Basic Energy Sciences

Funding Profile by Subprogram

(dollars in thousands)

	FY 2007 Current Appropriation	FY 2008 Original Appropriation	FY 2008 Adjustments	FY 2008 Current Appropriation	FY 2009 Request
Basic Energy Sciences					
Research					
Materials Sciences and Engineering	879,323	955,094	-1,034[ab]	954,060	1,125,579
Chemical Sciences, Geosciences, and Energy Biosciences	217,028	232,348	-9,771[ab]	222,577	297,113
Total, Research	1,096,351	1,187,442	-10,805[a]	1,176,637	1,422,692
Construction	125,029	94,122	-857[a]	93,265	145,468
Total, Basic Energy Sciences	1,221,380[c]	1,281,564	-11,662[a]	1,269,902	1,568,160
Stanford Linear Accelerator Center (SLAC) Linac Operations (non-add)	(37,550)	(61,500)	(—)	(61,500)	(96,700)
Basic Energy Sciences, excluding SLAC Linac Operations (non-add)[d]	(1,183,830)	(1,220,064)	(-11,662[a])	(1,208,402)	(1,471,460)

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"

Mission

The mission of the BES program—a multipurpose, scientific research effort—is to foster and support fundamental research to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. The portfolio supports work in the natural sciences by emphasizing fundamental research in materials sciences, chemistry, geosciences, and physical biosciences.

Basic research supported by the BES program touches virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. Research in materials

[a] Reflects a reduction for the 0.91% rescission in P.L. 110–161, the Energy and Water Development and Related Agencies Appropriations Act, 2008 as follows: Materials Sciences and Engineering ($-8,691,000); Chemical Sciences, Geosciences, and Energy Biosciences ($-2,114,000); and Construction ($-857,000).
[b] Includes a reallocation of funding within BES in accordance with the Energy and Water Conference Report, as follows: Materials Sciences and Engineering ($+7,657,000) and Chemical Sciences, Geosciences, and Energy Biosciences ($-7,657,000) to optimize funding for research and facility operations within the BES program.
[c] Total is reduced by $28,870,000: $25,777,000 of which was transferred to the Small Business Innovative Research (SBIR) program and $3,093,000 of which was transferred to the Small Business Technology Transfer (STTR) program.
[d] The SLAC linear accelerator (linac) supported operations of the B-Factory funded by High Energy Physics (HEP) through FY 2008. The linac also supports operations of the Linac Coherent Light Source currently under construction and funded by BES. SC has been transitioning funding of the SLAC linac from HEP to BES, with FY 2009 representing the first year of total funding by BES. BES totals without SLAC linac funding are presented to display program growth exclusive of this functional transfer.

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. History has taught us that seeking answers to fundamental questions results in a diverse array of practical applications as well as some remarkable revolutionary advances.

Strategic and GPRA Unit Program Goals

The Department's Strategic Plan identifies five Strategic Themes (one each for nuclear, energy, science, management, and environmental aspects of the mission) plus 16 Strategic Goals that tie to the Strategic Themes. The BES program supports the following goals:

Strategic Theme 3, Scientific Discovery & Innovation
Strategic Goal 3.1, Scientific Breakthroughs: Achieve the major scientific discoveries that will drive U.S. competitiveness; inspire America; and revolutionize our approaches to the nation's energy, national security, and environmental quality challenges.

Strategic Goal 3.2, Foundations of Science: Deliver the scientific facilities, train the next generation of scientists and engineers, and provide the laboratory capabilities and infrastructure required for U.S. scientific primacy.

The BES program has one 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 and the Chemical Sciences, Geosciences, and Energy Biosciences 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 and biological systems.

Develop new concepts and improve existing methods to assure a secure energy future, e.g., for solar energy conversion and for other energy sources.

Conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with high magnetic and electric fields.

Funding by Strategic and GPRA Unit Program Goal

(dollars in thousands)

	FY 2007	FY 2008	FY 2009
Strategic Goals 3.1, Scientific Breakthroughs and 3.2, Foundations of Science			
GPRA Unit Program Goal 3.1/2.50.00 Advance the Basic Science for Energy Independence			
Basic Energy Sciences	1,221,380	1,269,902	1,568,160

Annual Performance Results and Targets

FY 2004 Results	FY 2005 Results	FY 2006 Results	FY 2007 Results	FY 2008 Targets	FY 2009 Targets
GPRA Unit Program Goal 3.1/2.50.00 (Advance the Basic Science for Energy Independence)					
Materials Sciences and Engineering					
Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 100 nm and in the soft x-ray region was measured at 19 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 20 femtoseconds in duration with an intensity of 10,000 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: 91.9%). [Met Goal]	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]	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 two-dimensional combustion reacting flow simulation was performed involving 44 reacting species and 518,400 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 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.		

[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 2004 Results	FY 2005 Results	FY 2006 Results	FY 2007 Results	FY 2008 Targets	FY 2009 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: +1.3% cost variance and +0.8% 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: +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 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-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects. In FY08, it is at least 10% and 10%, respectively.	Cost-weighted mean percent variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects. In FY09, it is at least 10% and 10%, respectively.

Means and Strategies

The BES program supports fundamental peer-reviewed research to create new knowledge in areas important to the BES mission and supports the design, construction, and operation of a wide array of scientific user facilities for the preparation and examination of materials properties and their physical and chemical transformations. All research projects and facilities undergo regular peer review and merit evaluation based on procedures set down in 10 CFR 605 for the extramural grant program and under a similar process for the laboratory programs and scientific user facilities. All new projects are selected through peer review and merit evaluation.

External factors, in addition to budgetary constraints, that affect the level of performance include:

- changing mission needs as described by the DOE and SC mission statements and strategic plans;
- scientific opportunities as determined, in part, by scientific workshops and proposals received by researchers;
- the results of external program reviews and international benchmarking activities of entire fields or sub-fields, such as those performed by the National Academy of Sciences;
- unanticipated failures in critical components of scientific user facilities or major research programs; and
- strategic and programmatic decisions made by non-DOE funded domestic research activities and by major international research centers.

The BES program in fundamental science is coordinated with the activities of other programs within the Office of Science, with programs of the DOE technology office and the National Nuclear Security Administration, and with programs of other federal agencies. BES also promotes the transfer of the results of its basic research to contribute to DOE missions in areas of energy efficiency, renewable energy resources, improved use of fossil fuels, nuclear energy, reduced environmental impacts of energy production and use, national security, and future energy sources.

