our 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 2010, this activity will support research on energy conversion designed to achieve low cost power conversion. The research will 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 conversion efficiencies.

▪ **Neutron and X-ray Scattering**	**31,811**	**46,971**	**48,613**

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 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 2010, 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. Ultrafast materials science research will take advantage of new x-ray and neutron sources to perform research designed to understand the physics of strongly correlated systems, such as high temperature superconductors and magnetic materials with colossal magnetoresistance.

	FY 2008	FY 2009	FY 2010
▪ **Electron and Scanning Probe Microscopies**	**16,635**	**20,474**	**21,174**

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

In FY 2010, 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 femtosecond time scale. Ultrafast electron scattering will be developed as a companion tool to ultrafast photon probes.

	FY 2008	FY 2009	FY 2010
	(dollars in thousands)		
- **Experimental Program to Stimulate Competitive Research (EPSCoR)**	**14,680**	**16,755**	**8,520**

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 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 2010, support will continue for basic research related to all DOE mission areas and to enhance collaborative efforts with DOE user facilities. The FY 2010 request, after subtracting the additional funding provided by Congress in FY 2009, provides a funding increase for EPSCoR at a rate equivalent to increases for BES core research as a whole. Activities initiated with the additional funding provided by Congress in FY 2009 include additional implementation awards and research partnership awards. These activities are funded, to the extent possible, through their completion in FY 2011.

The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

	FY 2008	FY 2009	FY 2010
Alabama	1,074	135	—
Alaska	309	—	—
Arkansas	—	—	—
Delaware	980	980	—
Hawaii	—	—	—
Idaho	400	400	—
Iowa[a]	—	—	—
Kansas	405	—	—
Kentucky	—	650	700
Louisiana	522	440	300
Maine	650	650	—
Mississippi	—	—	—

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[a] Became eligible in FY 2009.

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Montana	531	350	450
Nebraska	784	—	—
Nevada	468	—	—
New Hampshire	545	569	—
New Mexico	1,455	—	750
North Dakota	450	—	—
Oklahoma	761	681	—
Puerto Rico	400	350	450
Rhode Island	—	—	—
South Carolina	1,315	785	—
South Dakota	405	—	—
Tennessee	1,821	135	314
U.S. Virgin Islands	—	—	—
Utah[a]	—	—	—
Vermont	—	—	—
West Virginia	1,318	—	—
Wyoming	—	—	—
Technical Support	87	250	250
Other[b]	—	10,380	5,306

	FY 2008	FY 2009	FY 2010
▪ **Synthesis and Processing Science**	**15,587**	**16,841**	**17,417**

This activity supports basic research to develop new techniques to synthesize new 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 objects 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 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. This activity includes operation of the Materials Preparation Center at the

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[a] Became eligible in FY 2009.
[b] Uncommitted funds in FY 2009 and FY 2010 will be competed among all EPSCoR states.

Ames Laboratory, which develops innovative and superior processes for materials preparation and provides small quantities of research-grade, controlled-purity materials and crystals not otherwise available to academic, governmental, and industrial research communities to be used for research purposes. Capital equipment funding is provided for crystal growth apparatus, heat treatment furnaces, lasers, chemical vapor 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 the 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 2010, research will seek to develop novel design rules for synthesizing nanostructured materials and assemblies for energy relevant systems. Research on advanced materials for electrical energy storage will include studies on the fundamental electrochemical characteristics of the nanoscale building blocks with varying size and shape and in confined geometry.

	FY 2008	FY 2009	FY 2010
▪ **Materials Chemistry and Biomolecular Materials**	**46,339**	**51,569**	**53,333**

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 controlled 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 atomic force 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 2010, basic research will be performed on the design and synthesis of new energy relevant materials and processes which include new three-dimensional nanostructured architectures that can be precisely tailored for batteries and ultracapacitors. 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. Nanoscale hybrid materials and advances in the understanding of nature's design 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.

	FY 2008	FY 2009	FY 2010
▪ **Energy Frontier Research Centers (EFRCs)[a]**	**—**	**55,300**	**55,300**

This activity supports those EFRCs with an emphasis on Materials Sciences and Engineering that are coordinated with the ongoing core research activities within the subprogram. EFRCs are multi-investigator and multi-disciplinary collaborations that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future. The EFRC program represents an important implementation of the BES strategic plan for grand challenge and use-inspired energy science that has been set forth in the series of BESAC and Basic Research Needs workshops over the last six years[b]. The scientific challenges emerging from these studies describe a new era of science—an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will. The EFRCs were established in FY 2009 through a competitive Funding Opportunity Announcement that was open to universities, DOE laboratories, for-profit companies, and nonprofit entities. EFRCs bring 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 and thus complement the ongoing BES core research activities. The EFRCs inspire, train, and support leading scientists of the future who will ultimately be called upon to solve the nation's energy challenges in the 21st century.

While EFRCs are inherently multi-disciplinary in nature, this activity includes EFRCs that are focused on the design, discovery, synthesis, and characterization of new materials for improved conversion of solar energy into electricity; that store electrical energy in innovative new ways with greatly increased capacity; 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; and that optimize and control photon management in solid state materials to improve energy efficiency. The Centers will enhance our fundamental understanding of complex materials by combining experimental research with theory, computation and advanced simulations. Unifying themes in the research include the synthesis and characterization of materials and phenomena on the nanometer length scale and ultrafast (femtoseconds to attoseconds) timescales. Observing the dynamics of energy flow in theses systems is necessary if we are to learn to control their behavior.

In FY 2010, emphasis will be placed on ensuring that the EFRCs established late in FY 2009 are progressing toward their full collaborative and scientific potential using management protocols develop for other large-scale activities.

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[a] A complimentary set of EFRCs is also supported in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

[b] http://www.sc.doe.gov/bes/reports/list.html

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
▪ **Energy Innovation Hub – Batteries and Energy Storage**	**—**	**—**	**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 vehicles; 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 affected 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.

In FY 2010, research will be included in the following areas. 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.

(dollars in thousands)

	FY 2008	FY 2009	FY 2010

- 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.

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

	FY 2008	FY 2009	FY 2010
▪ **General Plant Projects (GPP)**	**—**	**4,243**	**4,604**

GPP funding is provided for minor new construction, for other capital alterations and additions, and responsibilities to land, buildings, and utility systems as part of the BES stewardship responsibilities. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP is included in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram and the Scientific User Facilities subprogram. The total estimated cost of each GPP project will not exceed $10,000,000.

	FY 2008	FY 2009	FY 2010
SBIR/STTR	**—**	**8,831**	**9,922**

In FY 2008, $5,800,000 and $696,000 were transferred to the SBIR and STTR programs, respectively. The FY 2009 and FY 2010 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR program.

	FY 2008	FY 2009	FY 2010
Total, Materials Sciences and Engineering	**234,429**	**341,664**	**381,112**

Explanation of Funding Changes

	FY 2010 vs. FY 2009 ($000)
Materials Sciences and Engineering Research	
▪ **Experimental Condensed Matter Physics**	
Increased funding is provided for enhanced research in the area of complex and emergent behavior ($+1,587,000). Funding is provided to cover pension payments for ORNL (including Wackenhut) and LBNL ($+3,402,000).	$+4,989
▪ **Theoretical Condensed Matter Physics**	
Increased funding is provided for enhanced research to support multi-investigator projects in theory and modeling and simulation.	+1,007

FY 2010 vs.
FY 2009
($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. +490

- **Physical Behavior of Materials**

  Increased funding is provided for enhanced research on energy conversion designed to achieve low cost power conversion. +1,043

- **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. +1,642

- **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. +700

- **Experimental Program to Stimulate Competitive Research (EPSCoR)**

  The FY 2010 request accounts for the additional funding provided by Congress in FY 2009 ($-8,515,000), and provides a funding increase for EPSCoR at the same rate as BES core research ($+280,000). Additional funds provided in FY 2009 were used, to the extent possible, to fully fund grants and minimize outyear mortgages. -8,235

- **Synthesis and Processing Science**

  Increased funding is provided to develop novel design rules for synthesizing nanostructured materials and assemblies for energy relevant systems. +576

- **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 new three-dimensional nanostructured architectures that can be precisely tailored for batteries and ultracapacitors. +1,764

- **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

	FY 2010 vs. FY 2009 ($000)
- **General Plant Projects (GPP)**	
Increased funding is provided for GPP.	+361
Total, Materials Sciences and Engineering Research	**+38,357**
SBIR/STTR	
Increased funding in SBIR/STTR funding because of an increase in total operating expense.	+1,091
Total Funding Change, Materials Sciences and Engineering	**+39,448**

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Chemical Sciences, Geosciences, and Energy Biosciences			
Chemical Sciences, Geosciences, and Energy Biosciences Research	216,747	285,061	329,289
SBIR/STTR	—	7,809	9,068
Total, Chemical Sciences, Geosciences, and Energy Biosciences	216,747	292,870	338,357

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 chemical dynamics. There is a focus on cooperative phenomena in complex chemical systems, such as the effect of solvation on chemical structure, reactivity, and transport and the coupling of complex gas-phase chemistry with turbulent flow in combustion.