Validation and Verification

Progress against established plans is evaluated by periodic internal and external performance reviews. These reviews provide an opportunity to verify and validate performance. Monthly, quarterly, semiannual, and annual reviews consistent with specific program management plans are performed to ensure technical progress, cost and schedule adherence, and responsiveness to program requirements.

Program Assessment Rating Tool (PART)

The Department has implemented a tool to evaluate selected programs. PART was developed by the Office of Management and Budget (OMB) to provide a standardized way to assess the effectiveness of the Federal Government's portfolio of programs. The structured framework of the PART provides a means through which programs can assess their activities differently than through traditional reviews. The BES program has incorporated feedback from OMB into the FY 2009 budget request and has taken or will take the necessary steps to continue to improve performance.

In the FY 2003 PART review for the FY 2005 Budget, OMB gave the BES program a score of 93% overall, which corresponds to a rating of "Effective." OMB found the program to be strategically driven and well managed. Outside expert panels have validated the program's merit-based review processes ensuring that research supported is relevant and of very high quality. The assessment also found that BES has developed a limited number of adequate performance measures, which are continued for FY 2009. These measures have been incorporated into this budget request, BES grant solicitations, and the performance plans of senior managers. As appropriate, they will be incorporated into the performance based contracts of M&O contractors. Roadmaps, developed in consultation with the Basic Energy Sciences Advisory Committee (BESAC), will guide triennial reviews by BESAC of progress toward achieving the long term Performance Measures. These roadmaps are posted on the SC website. The Annual Performance Targets are tracked through the Department's Joule system and reported in the Department's Annual Performance and Accountability Report.

To improve public access to PART assessments and follow up actions, OMB has created the ExpectMore.gov web site. Information concerning BES PART assessments and current follow up actions can be found by searching on "basic energy sciences" at http://ExpectMore.gov.

Basic and Applied R&D Coordination

Electrical Energy Storage (EES): The Basic Energy Sciences program is proposing $33,938,000 in the request to support basic research in electrical energy storage (EES). Within this funding, $2,000,000 is targeted for a formally coordinated program with DOE applied technology offices. This R&D coordination focus area was the subject of a BES workshop held in April 2007. The workshop report noted that revolutionary breakthroughs in EES have been singled out as perhaps the most crucial need for this nation's secure energy future. The report concluded that the breakthroughs required for tomorrow's energy storage needs will be realized with fundamental research to understand the underlying processes involved in EES. The knowledge gained will in turn enable the development of novel EES concepts that incorporate revolutionary new materials and chemical processes. Such research will accelerate advances in developing novel battery concepts for hybrid and electric cars, lessening our dependence on oil. It will also help facilitate successful utilization and integration of renewable, intermittent power sources such as solar, wind, and wave energy into the utility sector, making these energy sources base load competitive.

Applied technology offices within DOE that could benefit from the Electrical Energy Storage research coordination effort include: the Offices of Electricity Delivery and Energy Reliability (for research on utility-scale electrical energy storage) and Energy Efficiency and Renewable Energy (the FreedomCAR and Vehicle Technologies program for research on batteries for vehicle technologies and Solar Energy Technologies program for research on energy storage for solar energy utilization).

Carbon Dioxide Capture and Storage: The Basic Energy Sciences program is proposing $10,915,000 in the request to support basic research in carbon dioxide capture and storage. The storage portion of this R&D coordination focus area was the subject of a BES workshop on Basic Research Needs for Geosciences in February 2007, which focused on the research challenges posed by carbon dioxide storage in deep porous geological formations. The workshop report noted that the chemical and geological processes involved in the storage of carbon dioxide are highly complex and its prediction would need an interdisciplinary approach that strongly couples experiments with theory, modeling, and computation bridging multiple length and time scales. Major research priorities were identified in the areas of multiphase fluid flow and materials transport in deep formations, dynamic imaging of flow and transport, fluid-induced rock deformation, transport properties, and *in situ* characterization of fluid trapping, isolation and immobilization, mineral fluid interface complexity and dynamics, and developing high-resolution modeling capabilities for predicting storage site performance. The report concluded that the breakthroughs in carbon dioxide storage required for carbon-free utilization of fossil fuels will be realized with fundamental research to understand the underlying chemical, geochemical, and geophysical processes involved in subsurface sequestration sites. Research in carbon dioxide capture would include fundamental studies of chemical processes and membranes for the separation of carbon dioxide from both post- and pre-combustion gas streams.

Applied technology offices within DOE that could benefit from the Carbon Dioxide Capture and Storage research coordination effort include the Office of Fossil Energy.

Characterization of Radioactive Waste: The Basic Energy Sciences program is proposing $8,492,000 in the request to support basic research in radioactive waste characterization. This R&D coordination focus area was the subject of a number of BES workshops, including the Basic Research Needs for Advanced Nuclear Energy Systems (July 2006), Basic Research Needs for Geosciences (February 2007), and Basic Research Needs for Materials under Extreme Environments (June 2007). The workshop reports noted that the materials and chemical processes involved in radioactive waste storage are highly complex and their characterization would need an interdisciplinary approach that strongly couples experiments with theory, modeling, and computation bridging multiple length and time scales. The reports concluded that the breakthroughs in radioactive waste characterization required for tomorrow's energy needs will be realized with fundamental research to understand the underlying physical and chemical processes that occur under the conditions of radioactive waste storage, which include extremes of temperature, pressure, radiation flux, and multiple complex phases. The knowledge gained will in turn enable finding the permanent solutions to nuclear waste disposal, making nuclear power a major component in primary energy usage and lessening our dependence on oil.

Applied technology offices within DOE that could benefit from the Characterization of Radioactive Waste research coordination effort include the Offices of Nuclear Energy, Environmental Management, and Civilian Radioactive Waste Management.

Predicting High Level Waste System Performance over Extreme Time Horizons: The Basic Energy Sciences program is proposing $8,492,000 in the request to support basic research in predicting high level waste (HLW) system performance over extreme time horizons. This R&D coordination focus area was the subject of a BES workshop on Basic Research Needs for Geosciences in February 2007, which focuses on research challenges posed by geological repositories for HLW. The workshop report noted that the chemical and geological processes involved in the performance of HLW systems over extreme time scales are highly complex and its prediction would need an interdisciplinary approach that strongly couples experiments with theory, modeling, and computation bridging multiple length and time scales. The report concluded that the breakthroughs in predicting HLW performance required for tomorrow's energy needs will be realized with fundamental research to understand the underlying chemical, geochemical, and geophysical processes involved in the highly radioactive environments. Major research priorities were identified in the areas of computational thermodynamics of complex fluids and solids, nanoparticulate and colloid physics and chemistry, biogeochemistry in extreme and perturbed environments, highly reactive subsurface materials and environments, and simulation of complex multi-scale systems for ultra-long times. The knowledge gained will in turn enable finding the permanent solutions to nuclear waste disposal, making nuclear power a major component in primary energy usage and lessening our dependence on oil. It will further advance the goal of addressing environmental remediation needs

Applied technology offices within DOE that could benefit from the Predicting High Level Waste System Performance over Extreme Time Horizons research coordination effort include: Offices of Nuclear Energy; Environmental Management; and the Civilian Radioactive Waste Management Program.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Electrical Energy Storage			
Materials Sciences and Engineering Research	—	—	16,969
Chemical Sciences, Geosciences, and Energy Biosciences	—	—	16,969
Total, Electrical Energy Storage	—	—	33,938
Carbon Dioxide Capture and Storage			
Chemical Sciences, Geosciences, and Energy Biosciences	5,915	5,915	10,915
Characterization of Radioactive Waste			
Chemical Sciences, Geosciences, and Energy Biosciences	—	—	8,492
Predicting High Level Waste System Performance Over Extreme Time Horizons			
Materials Sciences and Engineering Research	—	—	8,492
Total, Basic and Applied R&D Coordination	5,915	5,915	61,837

Overview

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 as it continued to evolve through legislation included in the Atomic Energy Act of 1954, the Energy Reorganization Act of 1974, the Department of Energy Organization Act of 1977, and the Energy Policy Acts of 1992 and 2005.

Today, the BES program is one of the nation's largest sponsors of research in the natural sciences. It is uniquely responsible for supporting fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences impacting energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. In FY 2007, the program funded research in more than 173 academic institutions located in 48 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. The BES synchrotron radiation light sources, the neutron scattering facilities, and the electron beam characterization centers represent the largest and best collection of such facilities supported by a single organization in the world. Annually, more than 10,000 researchers from universities, national laboratories, and industrial laboratories will perform experiments at these facilities in the coming years. Spurred by results of past investments and by innovations in accelerator concepts, the BES program continues its pioneering role in the development of new generations of scientific research instruments and facilities.

The 2001 “National Energy Policy” noted that the U.S. economy grew by 126% since 1973, but energy use increased by only 30%. Approximately one-half to two-thirds of the savings resulted from technological improvements in products and services that allow consumers to enjoy more energy services without commensurate increases in energy demand. At the heart of these improvements is fundamental research. The future holds even greater promise, largely because of our new atom-by-atom understanding of matter and the subsequent unprecedented ability to design and construct new materials at the nanoscale with properties that are not found in nature. The BES program has played a major role in enabling the nanoscale revolution. This impact results from a deliberate philosophy of identifying seminal challenges and establishing both coordinated programs and facilities that together transcend what individuals alone can do. The program in nanoscale science, including the construction and operation of Nanoscale Science Research Centers, continues that philosophy.

Advisory and Consultative Activities

Charges are provided to BESAC by the Under Secretary for Science, who also serves as the Director of the Office of Science. 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 prompted 10 follow-on “Basic Research Needs” workshops supported by BES in the past 5 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 CO_2); materials under extreme environments; and catalysis for energy applications. Together these workshops attracted over 1,500 participants from universities, industry, and DOE laboratories. BESAC is now charged with summarizing the results of these 10 workshops and relating this summary to the science themes identified in the 2007 BESAC Grand Challenges study.

Information and reports for all of the above mentioned advisory and consultative activities are available on the BESAC website (http://www.science.doe.gov/bes/BESAC/BESAC.htm). Other studies are commissioned as needed using the National Academy of Science’s National Research Council and other independent groups.

Facility Reviews

Facilities are reviewed using external, independent review committees operating according to the procedures established for peer review of BES laboratory programs and facilities (http://www.science.doe.gov/bes/labreview.html). 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.

These reviews have identified both best practices and issues, including those associated with mature facilities. For example, the light sources experienced a quadrupling of the number of users in the decade of the 1990s, and their reviews highlighted the change that occurred as they transitioned from a mode in which they served primarily expert users to one in which they served very large numbers of inexperienced users in a wide variety of disciplines. The outcomes of these reviews helped develop new models of operation for existing light sources and for the Spallation Neutron Source, which was completed in FY 2006, and the National Synchrotron Light Source-II (NSLS-II), which will begin 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" (http://www.science.doe.gov/opa/PDF/revhndbk.pdf). In general, once a project has entered the construction phase (e.g., the Linac Coherent Light Source), 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.

Planning and Priority Setting

Because the BES program supports a broad portfolio, planning is an ongoing activity. Many long-range planning exercises for elements of the BES program are performed under the auspices of BESAC. Inputs to prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities.

These considerations have led to the following: increased investments in science at the nanoscale to take advantage of the remarkable knowledge gained from atomic-scale understanding of materials; increased investments for operations of the major user facilities in recognition of the quadrupling of users in the past decade and to reap the rewards of the capital investments in the facilities themselves; increased investments for instrumentation at the facilities so that the quality of the instruments will match the world-class quality of the facilities; increased investments for ultrafast science to probe processes that happen on the timescale of chemical reactions; and increases for targeted program areas for which both scientific opportunity and mission need are high (e.g., basic research for effective solar energy utilization). Construction of new user facilities, such as the Spallation Neutron Source, follows from input from BESAC and from broad, national strategies that include the input from multiple federal agencies.

Significant Program Shifts

- The Intense Pulsed Neutron Source is closed in FY 2008 due to competing priorities. Funds are provided in FY 2009 to maintain the facility in a safe storage condition.

Additional research funding is provided in the following areas:

- **Basic research for the hydrogen economy (+$24,012,000).** Research to realize the potential of a hydrogen economy will be increased from $36,388,000 to $60,400,000. The research program is based on the BES workshop report "Basic Research Needs for the Hydrogen Economy."
- **Basic research for effective solar energy utilization (+$33,369,000).** Investments will be focused in three areas: solar-to-electric, solar-to-fuels, and solar-to-thermal conversions. Many of the proposed research directions identified in the 2005 BES workshop report "Basic Research Needs for Solar Energy Utilization" concern important cross-cutting issues such as (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties (e.g., polycrystalline materials versus expensive single crystal materials or plastics and polymers instead of metals and semiconductors); (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar

energy conversion infrastructure, such as transparent conductors and robust, inexpensive thermal management materials.