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. Inorganic and organic photochemical studies provide information on new chromophores, donor-acceptor complexes, and multi-electron photocatalytic cycles. Photoelectrochemical conversion is explored in studies of nanostructured semiconductors. Biological energy transduction systems are investigated, with an emphasis on the coupling of plant development and microbial biochemistry with the experimental and computational tools of the physical sciences.

In chemical transformations, research themes include the characterization, control, and optimization of chemical transformations, including efforts in catalysis science; separations and analytical science; 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. This research provides a fundamental basis for understanding the environmental contaminant fate and transport and for predicting the performance of repositories for radioactive waste or carbon dioxide ($CO_{2)}$ sequestration.

The proposed 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 2008 Research Accomplishments

- *Ultrafast snapshots of molecular dynamics.* New ultrafast laser techniques are allowing scientists to follow the concerted motion of the electrons and atoms that comprise a molecule as it undergoes chemical change. Distortions in the electron cloud that holds a molecule together can occur in less than one femtosecond, or one quadrillionth of a second. High harmonic generation (HHG) is a technique in which the intense, oscillating field from an ultrafast laser pulse first rips away an electron from a molecule and then slams it back into the ionic core of the molecule, generating soft x-ray photons. In recent studies of dinitrogen tetraoxide (N_2O_4), researchers first excited vibrational motion in the molecule with an optical ultrafast laser pulse and then used a second ultrafast pulse to produce soft x-rays from the vibrating molecule. HHG is highly sensitive to the nature of the molecular orbitals from which the electron is plucked and those orbitals (the electron cloud) are sensitive to the shape of the molecule. Thus, HHG could monitor the evolution of the molecular orbitals of N_2O_4 as it vibrated. This exciting result opens the door to future studies of the concerted motion of electrons and atoms in molecules that probe a foundational tenet of chemistry—that the rapid motion of electrons is separable from the slower motion of atoms in a molecule undergoing chemical change.
- *A molecular-scale understanding of carbon separation in advanced media.* Long-term solutions to global climate change require effective media to first separate CO_2 from pre- or post-combustion processes. Currently, this separation is done with amine-based solution chemistry, which is both expensive and requires large amounts of hazardous chemicals. New research aimed at finding molecular solids for this task has focused on calixarenes, which are a class of large molecules that form cage-like structures into which smaller molecules can enter and be retained. They feature an absorption selectivity that is a critical criterion for the separation of CO_2 from other components in process streams. The molecular solid of the calixarene p-tert-butylcalix[4]arene (TBC4) is a prototypical example of a compound that might be used in such a system. The motion of the guest molecules CO_2 and CH_4 were studied in TBC4 over a range of temperatures using molecular simulation technique. The results show key differences in the rattling motion and free energy of absorption for CO_2 and CH_4 and provide fundamental data for optimization of these molecular solids as CO_2 separation media.
- *Chemical imaging for solar photochemistry*. Chemical imaging is used to describe experimental methods in which chemical processes are imaged with both molecular specificity and high spatial resolution. A recent advance in confocal microscopy makes it possible to simultaneously spatially resolve the reaction of a single molecule and to measure the rate of that reaction with ultrafast time

resolution, thus adding temporal capability to chemical imaging. This new microscopy was used to measure rates of light-induced electron exchange between molecules and single semiconductor nanoparticles. Photo-induced electron transfer was studied at a single location on a semiconductor surface before the excited molecule had dissipated its thermal energy through molecular vibration. The new technique also allowed the migration of excitation on a nanoparticle to be visualized during an electron-transfer reaction that is of fundamental importance in converting sunlight into electricity. This creative redesign of confocal microscopy is simple and amenable to existing confocal microscopes, an important advance in the field of chemical imaging.

- *New catalysts from cheap and abundant metals*. The processing of petroleum into fuels and chemicals currently relies heavily on precious and scarce noble-metal catalysts because of their selectivity and activity. Sustainable catalytic conversion of biomass feedstocks into fuels requires the design and development of novel catalysts based on cheap and abundant metals. Research results from the fields of organometallic, bio-inspired, and solid-state chemistry are converging on a new set of catalysts based on common metals such as iron, zinc, nickel, copper, and manganese. With the aid of computational chemistry, new materials have been designed with tailored catalytic properties. Examples include a bio-inspired iron-oxo complex that selectively converts methane to methanol with much higher yields than natural enzymes and new alloys of zinc-nickel that are more active and selective in the conversion of acetylene to ethylene than classical palladium-silver alloys.
- *Minerals as semiconductors.* The semiconducting properties of a wide range of minerals are often ignored in the study of their geochemical behavior. Experiments on natural hematite (Fe_2O_3) have conclusively demonstrated that interfacial electron transfer reactions at one surface of a crystal in an electrolytic solution couple with those at another surface. This causes one crystal face to dissolve while other faces grow and creates gradients in the electrical potential within the crystal that can drive conductance from one crystal face to another. Bulk crystal conduction is likely to be a general phenomenon that occurs in a host of naturally abundant semiconducting minerals, leading to interfacial processes that are important, but previously under appreciated, in the geochemistry of soils and sediments.

Detailed Program Justification

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Chemical Sciences, Geosciences, and Energy Biosciences Research	**216,747**	**285,061**	**329,289**
▪ **Atomic, Molecular, and Optical Science**	**18,353**	**22,886**	**23,669**

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. The activity also supports research on the fundamental interactions of atoms, molecules, and ions of importance to fusion and fission energy research.

In FY 2010, continued emphasis will be placed on the development 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. In FY 2010, there is an increase for ultrafast science and for the control quantum systems.

- **Chemical Physics Research** **40,761** **47,886** **51,468**

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 chemical complexity of combustion has challenged predictive 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 2010, there will 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. In FY 2010, there is an increase for research related to the combustion of alternative fuels, for emergent behavior in condensed phase systems, and for interfacial science relevant to electrical energy storage, including studies for electrode-electrolyte interfaces.

There is also an increase in FY 2010 to cover pension payments for Oak Ridge National Laboratory (including Wackenhut) and Lawrence Berkeley National Laboratory.

	FY 2008	FY 2009	FY 2010
▪ **Solar Photochemistry**	**30,479**	**34,685**	**35,871**

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 the 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.

(dollars in thousands)

FY 2008	FY 2009	FY 2010

In FY 2010, continued emphasis will be placed on studies of semiconductor/polymer interfaces, multiple charge generation within semiconductor nanoparticles, and dye-sensitized solar cells. In FY 2010, there is an increase for research on inorganic/organic donor-acceptor molecular assemblies and the use of nanoscale materials in solar photocatalytic generation of chemical fuels.

	FY 2008	FY 2009	FY 2010
▪ **Photosynthetic Systems**	**15,715**	**17,884**	**18,496**

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 2010, 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. In FY 2010, there is an increase for solar energy conversion, including research on biological and bio-hybrid systems and enhanced efforts in understanding defect tolerance and self-repair in natural photosynthetic systems.

	FY 2008	FY 2009	FY 2010
▪ **Physical Biosciences**	**15,105**	**17,189**	**17,777**

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 2010, 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 2010, there is an increase for the application of physical characterization tools to biochemical systems, particularly those relevant to conversion of biomass into fuels.

	FY 2008	FY 2009	FY 2010
▪ **Catalysis Science**	**40,412**	**46,506**	**48,139**

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-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, 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 2010, 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. In FY 2010, there is an increase for chemical imaging of operating catalytic systems, experimental and theoretical studies of electrocatalytic processes relevant to solar energy conversion and electrical energy storage, and novel catalytic routes for the conversion of biological feedstocks into chemical fuels.

	FY 2008	FY 2009	FY 2010
▪ **Separations and Analysis**	**15,359**	**17,979**	**18,594**

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 the DOE's stewardship responsibility for transuranic chemistry; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important 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 2010, separations research will focus on fluid flow in nanoscale membranes and the formation of macroscopic separation systems via self-assembly of nanoscale building blocks. Chemical analysis research will emphasize the study of hydrogen separation and hydrogen transport within membrane systems; development of techniques with high spatial, temporal, and chemical resolution; and simultaneous application of multiple analytical techniques. In FY 2010, there is an increase for advanced chemical separations, particularly separation techniques relevant to capture of carbon dioxide and for analytical chemical imaging.