- **Basic research for advanced nuclear energy systems (+$16,984,000).** Basic research related to advanced fuel cycles is needed in areas such as (1) control and predictive capability of processes driven by small energy differences, e.g., aggregation and precipitation; (2) fundamental principles to guide ligand design; (3) investigation of new separations approaches based on magnetic and electronic differences; (4) development of environmentally benign separations processes, which produce no secondary wastes and consume no chemicals; and (5) development of modeling of separations processes to optimize waste minimization and minimize opportunities for diversion of nuclear materials (i.e. optimize proliferation resistance).
- **Complex systems or emergent behavior (+$5,000,000).** Emergent behaviors arise from the collective, cooperative behavior of individual components of a system. Current understanding of emergent behaviors is very limited. The challenge of understanding how emergent behavior results from the complexity of competing interactions is among the most compelling of our time, spanning physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magneto resistance, random field magnets, and spin liquids and glasses.
- **Ultrafast science (+$10,000,000).** Ultrafast science deals with physical phenomena that occur in the range of one-trillionth of a second (one picosecond) to less than one-quadrillionth of a second (one femtosecond). New investments in ultrafast science will focus on research applications of x-ray sources associated with BES facilities and beamlines: the Linac Coherent Light Source; the femtosecond "slicing" beamline at the Advanced Light Source; and the short pulse development at the Advanced Photon Source. Investments will also be made in the development and applications of laser-driven, table-top x-ray sources, including the use of high-harmonic generation to create bursts of x-rays on the even shorter than the femtosecond time scale.
- **Mid-scale instrumentation (+$19,600,000).** Scientific progress is predicated on observations of new phenomena, which often involve the building of better tools. There is a significant national need for mid-scale instruments that serve multiple users yet which are not as large as the synchrotron and neutron sources. High priority mid-scale instrumentation needs include end stations at the synchrotron light sources and neutron scattering facilities; laser systems for ultrafast or high-energydensity studies; micro- and atomic-scale characterization tools such as electron microcharacterization and scanning probe microscopy; high-field magnets; and facilities for providing large crystals and other unique materials for researchers throughout the Nation.
- **Chemical imaging (+$5,000,000).** Investments will develop and apply new methods to measure the chemical behavior of individual molecules and reactions, with high resolution in both space and time in order to elucidate fundamental principles of chemical processes at the nanoscale level. The research will build on current single-molecule spectroscopies and microscopies by adding simultaneous time-dependent characterization of evolving chemical processes, ultimately with femtosecond time resolution.
- **Electrical energy storage (EES) ($+33,938,000)**. The use of electricity generated from intermittent, renewable sources requires efficient EES in order to effectively integrate it into the baseload grid system and to use it in transportation applications. A number of specific areas of research for both batteries and electrochemical capacitors have been identified: (1) 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. (2) Charge transfer and transport—molecular scale understanding of interfacial

electron transfer. (3) Electrolytes—electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity. (4) 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. (5) Multi-scale modeling—computational tools with improved integration of length and time scales to understand the complex physical and chemical processes that occur in EES from the molecular to system scales.

- **Carbon Sequestration ($+5,000,000)**. Research will be undertaken to develop the scientific understanding that will underpin novel technological approaches to deep underground carbon sequestration. Research directions identified in the 2007 BES workshop report "Basic Research Needs for Geosciences" include: (1) understanding geochemical processes relevant to the dimensions of subsurface sequestration sites and incorporating realistic chemistry of reacting flowing fluids into predictive models of geological formations; (2) development of critical geophysical measurement techniques to enable remote probing and tracking of important chemical and physical processes within rock formations at depth, including capture of rock heterogeneity; and (3) development and application of fluid-flow measurement approaches and simulation tools that can link, and explicitly couple, chemical and physical processes at multiple scales.

Materials Sciences and Engineering

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Materials Sciences and Engineering			
Materials Sciences and Engineering Research	265,092	283,851	379,393
Facilities Operations	614,231	645,869	719,247
SBIR/STTR	—	24,340	26,939
Total, Materials Sciences and Engineering	879,323	954,060	1,125,579

Description

This subprogram includes two major activities. The first activity is fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties.

The second activity supported by this subprogram is the R&D, planning, and operation of scientific user facilities for the fabrication of materials and for the examination of materials 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.

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 focus 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.

In the R&D, planning, and operations of facilities, synchrotron radiation light source facilities, neutron scattering facilities, electron-beam microcharacterization centers, and nanoscale science research centers provide a unique set of analytical tools that reveal the atomic structure and functions of complex materials. Annually, the BES user facilities are visited by 10,000 scientists and engineers in many fields. These facilities are unique and improve the competitiveness of the U.S. scientific and technological establishment. Also supported are research activities leading to the improvement of today's facilities and to the development of next generation facilities.

Selected FY 2007 Research Accomplishments

- *Nanoscale building blocks for energy technologies.* Nanoscale materials hold great promise for enabling new concepts and approaches in energy applications, because the elementary steps of energy conversion take place at the nanometer length scale. There are many recent examples where quantum confinement in nanomaterials has produced unexpected phenomena exploitable in energy technologies. Taking advantage of the unique electronic structure in semiconductor quantum dots, containing only 50 atoms each, researchers have demonstrated white light emission with high luminescence efficiency, offering a revolutionary new nanomaterial for use in solid-state lighting. Equally interesting is the metallic quantum dot that exhibits exceptionally long electron-spin relaxation time due to discrete energy levels; the long relaxation time is needed for quantum information processing and for the development of quantum computers. Nanoscale phenomena have also been shown to produce a new-class of thermoelectrics, materials that convert heat into electricity. With reducing size, changes in the corresponding electronic structure afford independent control over the electron and phonon transport, enabling optimization of both electrical and thermal properties. Such control is not available in bulk materials. By embedding nanoscale structures into bulk thermoelectric materials, researchers have melded nanoscale electronic control with bulk-level microstructural tailoring, leading to very high thermoelectric conversion efficiencies. Such advances are especially critical for the conversion of waste heat in vehicles into useful electricity, which increases fuel efficiency. These results demonstrate that the control of materials and phenomena at the nanoscale can lead to revolutionary breakthroughs in energy relevant technologies.
- *New materials for radiation environments.* Materials capable of resisting damage from intense radiation are essential for advanced nuclear energy systems. The primary radiation-damage mechanism in materials involves the creation and accumulation of structural defects such as atomic dislocations, vacancies, and other anomalies. Multiple defects could lead to the collapse of the ordered crystalline structure of the material, adversely affecting the integrity of material components used in nuclear energy systems. Recent studies have shown that materials can be made radiation-damage resistant by creating structures that actually accommodate radiation-induced structural disorder on the atomic scale. Complex oxides are candidate materials for these structures, because they exhibit strong tendencies for natural atomic disordering. As a result, the formation of radiation-induced defects causes very little structural change, allowing the crystal structure to remain mechanically intact. The materials exhibit good radiation tolerance after high-level radiation exposure. Similarly, radiation damage can be accommodated in composite materials containing a high volume fraction of nanoscale interfaces. The interfaces are found to possess a strong affinity for defects, thereby catalytically removing them from the bulk of the material. The accumulation of large numbers of defects would otherwise lead to embrittlement and loss of mechanical integrity.

The research has provided fundamental insight into tailoring the atomic structure of materials to achieve substantial improvements in radiation damage tolerance.

- *Emergent electronic behavior from graphene.* Researchers have found through electrical transport measurements that electron dynamics are relativistic in graphene, essentially an unrolled single-walled carbon nanotube. Specifically, under proper conditions, the electrons in graphene behave like massless particles such as photons and move through the material at a constant speed with very little scattering. Furthermore, the electrons in graphene exhibit the quantum Hall effect (QHE) at room temperature, which surprised the condensed matter physics community since QHE was only observed at ultra low temperature previously. This may lead to the development of ultrafast energy-efficient devices fabricated from materials as simple as a single atomic layer of carbon atoms.
- *Ultrafast movies of the turbulent magnetic nanoworld.* The extremely short timescale of magnetic switching, normally in the nanosecond or shorter regime, has prevented the direct visualization of the switching process until now. With recent advances in ultrafast x-ray techniques in conjunction with the advent of state-of-the-art x-ray microscopy, researchers have succeeded for the first time in observing the spin-injection process by motion pictures with 200 picoseconds (2×10^{-10} seconds) frame speed and 30 nm spatial resolution.
- *Catalytic breakthrough boosts hydrogen fuel cells.* Catalysis is vital to the operation of hydrogen fuel cells for reducing kinetic barriers and improving electrochemical reaction efficiencies. By alloying platinum single crystals with nickel, which preferentially enriches the second layer beneath the surface, researchers have altered the electronic structure of surface states that control catalytic activity. The study has revealed that the sub-surface layers could play a significant role in controlling the catalytic activity. The knowledge gained has enabled further control of the bond strengths among the catalyst, reactant, and blocking species, leading to significant improvements in catalytic stability and performance, including a 90-fold improvement in activity over pure platinum for the oxygen-reducing cathodic fuel cell reaction. This novel basic science approach demonstrates a new route for an advanced concept in nanoscale catalyst assembly.

Selected FY 2007 Facility Accomplishments

- *The Spallation Neutron Source (SNS) completes its first full year of operation.* The SNS beam power has been steadily increased during the first operation year to a power of 185 kilowatts, a world record for pulsed spallation sources. During FY 2007, the SNS delivered 3,500 hours of neutron production time, including more than 1,800 hours for users on three instruments, a backscattering spectrometer and two reflectometers. The SNS has actively reached out to users by coordinating the “Imaging and Neutrons 2006” conference; supporting a short course, “Neutron Scattering in Earth Sciences;” and sponsoring a booth at the American Crystallographic Association annual meeting.
- *The High Flux Isotope Reactor (HFIR) resumes regular operation after major upgrades.* HFIR has resumed operation after several infrastructure and system modifications. A super-critical hydrogen cold source, which operates at 18 Kelvin and provides world-class cold neutron brightness to instruments through four super-mirror neutron guides, has been installed in one of the HFIR beamlines. Several facility modifications have been performed to provide the new systems and infrastructure necessary to safely operate the cold source at cryogenic temperatures in a reactor environment and to enable safe and reliable transmission of the cold neutron beam to the adjacent cold neutron scattering guide hall. In FY 2007, HFIR has operated for three complete cycles. With successful cold source operation, two small-angle neutron scattering instruments were added in 2007 and are currently being commissioned. Nearly 100 users conducted experiments at HFIR in

FY 2007. In addition to neutron production, 234 experiment capsules were irradiated for medical and commercial isotope development and for fusion energy development, including for ITER and US/Japan Collaborative programs.

- *Synchrotron radiation light sources again host more than 8,000 users.* The steady increase in numbers of light source users from 1,657 in FY 1990 to 8,538 in FY 2007 is expected to continue through FY 2009. In anticipation of further expansion of the number of users, BES is increasing user support funding at all of the light sources and is adding new space, with the new User Support Building at the ALS as one example. In FY 2007, SSRL studies on carbon-hydrogen bonds in carbon nanotubes showed that almost complete hydrogenation is possible, corresponding to a hydrogen storage capacity of more than seven weight percent. At the APS, it was shown that the lowest thermal conductivity ever measured for a dense solid resulted from synthesizing a tungsten diselenide sample with random crystal plane stacking; materials with low thermal conductivity could lead to more energy efficient engine design in the future.
- *Full operations at four of the five Nanoscale Science Research Centers.* The first of the five BES Nanoscale Science Research Centers (NSRCs) completed its first full year of operation as a user facility in FY 2006. Three more NSRCs completed installation of initial technical equipment and transitioned to full user operations mode in FY 2007, with the fifth NSRC completing building construction. They are major scientific user facilities in which leading-edge synthesis and processing capabilities are integrated with exceptional tools and expertise for characterization and with corresponding resources for theory, modeling, and simulation. The NSRCs have established a joint ES&H (Environmental, Safety, and Health) working group, which has documented an “Approach to Nanomaterials ES&H” that provides guidance and suggestions on practices and procedures; this document has been widely disseminated and accepted both within and beyond the DOE community.
- *Electron microscopy centers reveal new materials properties and crystal growth modes.* Scientific advances enabled by electron scattering at these facilities span a wide range of materials and phenomena. One example is *in-situ* microscopy use to reveal that epitaxial growth of palladium islands on ruthenium surfaces occurs via a “snake-like” motion that gives rise to nanoscale labyrinth patterns, rather than a more standard and expected “step-like” linear growth mechanism. These studies are a first step in understanding the connection between surface morphology and alloying, and towards controlling surface structure and composition patterns.