	FY 2008	FY 2009	FY 2010
▪ **Heavy Element Chemistry**	**9,002**	**10,744**	**11,111**

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 determinations of the 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 2010, 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. In FY 2010, there is an increase for enhanced efforts on actinide chemistry and separations science related to advanced nuclear energy systems.

	FY 2008	FY 2009	FY 2010
▪ **Geosciences Research**	**20,463**	**23,787**	**24,601**

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 2010, continued emphasis will 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 2010, there is an increase for solid earth geophysics and geochemistry.

	FY 2008	FY 2009	FY 2010
▪ **General Plant Projects (GPP)**	**11,098**	**815**	**843**

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 the 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 $10,000,000.

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 2008	FY 2009	FY 2010
▪ **Energy Frontier Research Centers (EFRCs)**[a]	**—**	**44,700**	**44,700**

This activity supports those EFRCs with an emphasis on Chemical Sciences, Geosciences, and Energy Biosciences that are coordinated with the ongoing core research activities within the subprogram EFRCs are multi-investigator and multi-disciplinary collaborations that foster, encourage, and accelerate basic research to provide the basis for transformative energy technologies of the future. The EFRC program represents an important implementation of the BES strategic plan for grand challenge and use-inspired energy science that has been set forth in the series of BESAC and Basic Research Needs workshops over the last six years[b]. The scientific challenges emerging from these studies describe a new era of science—an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will. The EFRCs were established in FY 2009 through a competitive Funding Opportunity Announcement that was open to universities, DOE laboratories, for-profit companies and nonprofit entities. EFRCs bring 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 and thus complement the ongoing BES core research activities. The EFRCs inspire, train, and support leading scientists of the future who will ultimately be called upon to solve the nation’s energy challenges in the 21st century.

While EFRCs are inherently multi-disciplinary in nature, this activity includes EFRCs that are focused on design, discovery, control, and characterization of chemical, biochemical, and geological moieties and processes for the advanced conversion of solar energy into chemical fuels; for improved electrochemical storage of energy; for the creation of next-generation biofuels via catalytic chemistry and biochemistry; for the clean and efficient combustion of advanced transportation fuels; and for science-based geological carbon capture and sequestration. Unifying themes in the research include the fundamental understanding of interfacial phenomena underlying the transport of electrons, atoms, molecules, and energy at the nanoscale and the development and application of

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[a] A complimentary set of EFRCs is also supported in the Materials Sciences and Engineering subprogram.
[b] http://www.sc.doe.gov/bes/reports/list.html

new experimental and theoretical tools for molecular-scale understanding of complex chemical, biochemical, and geological processes.

In FY 2010, emphasis will be placed on ensuring that the EFRCs established late in FY 2009 are progressing toward their full collaborative and scientific potential using management protocols developed for other large-scale activities.

	FY 2008	FY 2009	FY 2010
▪ **Energy Innovation Hub - Fuels from Sunlight**	**—**	**—**	**34,020**

Nature has understood for nearly 3 billion years how to turn sunlight into energy-rich chemical fuels starting from the abundant feedstocks of water and carbon dioxide. All of the fuels we use today to power our vehicles and create electricity, whether from fossil or biomass resources, are derived from the natural photosynthetic process. While biofuels derived from plant feedstocks avoid the environmental consequences of burning fossil fuels, the scalability and sustainability of this approach remains a concern. More fundamentally, the overall efficiency in converting sunlight to plant material and then converting biomass into fuels is low. Imagine the potential if we could bypass the plant medium entirely and generate fuels directly from sunlight, carbon dioxide, and water just as a plant does. The impact of replacing fossil fuels with bio-inspired fuels created directly from sunlight would be immediate and completely transformative, providing an abundant supply of environmentally benign fuel for our transportation needs. Recognizing this fact, the BESAC report, *New Science for Secure and Sustainable Energy Future,* listed the production of fuels directly from sunlight as one its three strategic goals for which transformational science breakthroughs are urgently needed.

Basic research has provided enormous advances in our understanding of the subtle and complex photochemistry associated with the natural photosynthetic system. Similar advances have been made in purely inorganic photo-catalytic approaches to split water or photoreduce carbon dioxide. Yet, we still lack sufficient knowledge of the natural process and adequate control of artificial systems to design solar fuel generation processes with the efficiency, sustainability, or economic viability required. A Hub focused on making fuels from sunlight would aim at developing a direct solar fuel conversion system with overall conversion efficiency that produces fuels with sufficient energy content to enable the transition to proof-of-concept prototyping. The scale of the scientific challenge associated with this goal is daunting, but not insurmountable, and will require drawing expertise and premier scientific talent from the disciplines of chemistry, physics, materials sciences, biology, and engineering.

In FY 2010, research will be included in the following areas. Potential approaches to the challenge of producing fuels from sunlight that the Hub might adopt include the following:

- Replicating or reverse engineering the natural photosynthetic system with inorganic materials or hybrid bio-inorganic systems. Advances here require a more profound understanding of the subtle and complex chemistry of plant life, particularly in understanding the marvelous ability by which plants regulate the photosynthetic apparatus and repair themselves when damaged, both critical factors in the construction of a robust, man-made solar fuel generator.
- Using solar photovoltaics to drive the splitting of water or the reduction of carbon dioxide in an electrochemical cell, which requires the design and discovery of novel nano-engineered materials

(dollars in thousands)

	FY 2008	FY 2009	FY 2010

that catalyze the water splitting reaction and that are efficient, cost effective, environmentally benign, and have long term stability and reliability.

- Artificially connecting biochemical systems that can combine water, sunlight, and even carbon dioxide to produce hydrogen or another chemical fuel in a man-made chemical reactor. The key to this approach is identifying the "software" for the synthetic cell, which can guide the process to the desired product.
- One-time funding of $10,000,000 will be provided for Hub start-up needs, excluding any new construction.

SBIR/STTR	**—**	**7,809**	**9,068**

In FY 2008, $5,179,000 and $621,000 were transferred to the SBIR and STTR programs, respectively. The FY 2009 and FY 2010 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR program.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**216,747**	**292,870**	**338,357**

Explanation of Funding Changes

	FY 2010 vs. FY 2009 ($000)
Chemical Sciences, Geosciences, and Biosciences Research	
▪ **Atomic, Molecular and Optical Science**	
Increased funding is provided for ultrafast science and for the control of quantum systems.	+783
▪ **Chemical Physics Research**	
Increased funding is provided for research related to the combustion of alternative fuels, for emergent behavior in condensed phase systems, and for interfacial science relevant to electrical energy storage, including studies of electrode-electrolyte interfaces (+$1,638,000). Funding is provided to cover pension payments for ORNL (including Wackenhut) and LBNL ($+1,944,000).	+3,582
▪ **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.	+1,186
▪ **Photosynthetic Systems**	
Increased funding is provided for solar energy conversion, including research on biological and bio-hybrid systems and enhanced efforts in understanding defect	+612

	FY 2010 vs. FY 2009 ($000)
tolerance and self-repair in natural photosynthetic systems.	
▪ **Physical Biosciences**	
Increased funding is provided for the application of physical characterization tools to biochemical systems.	+588
▪ **Catalysis Science**	
Increased funding is provided for chemical imaging of operating catalytic systems, experimental and theoretical studies of electrocatalytic processes relevant to solar energy conversion and electrical energy storage, and novel catalytic routes for the conversion of biological feedstocks into chemical fuels.	+1,633
▪ **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.	+615
▪ **Heavy Element Chemistry**	
Increased funding is provided for enhanced efforts on actinide chemistry and separations science related to advanced nuclear energy systems.	+367
▪ **Geosciences Research**	
Increased funding is provided for research in solid earth geophysics and geochemistry.	+814
▪ **Energy Innovation Hub – Fuels from Sunlight**	
Funds are provided for an Energy Innovation Hub focused on making fuels from sunlight to develop a solar fuel conversion system that completely bypasses plants as the medium drawing from disciplines of chemistry physics, materials sciences, biology, and engineering.	+34,020
▪ **General Plant Projects (GPP)**	
Small increase for general plant projects.	+28
Total, Chemical Sciences, Geosciences and Energy Biosciences Research	**+44,228**
SBIR/STTR	
Increased funding in SBIR/STTR funding because of an increase in operating expenses.	+1,259
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	**+45,487**

Scientific User Facilities

Funding Schedule by Activity[a]

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Scientific User Facilities			
Research	11,439	20,370	24,713
Major Items of Equipment	30,543	34,000	25,000
Facilities Operations	666,333	718,968	742,749
SBIR/STTR	—	18,632	19,329
Total, Scientific User Facilities	708,315	791,970	811,791

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 provide 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 the x-ray range, 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 them, assemble them, 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 1990's to over 40% in 2008. 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.