Detailed Justification

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Materials Sciences and Engineering Research	**265,092**	**283,851**	**379,393**
▪ **Experimental Condensed Matter Physics**	**42,720**	**40,720**	**50,509**

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 nanoscale 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 2009, funding will be provided ($+2,500,000) to initiate a national network for the synthesis of new materials and the growth of high quality single crystals for the exploration of new physical phenomena. This activity will enable U.S. scientists with the state-of-the-art synthetic capabilities to produce crystals of novel materials with the highest quality; and to train the next generation of scientists capable of growing high quality crystals. The single crystal growth efforts will provide high-quality single crystal samples to enable researchers to fully utilize the capabilities at the advanced neutron and x-ray light sources. Major activities will continue in the development of nanomaterials for hydrogen storage ($+3,350,000), which exhibit size-dependent properties that are not seen in macroscopic solid-state materials. Enhanced electrical, thermal, mechanical, optical, and chemical properties have shown that these new nanomaterials could lead to dramatic improvements in the technologies relevant to fuel cells, batteries, capacitors, nanoelectronics, sensors, thermal management, super-strong lightweight materials, hydrogen storage, and electrical power transmission. A particular emphasis is the study of photovoltaics for solar energy use ($+3,939,000).

	FY 2007	FY 2008	FY 2009
▪ **Theoretical Condensed Matter Physics**	**23,208**	**25,832**	**36,190**

This activity was formerly named Condensed Matter Theory. The 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 the 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 leading to 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.

	(dollars in thousands)	
FY 2007	FY 2008	FY 2009

In FY 2009, there is an increase to support theory, modeling and simulation to understand mechanisms governing the complex physical and chemical processes for high density electrical energy storage ($+2,000,000). Emphasis will be on developing multi-scale computational tools and methods with integration of length and time scales to aid design of interfaces in batteries and ultracapacitors. Predictive models of the kinetics of materials phase changes, especially those accompanying charge transfer, transport, and evolution in electrode microstructures, will be critical to provide detailed insight into electrochemical processes at the molecular level. An enhancement will be made to theoretical efforts concerning emergent behavior research ($+1,500,000). The research aims at 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 or smaller. The proposed program will encompass both theoretical and computational approaches capable of interrogating systems to gain direct insight on the mechanisms underpinning the cooperative behavior. Within this funding, there is an increase to support new theory, modeling, and simulation of materials for high-capacity solid-state hydrogen storage ($+2,938,000) and materials for solar energy use ($+1,920,000). A major emphasis of the program is obtaining a theoretical understanding of nanoscale phenomena in materials for energy use, storage, and transmission ($+2,000,000).

	FY 2007	FY 2008	FY 2009
▪ **Mechanical Behavior and Radiation Effects**	**12,626**	**13,620**	**23,112**

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 abilities to predict materials performance and reliability and to address service life extension issues are 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 2009, there is an increase to enhance core research in high-temperature mechanical behavior and radiation effects in materials under extreme conditions ($+1,000,000). Of particular interest are environments involving energetic flux, chemical reactive stimulants, thermomechanical processes, and magnetic and electric fields. The primary emphasis will be on discovering novel phenomena and materials for improved performance with superior functionality. Additional funds are also requested for new basic research to develop a new generation of robust materials for utilization in high-temperature and irradiation-probe environments for advanced nuclear energy systems ($+8,492,000). The emphasis of this research will be devoted to establishing unified models to predict the mechanical and degradation behavior of solids over multiple length and time scales through new and emerging advanced scientific facilities and high-performance parallel-computing platforms. Novel in-situ experiments in realistic environments 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. Such advances in this area will provide the underpinning science that will enable licensing nuclear waste packages for emplacement in the Yucca Mountain repository and the discovery of new materials for use within Generation-IV nuclear reactors and other nuclear energy systems, such as accelerator-driven nuclear fission and transmutation.

	FY 2007	FY 2008	FY 2009
▪ **Physical Behavior of Materials**	**25,964**	**25,960**	**33,539**

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 underpins the DOE mission by developing the basic science necessary for improving materials reliability in chemical, electrical, and electrochemical applications and for improving the generation and storage of energy. With increased demands being placed on materials in energy-relevant environments, such as extreme temperatures, strong magnetic fields, and hostile chemical conditions, understanding how materials behavior is linked to the surroundings and treatment history is critical. DOE mission-relevant topics include corrosion; photovoltaics for solar energy conversion; fast-ion conducting electrolytes for batteries and fuel cells; novel magnetic materials for low magnetic loss power generation; magnetocaloric materials for high-efficiency refrigeration; new materials for high-temperature gasification.

In FY 2009, there is an increase to initiate new research to develop new concepts underpinning electrolyte development ($+1,500,000). The emphasis of this research will be on establishing a fundamental understanding of the interactions that occur in electrolyte systems—ion-ion, ion-solvent, and ion-electrode. Such knowledge will permit the formulation of novel designed electrolytes with significant improvements in electrical energy storage devices. Funding will include support for new solar conversion research ($+3,379,000). To achieve low solar cost-to-power ratios, basic research into new materials and processes are needed, which include new photoconversion materials, such as polycrystalline, nanocrystalline, and organic materials to replace expensive single

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

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 at modest cost. The program will continue to emphasize the vigorous exploration of nanoscale phenomena ($+2,000,000), which will afford new opportunities to dramatically improve energy relevant materials. Research related to the hydrogen economy will also be supported ($+700,000).

	FY 2007	FY 2008	FY 2009
▪ **Neutron and X-ray Scattering**	**38,943**	**38,940**	**52,098**

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 2009, neutron and x-ray scattering research will be increased to initiate activities to determine electrode and electrolyte structure in electrical energy storage devices at various states of charge and discharge, cycle life, and operating conditions ($+3,000,000). The increased neutron and x-ray fluxes and optimized beamline optics at BES user facilities, combined with specialized instrumentation, present unique and exciting opportunities for the design of an entirely new set of experiments to follow electrochemical processes in real time. Emphasis will be on using elastic and inelastic neutron scattering to determine structure and local dynamics and on neutron reflectivity to examine electrode/electrolyte interfaces. Time-resolved measurements will be used to study phase transformation kinetics in both amorphous and crystalline phases. Additional core research activities will be initiated to support scattering research for materials under extreme conditions ($+1,758,000) . Of particular interest are environments involving ultrahigh pressure for exploring novel phase and phenomena not accessible via ambient conditions. Additional funding ($+4,000,000) will support photon-based ultrafast materials science research with an emphasis on the understanding of the physics of strongly correlated systems, such as high temperature superconductors and magnetic materials with colossal magneto-resistance. The common characteristic of this class of materials is a significant interplay among the electronic-, lattice-, spin-, and/or orbital degrees of freedom, which can be probed by ultrafast techniques. Increase in this area of research will support new activities in ultrafast science at universities and DOE laboratories, including Stanford/SLAC—the home of the Linac Coherent Light Source, which is the BES centerpiece for activities in ultrafast sciences. Funding will also support mid-scale instrumentation needs including end stations at the synchrotron light sources and neutron scattering facilities ($+10,600,000). With its sensitivity to light elements, neutron scattering and instrumentation will continue to play a key role in hydrogen research ($+2,300,000). Funding for support of HFIR research and user support staff at ORNL is transferred to SNS facility operations ($-8,500,000); this funding is now part of the joint SNS-HFIR user support program. The HFIR operations budget continues to support operations of the reactor only.