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[a] This table shows the FY 2008 and FY 2009 funding in the new (comparable) budget structure to assist in comparing year-to-year funding trends. A crosswalk of the new and old structure is provided at the end of this chapter, describing in detail the modification to the budget structure.

Selected FY 2008 Facility Accomplishments

- *The Spallation Neutron Source (SNS)* continues on its path to megawatt-level beam powers. The SNS raised its beam power to 700 kW, which is four times higher than any other spallation neutron source in the world. In addition, 11 neutron scattering instruments will be available to users in FY 2009. At the *High Flux Isotope Reactor (HFIR)* the new cold source provided beam to new instruments at cold neutron flux levels unsurpassed by any other research reactor facility in the world. The number of instruments at HFIR available to users has increased to nine and the reactor has operated safely and with excellent reliability.
- *Studies at the SNS* of a new class of nanostructured materials—weakly-coupled polyelectrolyte multilayers—show that pH level can trigger release disorders in the film. The results suggest possible applications where macromolecular components can be released through the disordered films, such as in a drug delivery system.
- *Synchrotron radiation light sources.* In FY 2008, there were significant advances in nanoscale imaging. The hard x-ray nanoprobe at the *Advanced Photon Source*, operated jointly with the *Center for Nanoscale Materials*, provides x-ray imaging with an initial spatial resolution of 30 nanometers using zone plate lenses. The coherently focused beams are used to map crystal lattice spacing modulations to determine the strain and crystallographic structure of nanoscale regions of complex materials and devices. The nanobeam x-ray analysis showed that metal surface scales are a mixture of oxides and metal nanoparticles. These nanoparticles can self-assemble into nano-networks forming continuous channels for transport of elements such as carbon and hydrogen through the oxide scales, causing corrosion and embrittlement. Metal oxide scales without spinel phases have been found to prevent the formation of these nanoparticles. Based on these studies laboratory-sized batches of materials have been developed that exhibit as much as ten times longer life than commercial alloys with similar chromium content. These alloys are of considerable interest to the chemical, petrochemical and refining industries.

  X-ray focusing technique has been employed at the *National Synchrotron Light Source* where a compound lens composed of a series of refractive silicon lenses is able to surpass a critical incident x-ray angle limit to deliver superior focusing properties. This is an important step towards the *National Synchrotron Light Source II (NSLS-II),* a state-of-the-art synchrotron facility in development that will produce x-rays up to 10,000 times brighter than those generated by the current NSLS.

  Research done at the *Advanced Light Source (ALS)* shows that relativistic Dirac particles and the quantum coexist and are in fact highly coupled in electrically insulating single crystalline bismuth antimony alloys. This may be important in the design of new devices for low power consumption spin based electronics technologies and may also provide a basis for quantum computing.
- *Full operations of the five Nanoscale Science Research Centers (NSRC).* The NSRCs hosted more than 1,200 users in FY 2008, resulting in over 400 publications in the scientific literature. These BES facilities have been used to synthesize and characterize new materials. At the *Molecular Foundry* a class of sequence-specific bio-inspired polymers called peptoids have been synthesized from readily available starting materials by solid-phase synthesis and folded into defined structures. Peptoid oligomers and polymers are finding wide applications by a variety of groups in drug discovery, diagnostics, drug delivery, and materials science, since they combine the advantages of proteins with those of synthetic polymers.

Scientists at the *Center for Functional Nanomaterials* discovered a process that enables controlled layer-by-layer deposition of large areas of graphene on the metal substrate, ruthenium. Graphene, an atom-thick honeycomb layer of carbon atoms, has shown exceptional properties with potential for a broad range of applications. For instance, graphene's very high electron mobility at room temperature and its sensitivity to single-molecule gas detection make graphene very promising for applications in electronics and sensing.

An indirect imaging technique was developed at the *Center for Nanophase Material Science* whereby a hidden nanoscale structure can be inferred from the fluctuations of neighboring structures that can be imaged. This technique was used to discover key operational details of a biochemical switch that determines the fate of HIV-infected cells. Another novel method to probe bias-induced phase transitions based on a scanning probe microscopy platform has provided new insights into ferroelectric switching, and also garnered an R&D 100 award.

- *Major advances in imaging at the electron beam micro-characterization and nanoscale science research centers*. An unprecedented 0.05 nm spatial information limit was demonstrated in the course of development of the Transmission Electron Aberration-corrected Microscope (TEAM), a project led by the *National Center for Electron Microscopy* and involved numerous other partners to create the first of a new generation of electron microscopes. Also as part of the TEAM effort, researchers at the *Electron Microscopy Center for Materials* improved by an order of magnitude the resolution of energy-filtered transmission microscopy by correcting for the chromatic aberrations of the electron microscope's lenses. This technique enables the study of variations in chemistry at the sub-nanometer scale which is essential to improving the properties of materials.

Detailed Program Justification

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Research	**11,439**	**20,370**	**24,713**
▪ **Electron-beam Microcharacterization**	**8,192**	**11,250**	**11,652**

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 2008	FY 2009	FY 2010

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 2010, full user operations are supported on the Transmission Electron Aberration Corrected Microscope (TEAM), which will be available to the research community as part of the National Center for Electron Microscopy at LBNL. This instrument 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.

▪ **Accelerator and Detector Research**	**2,747**	**9,120**	**13,061**

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Research includes studies of ultra-high brightness electron beams to drive self amplified spontaneous emission free electron lasers, such as the Linac Coherent Light Source (LCLS); 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 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 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 DOE Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) program awards for the development of x-ray detectors and advanced accelerator technology.

Additional funds provided in FY 2010 will increase selected R&D activities related to light sources. These include 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. 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.

▪ **Nanoscale Science Research Centers**	**500**	**—**	**—**

Funding for Other Project Costs for the Nanoscale Science Research Centers has been completed.

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Major Items of Equipment	**30,543**	**34,000**	**25,000**
▪ **Spallation Neutron Source Instrumentation I (SING I)**	**11,856**	**12,000**	**5,000**

Funds are provided to continue 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.

▪ **Spallation Neutron Source Instrumentation II (SING II)**	**6,000**	**7,000**	**18,000**

Funds are provided for 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 be 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 2011. The SING II instruments are in addition to the five instruments to be provided by the SING I MIE. The baseline TPC is now approved at the Approve Performance Baseline, CD-2, for three of the four instruments. The FY 2010 Request is for engineering design of the final instrument and fabrication of the others.

▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)**	**6,000**	**15,000**	**—**

Funds are provided for a Major Item of Equipment with a total project cost of $60,000,000 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. No funds are requested in FY 2010. The project is fully funded as of FY 2009.

▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	**6,687**	**—**	**—**

Funding for the Transmission Electron Aberration Corrected Microscope (TEAM) Major Item of Equipment was completed in FY 2008.

▪ **SNS Power Upgrade Project (PUP)**	**—**	**—**	**2,000**

Funds are provided for a Major Item of Equipment with a preliminary Total Project Cost range of $86,500,000–$98,400,000 for activities to design, build, install, test, and commission the equipment necessary to increase the Spallation Neutron Source (SNS) proton beam energy. CD-0 was approved on November 22, 2004. 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 funding is provided for engineering design only. Engineering design may include limited fabrication and testing of design concepts.

	FY 2008	FY 2009	FY 2010
Facilities Operations	**666,333**	**718,968**	**742,749**

This activity supports the operation of the BES scientific user facilities, which consist of light sources, neutron sources, nanoscience centers, and the linear accelerator for the Linac Coherent Light Source project under construction 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 to all areas of science and technology, 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 2000–2008, 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 2010, operation of these scientific user facilities is funded at a level that will permit optimal service to users. Additional funds are provided in FY 2010 for full operation of the SLAC linac 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 as well as user support at the facilities. Increases in the NSRC budgets reflect full functionality and staffing of the five NSRCs. Small variations in the operations allocations across the five NSRCs reflect differing facility needs and priorities as well as the results of initial operations reviews of the four facilities in FY 2007 and FY 2008. Other project costs are provided for two facilities that are under construction and are described elsewhere in this budget: the Linac Coherent Light Source (LCLS) at SLAC and 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.

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 at the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front end components, monochromators, and power supplies. A summary of the funding for the facilities is provided below.