	FY 2007	FY 2008	FY 2009
▪ **Electron and Scanning Probe Microscopies**	**23,021**	**23,020**	**34,496**

This activity was formerly named Structure and Composition of Materials. The activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques, primarily at BES supported user facilities. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. This activity also supports the continual 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.

The properties of materials depend upon their structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon 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 2009, there is an increase to fund basic research to develop new concepts based on electron scattering and scanning probe techniques for in situ characterization of electrochemical reactions in electrical energy storage systems ($+1,500,000). The emphasis of this research will be the development of tools that will have radically improved spatial, time, and energy resolution to provide fundamental understanding of the electron and charge transfer processes and mechanisms by which ions interact with electrode materials. The main focus will be on characterization of transient nonequilibrium nanoscale structures, including adsorbed species in both vacuum and electrochemical environments, with near-atomic spatial resolution and femtosecond time scale. New research activities will also be initiated for developing ultrafast electron scattering probes as companion tools to ultrafast photon probes ($+1,000,000). Funds will also support activities in developing new experimental tools and techniques for atomic scale structural characterization, including scanning probes and electron-based scattering techniques, to further advance the nanoscale science ($+2,000,000). In addition, there are increases to support the development of advanced electron microscopy and scanning probe techniques for mid-scale instrumentation needs ($+2,000,000), and new experimental tools and techniques for atomic scale structural characterization for research related to the hydrogen economy ($+100,000), for solar energy

	FY 2007	FY 2008	FY 2009

(dollars in thousands)

conversion ($+3,876,000) and to enhance core research in developing novel electron and scanning probes for materials characterization under extreme conditions ($+1,000,000).

▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	**7,280**	**14,680**	**8,240**

This activity supports basic research spanning the broad range of science and technology programs within the DOE in states that have historically received relatively less Federal research funding. The EPSCoR states are Alabama, Alaska, Arkansas, Delaware, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, along with the Commonwealth of Puerto Rico and the U.S. Virgin Islands. 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, 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 2009, support will continue for basic research related to all DOE mission areas and to enhance collaborative efforts with DOE user facilities. The FY 2009 Request will allow EPSCOR to continue at a level consistent with the FY 2007 Appropriation and the FY 2008 Request.

The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

Alabama	393	264	—
Alaska	—	—	—
Arkansas	139	—	—
Delaware	629	980	980
Hawaii	—	—	—
Idaho	400	400	400
Kansas	—	—	—
Kentucky	450	650	650
Louisiana	440	440	440
Maine	450	650	650
Mississippi	—	—	—
Montana	134	131	—
Nebraska	269	140	—
Nevada	455	468	—

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
New Hampshire[a]	498	545	569
New Mexico	—	—	—
North Dakota	350	350	—
Oklahoma	713	661	681
Puerto Rico	—	—	—
Rhode Island	—	—	—
South Carolina	939	910	785
South Dakota	—	—	—
Tennessee[b]	275	275	135
Vermont	—	—	—
U.S. Virgin Islands	—	—	—
West Virginia	495	495	—
Wyoming	140	—	—
Technical Support	111	—	110
Other[c]	—	7,321	2,840
▪ **Synthesis and Processing Science**	**15,592**	**16,590**	**25,529**

This activity supports basic research 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; the preparation techniques for pristine single crystal and bulk materials with novel physical properties; the 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 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.

[a]Became eligible in FY 2006.
[b]Became ineligible in April 2006. Amounts shown represent continuation funds.
[c]Uncommited funds in FY 2008 and FY 2009 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

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.

In FY 2009, there are increases to fund new basic research in applying novel design rules for synthesizing nanostructured materials ($+2,000,000) and assemblies for electrical energy storage ($+1,500,000). The emphasis of this research will be on understanding the fundamental electrochemical characteristics of the nanoscale building blocks with varying size, shape, and in confined geometry. Additional support will fund new emergent behavior research ($+1,000,000). The research activity aims at providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations in ways to probe the atomistic basis of the emergent behavior. Within this funding, there are increases to support the synthesis and processing science of hydrogen-related materials ($+3,000,000), and materials for solar energy conversion ($+1,439,000).

▪ **Materials Chemistry and Biomolecular Materials**	**46,439**	**43,430**	**61,310**

This activity was formerly named Materials Chemistry. The 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 2009, there is an increase to support new basic research for electrical energy storage ($+7,469,000). To achieve efficient electric storage with high energy and power densities, basic research into the design and synthesis of new materials and processes is needed, including investigations into new three-dimensional nanostructured architectures that can be precisely tailored for power storage in batteries and ultracapacitors. Emphasis will be on developing a predictive understanding of the role of interfaces in the electrochemical processes underpinning energy storage

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

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 funding aims at accelerating the pace of advances in achieving functions such as the ability to repair or heal defects, self-regulate, self-clean, sequester impurities, and tolerate abuse, leading to radical improvements in electric energy storage performance. Additional funding is provided for new research on direct solar conversion to fuels ($+3,973,000). The emphasis will be on tailoring the absorption and charge separation via the control of photon and electron motion in materials, and to take full advantage of the nanotechnology/biotechnology revolutions to enable exquisite design of materials and the mimicking of natural function. The confluence of the emerging nanoscale hybrid materials and advances in the understanding of nature’s design rules of its photosynthetic and catalytic systems opens up opportunities for combining biological and inorganic/organic components in engineered assemblies with unprecedented efficiencies for the conversion of solar photons to fuels and chemicals. Also supported are activities in developing instrumentation to measure forces, atomic configuration, and physical and chemical properties with ultrahigh sensitivity to further advance the nanoscale science ($+2,000,000). Additional funding is provided for research related to the hydrogen economy ($+2,938,000) and for developing mid-scale synthesis and characterization tools ($+1,500,000).

	FY 2007	FY 2008	FY 2009
▪ **Engineering Research**	**475**	**—**	**—**

This activity supported studies of the conduction of heat in terms of the interactions of phonons (or crystal lattice vibrations) with crystalline defects and impurities and the transfer of mass and energy in turbulent flow in geometrically constrained systems and the mechanics of nanoscale systems. In FY 2008, the remaining engineering research activities were terminated because of competing priorities.