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
All Facilities			
Achieved Operating Hours	29,137	N/A	N/A
Planned Operating Hours	28,580	31,800	34,000
Optimal Hours	35,800	34,000	34,000
Percent of Optimal Hours	76%	94%	100%
Unscheduled Downtime	8.5%	<10%	<10%
Number of Users	10,538	11,345	12,390

	FY 2008	FY 2009	FY 2010
▪ **Synchrotron Radiation Light Sources**	**328,253**	**366,373**	**375,700**
Advanced Light Source, LBNL	50,194	52,016	53,869
Advanced Photon Source, ANL	112,290	118,061	127,140
National Synchrotron Light Source, BNL	37,572	40,573	42,021
National Synchrotron Light Source-II, BNL	20,000	10,000	2,000
Stanford Synchrotron Radiation Light Source, SLAC	32,197	34,023	35,196
Linac Coherent Light Source (LCLS), SLAC	15,500	20,000	20,500
Linac for LCLS, SLAC	60,500	91,700	94,974

BES operates four light source facilities: the Advanced Light Source at LBNL, the Advanced Photon Source at ANL, the National Synchrotron Light Source at BNL, and the Stanford Synchrotron Radiation Light Source at SLAC. The unique properties of synchrotron radiation include its continuous spectrum, high flux and brightness, and high coherence, which make 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.

Additional funds are provided in FY 2010 to continue full operation of the SLAC linac and to support operation of the Linac Coherent Light Source (LCLS) starting in the middle of the FY 2010. The budget also reflects an increase in the operating hours as well as user support at the facilities. Other project costs are provided for two facilities under construction - the National Synchrotron Light Source II at BNL and the LCLS at SLAC. The facility operations budget for the light sources also includes operating funds, capital equipment funds, and accelerator and reactor improvement project (AIP) funding under $5,000,000. The AIP funding will support additions and modifications to the accelerator and reactor facilities. Capital equipment is needed at the facilities for items such as beam monitor, interlock systems, vacuum transport systems, beamline front ends and optical components.

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Advanced Light Source			
Achieved Operating Hours	4,721	N/A	N/A
Planned Operating Hours	5,000	5,400	5,600
Optimal Hours	5,600	5,600	5,600
Percent of Optimal Hours	84.3%	96.4%	100%
Unscheduled Downtime	8.3%	<10%	<10%
Number of Users	1,939	2,100	2,200
Advanced Photon Source			
Achieved Operating Hours	4,503	N/A	N/A
Planned Operating Hours	4,380	4,800	5,000
Optimal Hours	5,000	5,000	5,000
Percent of Optimal Hours	90%	96%	100%
Unscheduled Downtime	2.4%	<10%	<10%
Number of Users	3,270	3,500	3,700
National Synchrotron Light Source			
Achieved Operating Hours	5,006	N/A	N/A
Planned Operating Hours	4,900	5,200	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	93%	96%	100%
Unscheduled Downtime	6.0%	<10%	<10%
Number of Users	2,128	2,100	2,100

(dollars in thousands)

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Stanford Synchrotron Radiation Light Source			
Achieved Operating Hours	5,027	N/A	N/A
Planned Operating Hours	4,500	5,000	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	93%	93%	100%
Unscheduled Downtime	2.9%	<10%	<10%
Number of Users	1,147	1,300	1,400

	FY 2008	FY 2009	FY 2010
▪ **High-Flux Neutron Sources**	**247,880**	**251,403**	**260,246**
High Flux Isotope Reactor, ORNL	54,381	58,744	60,841
Intense Pulsed Neutron Source, ANL	8,400	4,000	4,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,655	11,136	11,533
Spallation Neutron Source, ORNL	174,444	177,523	183,872

BES operates three neutron scattering user facilities—one research reactor, the High Flux Isotope Reactor at ORNL, and two spallation neutron sources, the Spallation Neutron Source at ORNL and the Manuel Lujan Jr. Neutron Scattering Center at LANL. 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 take measurements leading to an understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of solids.

Additional funds are provided in FY 2010 for new operating beamlines at the Spallation Neutron Source and the High Flux Isotope Reactor at ORNL. The budget also reflects an increase in the operating hours as well as user support at the neutron scattering facilities. The Intense Pulsed Neutron Source is closed and funds are provided to continue decommissioning of the target assembly.

The facility operations budget for the neutron sources also includes operating funds, capital equipment funds, and accelerator and reactor improvement project (AIP) funding under $5,000,000. The AIP funding will support additions and modifications to accelerator and reactor facilities. Capital equipment is needed at the facilities for items such as beam monitor, interlock systems, vacuum transport systems, beamline front ends and optical components.

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
High Flux Isotope Reactor			
Achieved Operating Hours	3,539	N/A	N/A
Planned Operating Hours	3,100	3,900	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	79%	87%	100%
Unscheduled Downtime	1.3%	<10%	<10%
Number of Users	258	450	500
Intense Pulsed Neutron Source			
Achieved Operating Hours	1,013	—	—
Planned Operating Hours	1,000	—	—
Optimal Hours	3,600	—	—
Percent of Optimal Hours	28%	—	—
Unscheduled Downtime	4.5%	—	—
Number of Users	89	—	—
Manuel Lujan, Jr. Neutron Scattering Center			
Achieved Operating Hours	2,509	N/A	N/A
Planned Operating Hours	3,000	3,500	3,600
Optimal Hours	3,600	3,600	3,600
Percent of Optimal Hours	70%	97%	100%
Unscheduled Downtime	23.0%	<10%	<10%
Number of Users	261	280	300
Spallation Neutron Source			
Achieved Operating Hours	2,819	N/A	N/A
Planned Operating Hours	2,700	4,000	4,500
Optimal Hours	2,700	4,500	4,500
Percent of Optimal Hours	63%	89%	100%
Unscheduled Downtime	23.1%	<10%	<10%
Number of Users	165	250	700

	FY 2008	FY 2009	FY 2010
	(dollars in thousands)		
▪ **Nanoscale Science Research Centers (NSRCs)**	**90,200**	**101,192**	**106,803**
Center for Nanophase Materials Sciences, ORNL	18,650	19,956	21,068
Center for Integrated Nanotechnologies, SNL/LANL	18,000	20,100	21,218
Molecular Foundry, LBNL	17,700	20,142	21,260
Center for Nanoscale Materials, ANL	18,150	20,852	21,997
Center for Functional Nanomaterials, BNL	17,700	20,142	21,260

BES operates five NSRCs to support the synthesis, processing, fabrication, and analysis of materials at the nanoscale: the Center for Nanophase Materials Sciences at ORNL, the Molecular Foundry at LBNL, the Center for Integrated Nanotechnologies at SNL/LANL, the Center for Nanoscale Materials at ANL, and the Center for Functional Nanomaterials at BNL. These facilities are the Department of Energy'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 focuses on a different area of nanoscale research, such as materials derived from or inspired by nature; hard and crystalline materials, including the structure of macromolecules; magnetic and soft materials, including polymers and ordered structures in fluids; and nanotechnology integration. Each center is housed in a new laboratory building near one or more existing BES facilities for x-ray, neutron, or electron scattering. These new buildings contain clean rooms, laboratories for nanofabrication, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities.

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Number of Users[a]			
Center for Nanophase Materials Sciences	404	420	440
Center for Integrated Nanotechnologies	272	280	300
Molecular Foundry	303	315	330
Center for Nanoscale Materials	196	210	220
Center for Functional Nanomaterials	106	140	200

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[a] Facility operating hours are not measured at user facilities that do not rely on one central machine because such maintenance does not govern how many hours per year the whole facility can accommodate users.

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
SBIR/STTR	**—**	**18,632**	**19,329**

In FY 2008, $16,384,000 and $1,966,000 were transferred to the SBIR and STTR programs, respectively. The FY 2009 and FY 2010 amounts shown are the estimated requirements for the continuation of the congressionally mandated SBIR and STTR program.

Total, Scientific User Facilities	**708,315**	**791,970**	**811,791**

Explanation of Funding Changes

	FY 2010 vs. FY 2009 ($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.	+402
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.	+3,941
Total Research	**+4,343**
Major Items of Equipment	
Spallation Neutron Source Instrumentation I	
Scheduled decrease for the Major Item of Equipment for the Spallation Neutron Source Instrumentation I.	-7,000
Spallation Neutron Source Instrumentation II	
Scheduled increase for the Major Item of Equipment for the Spallation Neutron Source Instrumentation II.	+11,000
Linac Coherent Light Source Ultrafast Science Instruments (LUSI)	
Scheduled decrease for the Major Item of Equipment for the Linac Coherent Light Source Ultrafast Science Instruments. Project was fully funded as of FY 2009.	-15,000
SNS Power Upgrade, ORNL	
Increase to begin SNS Power Upgrade MIE	+2,000
Total, Major Items of Equipment	**-9,000**

	FY 2010 vs. FY 2009 ($000)
Facilities Operations	
▪ **Operation of National User Facilities**	
Increase for the Advanced Light Source to support accelerator operations and users.	+1,853
Increase for Advanced Photon Source to support accelerator operations and users.	+9,079
Increase for National Synchrotron Light Source to support accelerator operations and users.	+1,448
Decrease for National Synchrotron Light Source-II – Other Project Costs per the project schedule.	-8,000
Increase for the Stanford Synchrotron Radiation Light Source to support accelerator operations and users.	+1,173
Decrease for Linac Coherent Light Source Other Project Costs per the project schedule ($-5,500,000) and increase to begin operations of the LCLS portion of the Linac that has been commissioned ($+6,000,000).	+500
Increase for SLAC Linac to support operations.	+3,274
Increase for High Flux Isotope Reactor to support reactor operations.	+2,097
Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and users at approximately the FY 2008 level.	+397
Increase for Spallation Neutron Source to support operations and users	+6,349
Increase for the Center for Nanophase Materials to support operations and users.	+1,112
Increase for the Center for Integrated Nanotechnologies to support operations and users.	+1,118
Increase for the Molecular Foundry to support operations and users.	+1,118
Increase for the Center to Nanoscale Materials to support operations and users.	+1,145
Increase for the Center for Functional Nanomaterials to support operations and users.	+1,118
Total, Facilities Operations	**+23,781**
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expense.	+697
Total Funding Change, Scientific User Facilities	**+19,821**

Construction

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Construction			
Advanced Light Source User Support Building, LBNL	4,954	11,500	—
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	6,391	3,728	—
Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	941	—	—
National Synchrotron Light Source-II, BNL	29,727	93,273	139,000
Linac Coherent Light Source, SLAC	50,889	36,967	15,240
Center for Functional Nanomaterials, BNL	363	—	—
Total, Construction	93,265	145,468	154,240

Description

Construction is needed to support the research in the BES subprograms. Experiments in support of basic research require that state-of-the-art facilities be built or 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 required. 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 of 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 2008	FY 2009	FY 2010
Advanced Light Source (ALS) User Support Building, LBNL	**4,954**	**11,500**	**—**

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.

FY 2008 funds were used to complete preparation of the construction solicitation package(s) for USB and perform Title II design services. The FY 2009 construction funding is being 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 being used to remobilize the design-build construction contractor, erect the steel, complete exterior cladding and commence interior construction project efforts.

Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	**6,391**	**3,728**	**—**

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 will be 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 will be renovated to meet the new PULSE programs needs for offices, laboratories, and conference rooms.

The FY 2008 funds were used to begin the PULSE Building Renovation. FY 2009 funding will be used to complete construction.

Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	**941**	**—**	**—**

Project Engineering and Design funds for the Photon Ultrafast Laser Science and Engineering Building Renovation, described above, were provided in FY 2008.

National Synchrotron Light Source-II (NSLS-II), BNL	**29,727**	**93,273**	**139,000**

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 atom. 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 2008, Project Engineering and Design (PED) allowed the project to begin detailed design. These funds provide detail estimates of construction based on the approved design, final working drawings and specifications, and provided schedules for construction and procurements.

(dollars in thousands)

	FY 2008	FY 2009	FY 2010

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

In FY 2010, funds will be used to continue civil construction activities and advancing experimental and accelerator systems. Additional information is provided in the construction project data sheet 07-SC-06.

Linac Coherent Light Source, SLAC	**50,889**	**36,967**	**15,240**

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 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 2008, construction funding was used to complete most of the LCLS conventional facilities—including the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and Far Experimental Hall—and for continued procurement and installation of the technical hardware. The project was impacted by the delay and reduction in FY 2007 funding the procurement for the x-ray optics, diagnostics, and end stations and the project revised its cost and schedule baseline in January 2008.

In FY 2009, funding is being used for undulator and photon diagnostics installations, experimental halls installations, renovation of existing buildings at SLAC to provide office space in support of LCLS operations, and installation of technical hardware for x-ray transport system. Commissioning of the facility will also continue on a phased schedule.

In FY 2010, funds will complete the construction and commissioning elements of the project. FY 2011 is expected to be the first full year of LCLS facility operations. Additional information on the LCLS project is provided in the LCLS construction project data sheet, project number 05-R-320.

Center for Functional Nanomaterials, BNL	**363**	**—**	**—**

The Center for Functional Nanomaterials (CFN), a BES Nanoscale Science Research Center, was completed 40 days ahead of schedule and within budget in FY 2008.

Total, Construction	**93,265**	**145,468**	**154,240**

Explanation of Funding Changes

	FY 2010 vs. FY 2009 ($000)
Advanced Light Source (ALS) User Support Building, LBNL	
Decrease in funding for construction of the ALS User Support Building, as scheduled.	-11,500
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	
Decrease in funding representing the completion of construction in FY 2009, as scheduled.	-3,728
National Synchrotron Light Source-II (NSLS II), BNL	
Increase in funding to continue construction of the NSLS II project, as scheduled.	+45,727
Linac Coherent Light Source, SLAC	
Decrease in funding to continue construction of the LCLS project, representing the scheduled ramp down of activities.	-21,727
Total Funding Change, Construction	**+8,772**

Supporting Information

Operating Expenses, Capital Equipment and Construction Summary

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Operating Expenses	1,066,750	1,259,706	1,368,531
Capital Equipment	65,543	127,702	122,029
General Plant Projects	14,698	6,505	6,946
Accelerator Improvement Projects	12,500	32,591	33,754
Construction	93,265	145,468	154,240
Total, Basic Energy Sciences	1,252,756	1,571,972	1,685,500

Funding Summary

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Research	451,517	633,206	719,745
Scientific User Facilities Operations	666,333	718,968	742,749
Major Items of Equipment	30,543	34,000	25,000
Construction Projects	93,265	145,468	154,240
Other	11,098	40,330	43,766
Total, Basic Energy Sciences	1,252,756	1,571,972	1,685,500

Scientific User Facility Operations

(dollars in thousands)

	FY 2008	FY 2009	FY 2010
Advanced Light Source, LBNL	50,194	52,016	53,869
Advanced Photon Source, ANL	112,290	118,061	127,140
National Synchrotron Light Source, BNL	37,572	40,573	42,021
National Synchrotron Light Source-II, BNL	20,000	10,000	2,000
Stanford Synchrotron Radiation Light Source, SLAC	32,197	34,023	35,196
High Flux Isotope Reactor, ORNL	54,381	58,744	60,841
Intense Pulsed Neutron Source, ANL	8,400	4,000	4,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,655	11,136	11,533
Spallation Neutron Source, ORNL	174,444	177,523	183,872
Center for Nanophase Materials Sciences, ORNL	18,650	19,956	21,068
Center for Integrated Nanotechnologies, SNL/LANL	18,000	20,100	21,218
Molecular Foundry, LBNL	17,700	20,142	21,260

	(dollars in thousands)		
	FY 2008	FY 2009	FY 2010
Center for Nanoscale Materials, ANL	18,150	20,852	21,997
Center for Functional Nanomaterials, BNL	17,700	20,142	21,260
Linac Coherent Light Source (LCLS), SLAC	15,500	20,000	20,500
Linac for LCLS, SLAC	60,500	91,700	94,974
Total, Scientific User Facility Operations	666,333	718,968	742,749

Facilities Users and Hours

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Advanced Light Source			
Achieved Operating Hours	4,721	N/A	N/A
Planned Operating Hours	5,000	5,400	5,600
Optimal Hours	5,600	5,600	5,600
Percent of Optimal Hours	84.3%	96.4%	100%
Unscheduled Downtime	8.3%	<10%	<10%
Number of Users	1,939	2,100	2,200
Advanced Photon Source			
Achieved Operating Hours	4,503	N/A	N/A
Planned Operating Hours	4,380	4,800	5,000
Optimal Hours	5,000	5,000	5,000
Percent of Optimal Hours	90%	96%	100%
Unscheduled Downtime	2.4%	<10%	<10%
Number of Users	3,270	3,500	3,700
National Synchrotron Light Source			
Achieved Operating Hours	5,006	N/A	N/A
Planned Operating Hours	4,900	5,200	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	93%	96%	100%
Unscheduled Downtime	6.0%	<10%	<10%
Number of Users	2,128	2,100	2,100

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Stanford Synchrotron Radiation Light Source			
Achieved Operating Hours	5,027	N/A	N/A
Planned Operating Hours	4,500	5,000	5,400
Optimal Hours	5,400	5,400	5,400
Percent of Optimal Hours	93%	93%	100%
Unscheduled Downtime	2.9%	<10%	<10%
Number of Users	1,147	1,300	1,400
High Flux Isotope Reactor			
Achieved Operating Hours	3,539	N/A	N/A
Planned Operating Hours	3,100	3,900	4,500
Optimal Hours	4,500	4,500	4,500
Percent of Optimal Hours	79%	87%	100%
Unscheduled Downtime	1.3%	<10%	<10%
Number of Users	258	450	500
Intense Pulsed Neutron Source			
Achieved Operating Hours	1,013	—	—
Planned Operating Hours	1,000	—	—
Optimal Hours	3,600	—	—
Percent of Optimal Hours	28%	—	—
Unscheduled Downtime	4.5%	—	—
Number of Users	89	—	—
Manuel Lujan, Jr. Neutron Scattering Center			
Achieved Operating Hours	2,509	N/A	N/A
Planned Operating Hours	3,000	3,500	3,600
Optimal Hours	3,600	3,600	3,600
Percent of Optimal Hours	70%	97%	100%
Unscheduled Downtime	23.0%	<10%	<10%
Number of Users	261	280	300

	FY 2008 Actual	FY 2009 Estimate	FY 2010 Estimate
Spallation Neutron Source			
Achieved Operating Hours	2,819	N/A	N/A
Planned Operating Hours	2,700	4,000	4,500
Optimal Hours	2,700	4,500	4,500
Percent of Optimal Hours	63%	89%	100%
Unscheduled Downtime	23.1%	<10%	<10%
Number of Users	165	250	700
Center for Nanophase Materials Sciences[a]			
Number of Users	404	420	440
Center for Integrated Nanotechnologies[a]			
Number of Users	272	280	300
Molecular Foundry[a]			
Number of Users	303	315	330
Center for Nanoscale Materials[a]			
Number of Users	196	210	220
Center for Functional Nanomaterials[a]			
Number of Users	106	140	200
Total, All Facilities			
Achieved Operating Hours	29,137	N/A	N/A
Planned Operating Hours	28,580	31,800	34,000
Optimal Hours	35,800	34,000	34,000
Percent of Optimal Hours	76%	94%	100%
Unscheduled Downtime	8.5%	<10%	<10%
Number of Users	10,538	11,345	12,390

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[a] Facility operating hours are not measured at user facilities that do not rely on one central machine because such maintenance does not govern how many hours per year the whole facility can accommodate users.

Major Items of Equipment

(dollars in thousands)

	Prior Years	FY 2008	FY 2009	FY 2009 Additional Approp.	FY 2010	Outyears	Total
Spallation Neutron Source Instrumentation I (31MK), ORNL[a]							
TEC/TPC	39,244	11,856	12,000	—	5,000	400	68,500
Spallation Neutron Source Instrumentation II (71RB), ORNL[b]							
TEC/TPC	500	6,000	7,000	—	18,000	28,500	60,000
Linac Coherent Light Source Instrumentation (71RA), SLAC[c]							
TEC	500	6,000	15,000	+33,600	—	—	55,100
OPC	4,900	—	—	—	—	—	4,900
TPC	5,400	6,000	15,000	+33,600	—	—	60,000
Transmission Electron Aberration Corrected Microscope (61PC), LBNL							
TEC	5,500	6,100	—	—	—	—	11,600
OPC	14,900	587	—	—	—	—	15,487
TPC	20,400	6,687	—	—	—	—	27,087
SNS Power Upgrade Project ORNL							
TEC	—	—	—	—	2,000	TBD	TBD
OPC	—	—	—	—	—	TBD	TBD
TPC	—	—	—	—	2,000	TBD	TBD
Total, Major Items of Equipment							
TEC		29,956	34,000	+33,600	25,000		
OPC		587	—	—	—		
TPC		30,543	34,000	+33,600	25,000		

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[a] This FY 2003 MIE includes five instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Spectrometer.

[b] Mission Need (CD-0) was approved on October 31, 2005 with a TPC range of $40–60M. The baseline TPC will be approved at CD-2 (Approve Performance Baseline).

[c] Mission Need (CD-0) was approved on August 10, 2005 with a TPC range of $50–60M. The baseline TPC will be approved at CD-2 (Approve Performance Baseline).

Construction Projects

(dollars in thousands)

	Prior Years	FY 2008	FY 2009	FY 2009 Additional Approp.	FY 2010	Outyears	Total
08-SC-01 Advanced Light Source User Support Building, LBNL							
TEC	1,500	4,954	11,500	14,546	—	—	32,500[a]
OPC	2,480	—	4	136	—	—	2,620
TPC	3,980	4,954	11,504	14,682	—	—	35,120
08-SC-10 PED, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC							
TEC/TPC	—	941	—	—	—	—	941
08-SC-11 Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC							
TEC	—	6,391	3,728	—	—	—	10,119
OPC	—	100	40	—	—	—	140
TPC	—	6,491	3,768	—	—	—	10,259
07-SC-06, National Synchrotron Light Source-II, BNL							
TEC	3,000	29,727	93,273	150,000	139,000	376,200	791,200
OPC	27,800	20,000	10,000	—	2,000	61,000	120,800
TPC	30,800	49,727	103,273	150,000	141,000	437,200	912,000
05-R-320 Linac Coherent Light Source, SLAC							
TEC	248,904	50,889	36,967	—	15,240	—	352,000[b]
OPC	24,000	15,500	17,000	—	11,500	—	68,000
TPC	272,904	66,389	53,967	—	26,740	—	420,000
05-R-321 Center for Functional Nanomaterials, BNL							
TEC	79,334	363	—	—	—	—	79,697[c]
OPC	800	500	—	—	—	—	1,300
TPC	80,134	863	—	—	—	—	80,997

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[a] Includes $1,500,000 of PED included in the 07-SC-12 PED, LBNL Advanced Light Source User Support Building datasheet.

[b] Includes 35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source datasheet.

[c] Includes $5,966,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

(dollars in thousands)

	Prior Years	FY 2008	FY 2009	FY 2009 Additional Approp.	FY 2010	Outyears	Total
Total, Construction							
TEC		93,265	145,468	164,546	154,240		
OPC		36,100	27,044	136	13,500		
TPC		129,365	172,512	164,682	167,740		

Scientific Employment

(estimated)

	FY 2008	FY 2009	FY 2010
# of University Grants	1,000	1,200	1,300
Average Size per year	150,000	175,000	175,000
# Permanent Ph.D's (FTEs)	3,650	4,570	4,910
# Postdoctoral Associates (FTEs)	960	1,270	1,390
# Graduate Students (FTEs)	1,490	2,000	2,200

Budget Structure Funding Crosswalk

(dollars in thousands)

	FY 2008 Current Approp.	FY 2008 Comp. Adjust.	FY 2008 Comp. Approp.	FY 2009 Current Approp.	FY 2009 Comp. Adjust.	FY 2009 Comp. Approp.	FY 2010 Request
Materials Sciences and Engineering							
Materials Sciences and Engineering Research							
Experimental Condensed Matter Physics	40,628	—	40,628	46,398	—	46,398	51,387
Theoretical Condensed Matter Physics	27,255	—	27,255	29,448	—	29,448	30,455
Mechanical Behavior and Radiation Effects	13,268	—	13,268	14,336	—	14,336	14,826
Physical Behavior of Materials	28,226	—	28,226	30,498	—	30,498	31,541
Neutron and X-Ray Scattering	40,311	-8,500	31,811	46,971	—	46,971	48,613
Electron and Scanning Probe Microscopies	16,635	—	16,635	20,474	—	20,474	21,174
Experimental Program to Stimulate Competitive Research (EPSCoR)	14,680	—	14,680	16,755	—	16,755	8,520
Synthesis and Processing Science	15,587	—	15,587	16,841	—	16,841	17,417
Materials Chemistry and Biomolecular Materials	46,339	—	46,339	51,569	—	51,569	53,333
Energy Frontier Research Centers (EFRCs)	—	—	—	55,300	—	55,300	55,300
Electron-beam Microcharacterization	8,192	-8,192	—	11,250	-11,250	—	—
Energy Innovation Hub - Batteries and Energy Storage	—	—	—	—	—	—	34,020
Accelerator and Detector Research	2,747	-2,747	—	9,120	-9,120	—	—
Nanoscale Science Research Centers (OPC)	500	-500	—	—	—	—	—
Spallation Neutron Source Instrumentation I (SING I)	11,856	-11,856	—	7,000	-7,000	—	—
Spallation Neutron Source Instrumentation II(SING II)	6,000	-6,000	—	12,000	-12,000	—	—
Linac Coherent Light Source Ultrafast Science Instruments (LUSI)	6,000	-6,000	—	15,000	-15,000	—	—

(dollars in thousands)

	FY 2008 Current Approp.	FY 2008 Comp. Adjust.	FY 2008 Comp. Approp.	FY 2009 Current Approp.	FY 2009 Comp. Adjust.	FY 2009 Comp. Approp.	FY 2010 Request
Transmission Electron Aberration Corrected Microscope (TEAM)	6,687	-6,687	—	—	—	—	—
General Plant Projects	—	—	—	4,243	—	4,243	4,604
Total, Materials Sciences and Engineering Research	284,911	-50,482	234,429	387,203	-54,370	332,833	371,190
Facilities Operations							
Advanced Light Source, LBNL	50,194	-50,194	—	52,016	-52,016	—	—
Advanced Photon Source, ANL	112,290	-112,290	—	118,061	-118,061	—	—
National Synchrotron Light Source, BNL	37,572	-37,572	—	40,573	-40,573	—	—
National Synchrotron Light Source-II, BNL	20,000	-20,000	—	10,000	-10,000	—	—
Stanford Synchrotron Radiation Light Source, SLAC	32,197	-32,197	—	34,023	-34,023	—	—
Linac Coherent Light Source (LCLS), SLAC	15,500	-15,500	—	20,000	-20,000	—	—
Linac for LCLS, SLAC	60,500	-60,500	—	91,700	-91,700	—	—
High Flux Isotope Reactor, ORNL	54,381	-54,381	—	58,744	-58,744	—	—
Intense Pulsed Neutron Source, ANL	8,400	-8,400	—	4,000	-4,000	—	—
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,655	-10,655	—	11,136	-11,136	—	—
Spallation Neutron Source, ORNL	165,944	-165,944	—	177,523	-177,523	—	—
Center for Nanophase Materials Sciences, ORNL	18,650	-18,650	—	19,956	-19,956	—	—
Center for Integrated Nanotechnologies, SNL/LANL	18,000	-18,000	—	20,100	-20,100	—	—
Molecular Foundry, LBNL	17,700	-17,700	—	20,142	-20,142	—	—
Center for Nanoscale Materials, ANL	18,150	-18,150	—	20,852	-20,852	—	—
Center for Functional Nanomaterials, BNL	17,700	-17,700	—	20,142	-20,142	—	—
Total, Facilities Operation	657,833	-657,833	—	718,968	-718,968	—	—
SBIR/STTR	—	—	—	27,463	-18,632	8,831	9,922
Total, Materials Sciences and Engineering Research	942,744	-708,315	234,429	1,133,634	-791,970	341,664	381,112

(dollars in thousands)

	FY 2008 Current Approp.	FY 2008 Comp. Adjust.	FY 2008 Comp. Approp.	FY 2009 Current Approp.	FY 2009 Comp. Adjust.	FY 2009 Comp. Approp.	FY 2010 Request
Chemical Sciences, Geosciences, and Energy Biosciences							
Chemical Sciences, Geosciences, and Energy Biosciences Research							
Atomic, Molecular, and Optical Science	18,353	—	18,353	22,886	—	22,886	23,669
Chemical Physics Research	34,006	+6,755	40,761	47,886	—	47,886	51,468
Solar Photochemistry	30,479	—	30,479	34,685	—	34,685	35,871
Photosynthetic Systems	15,715	—	15,715	17,884	—	17,884	18,496
Physical Biosciences	15,105	—	15,105	17,189	—	17,189	17,777
Catalysis Science	40,412	—	40,412	46,506	—	46,506	48,139
Separations and Analysis	15,359	—	15,359	17,979	—	17,979	18,594
Heavy Element Chemistry	9,002	—	9,002	10,744	—	10,744	11,111
Geosciences Research	20,463	—	20,463	23,787	—	23,787	24,601
General Plant Projects	11,098	—	11,098	815	—	815	843
Energy Frontier Research Centers (EFRCs)	—	—	—	44,700	—	44,700	44,700
Energy Innovation Hub – Fuels from Sunlight	—	—	—	—	—	—	34,020
Total, Chemical Sciences, Geosciences, and Energy Biosciences Research	209,992	+6,755	216,747	285,061	—	285,061	329,289
Facilities Operations							
Combustion Research Facility	6,755	-6,755	—	—	—	—	—
SBIR/STTR	—	—	—	7,809	—	7,809	9,068
Total, Chemical Sciences, Geosciences, and Energy Biosciences	216,747	—	216,747	292,870	—	292,870	338,357
Scientific User Facilities							
Research							
Electron-Beam Microcharacterization	—	+8,192	8,192	—	+11,250	11,250	11,652
Accelerator and Detector Research	—	+2,747	2,747	—	+9,120	9,120	13,061
Nanoscale Science Research Centers (OPC)	—	+500	500	—	—	—	—
Total, Research	—	+11,439	11,439	—	+20,370	20,370	24,713

(dollars in thousands)

	FY 2008 Current Approp.	FY 2008 Comp. Adjust.	FY 2008 Comp. Approp.	FY 2009 Current Approp.	FY 2009 Comp. Adjust.	FY 2009 Comp. Approp.	FY 2010 Request
Major Items of Equipment							
Spallation Neutron Source Instrumentation I (SING I)	—	+11,856	11,856	—	+7,000	7,000	—
Spallation Neutron Source Instrumentation II (SING II)	—	+6,000	6,000	—	+12,000	12,000	5,000
Linac Coherent Light Source Ultrafast Science Instruments (LUSI)	—	+6,000	6,000	—	+15,000	15,000	18,000
Transmission Electron Aberration Corrected Microscope (TEAM)	—	+6,687	6,687	—	—	—	—
SNS Power Upgrade Project (PUP)	—	—	—	—	—	—	2,000
Total, Major Items of Equipment	—	+30,543	30,543	—	+34,000	34,000	25,000
Facilities Operations							
Advanced Light Source, LBNL	—	+50,194	50,194	—	+52,016	52,016	53,869
Advanced Photon Source, ANL	—	+112,290	112,290	—	+118,061	118,061	127,140
National Synchrotron Light Source, BNL	—	+37,572	37,572	—	+40,573	40,573	42,021
National Synchrotron Light Source-II, BNL	—	+20,000	20,000	—	+10,000	10,000	2,000
Stanford Synchrotron Radiation Light Source, SLAC	—	+32,197	32,197	—	+34,023	34,023	35,196
Linac Coherent Light Source (LCLS), SLAC	—	+15,500	15,500	—	+20,000	20,000	20,500
Linac for LCLS, SLAC	—	+60,500	60,500	—	+91,700	91,700	94,974
High Flux Isotope Reactor, ORNL	—	+54,381	54,381	—	+58,744	58,744	60,841
Intense Pulsed Neutron Source, ANL	—	+8,400	8,400	—	+4,000	4,000	4,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	—	+10,655	10,655	—	+11,136	11,136	11,533
Spallation Neutron Source, ORNL	—	+174,444	174,444	—	+177,523	177,523	183,872
Center for Nanophase Materials Sciences, ORNL	—	+18,650	18,650	—	+19,956	19,956	21,068

(dollars in thousands)

	FY 2008 Current Approp.	FY 2008 Comp. Adjust.	FY 2008 Comp. Approp.	FY 2009 Current Approp.	FY 2009 Comp. Adjust.	FY 2009 Comp. Approp.	FY 2010 Request
Center for Integrated Nanotechnologies, SNL/LANL	—	+18,000	18,000	—	+20,100	20,100	21,218
Molecular Foundry, LBNL	—	+17,700	17,700	—	+20,142	20,142	21,260
Center for Nanoscale Materials, ANL	—	+18,150	18,150	—	+20,852	20,852	21,997
Center for Functional Nanomaterials, BNL	—	+17,700	17,700	—	+20,142	20,142	21,260
Total, Facilities Operations	—	+666,333	666,333	—	+718,968	718,968	742,749
SBIR/STTR	—	—	—	—	+18,632	18,632	19,329
Total, Scientific User Facilities	—	+708,315	708,315	—	+791,970	791,970	811,791
Construction							
Advanced Light Source User Support Building, LBNL	4,954	—	4,954	11,500	—	11,500	—
Photon Ultrafast Laser and Science and Engineering Building Renovation, SLAC	6,391	—	6,391	3,728	—	3,728	—
Project Engineering and Design, Photon Ultrafast Laser and Science and Engineering Building Renovation, SLAC	941	—	941	—	—	—	—
National Synchrotron Light Source-II, BNL	29,727	—	29,727	93,273	—	93,273	139,000
Linac Coherent Light Source, SLAC	50,889	—	50,889	36,967	—	36,967	15,240
Center for Functional Materials, BNL	363	—	363	—	—	—	—
Total, Construction	93,265	—	93,265	145,468	—	145,468	154,240
Total, Basic Energy Sciences	1,252,756	—	1,252,756	1,571,972	—	1,571,972	1,685,500