	FY 2007	FY 2008	FY 2009
▪ **Electron-beam Microcharacterization**	**8,040**	**8,183**	**11,250**

This activity supports operation of three electron-beam microcharacterization centers, which support research on next-generation electron-beam instrumentations and operate as user facilities. These centers are: (1) the Electron Microscopy Center for Materials Research at ANL, (2) the National Center for Electron Microscopy at LBNL, and (3) the Shared Research Equipment Program at ORNL. These centers contain various specialized instruments to provide information on the structure, chemical composition, and properties of materials from the atomic level up using direct imaging, diffraction, spectroscopy, and other techniques based primarily on electron scattering. Atomic arrangements, local bonding, defects, interfaces and boundaries, chemical segregation and gradients, phase separation, and surface phenomena are all aspects of the nanoscale and atomic structure of materials, which ultimately controls the mechanical, thermal, electrical, optical, magnetic, and many other properties and behaviors. Electron probes are valuable for investigating such structure because of their strong interactions with atomic nuclei and bound electrons, allowing signal collection from small numbers of atoms—or, in ideal cases, just one. The use of charged particles allows electromagnetic control and lensing of electron beams, resulting in spatial resolution that can approach single atomic separations or better. 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

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

probe microscopes, and/or auxiliary tools such as spectrometers, detectors, and advanced sample preparation equipment.

In FY 2009, additional funds are provided for enhanced user support, scientific research of staff scientists, and development of new instruments or techniques ($+3,067,000). This includes staffing, maintenance, and other operational support for the Transmission Electron Aberration Corrected Microscope (TEAM), which will be in operation as part of the National Center for Electron Microscopy at LBNL.

	FY 2007	FY 2008	FY 2009
▪ **Accelerator and Detector Research**	**1,476**	**1,833**	**9,120**

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 interacts 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 2009 will increase selected ongoing activities in accelerator-based research activities ($+7,287,000). 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.

	FY 2007	FY 2008	FY 2009
▪ **Nanoscale Science Research Centers**	**500**	**500**	**—**

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

	FY 2007	FY 2008	FY 2009
▪ **Spallation Neutron Source Instrumentation I (SING I)**	**10,500**	**11,856**	**12,000**

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 will be installed at the SNS on a phased schedule between FY 2008–2011.

	FY 2007	FY 2008	FY 2009
▪ **Spallation Neutron Source Instrumentation II (SING II)**	**500**	**6,000**	**7,000**

Funds are provided for a Major Item of Equipment with a Total Project Cost in the range of $40,000,000 to $60,000,000 for 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. The TEC range will be narrowed to a cost and schedule performance baseline following completion of Title I design and Independent Project Reviews. 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 Alternative Selection and Cost Range (CD-1) was approved on September 27, 2007, with an estimated cost range of $40,000,000 to $60,000,000. The baseline TPC will be approved at Approve Performance Baseline, CD-2 for each of the four instruments. The FY 2009 Budget Request is for engineering design only. Engineering design may include limited fabrication and testing of design concepts. Funds for full fabrication will be requested after approval of the Performance Baseline, CD-2.

	FY 2007	FY 2008	FY 2009
▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)**	**2,000**	**6,000**	**15,000**

Funds are provided for a Major Item of Equipment with a total project cost in the range of $50,000,000 to $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 Stanford Linear Accelerator Center. The TEC will be narrowed to a cost and schedule performance baseline following completion of Title I design and Independent Project Reviews. It is anticipated that these three instruments will be installed at the LCLS on a phased schedule between FY 2010–2012.

The Alternative Selection and Cost Range (CD-1) was approved on September 27, 2007, with an estimated cost range of $50,000,000 to $60,000,000. The baseline TPC will be approved at Approve Performance Baseline, CD-2. The FY 2009 Budget Request is for engineering design only. Engineering design may include limited fabrication and testing of design concepts. Funds for full fabrication will be requested after approval of the Performance Baseline, CD-2.

	FY 2007	FY 2008	FY 2009
▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	**5,508**	**6,687**	**—**

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

	FY 2007	FY 2008	FY 2009
▪ **General Plant Projects (GPP)**	**300**	**—**	**—**

GPP funding supports minor new construction, other capital alterations and additions, and improvements to land, buildings, and utility systems. 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. The total estimated cost of each GPP project will not exceed $5,000,000. In FY 2009 GPP funds are transferred to the Science Laboratories Infrastructure (SLI) program to support the SC Infrastructure Modernization Initiative.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Facilities Operations	**614,231**	**645,869**	**719,247**

This activity supports the operation of four synchrotron radiation light sources,

- the Advanced Light Source (ALS) at LBNL,
- the Advanced Photon Source (APS) at ANL,
- the National Synchrotron Light Source (NSLS) at BNL, and
- the Stanford Synchrotron Radiation Laboratory (SSRL) at SLAC;

three neutron scattering facilities,

- the High Intensity Flux Reactor (HFIR) at ORNL,
- the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) at LANL, and
- the Spallation Neutron Source (SNS) at ORNL;

five Nanoscale Science Research Centers (NSRCs),

- 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;

and one linear accelerator for a project under construction,

- the Linac Coherent Light Source (LCLS) linac at SLAC.

The BES scientific user facilities, which include light sources, neutron sources, and nanoscience centers, serve researchers from universities, national laboratories, and industry, providing specialized instrumentation and expertise that enables scientific users to carry out experiments or develop theories that could not be done by individual investigators at their home institutions. For approved, peer-reviewed projects, operating time is available without charge to those scientists who intend to publish their results in the open literature. More than 10,000 scientists are users of BES facilities annually. The number of users for the synchrotron radiation sources and neutron scattering facilities are shown in the table below, and a table of the number of users for all BES facilities, FY 2000–2007, is provided at: http://www.sc.doe.gov/bes/users.htm. The synchrotron light sources, producing mostly soft and hard x-rays, examine the fundamental parameters used to perceive the physical world (energy, momentum, position, and time) using the techniques of spectroscopy, scattering, and imaging applied over various time scales. Neutron sources take advantage of neutrons' electrical neutrality and special magnetic properties to probe atoms and molecules, and their assembly into materials. The suite of Nanoscale Science Research Centers provides the ability to fabricate complex nanostructures using chemical, biological, and other synthesis techniques, to characterize them, to assemble them, and to integrate them into devices. The FY 2008 budget allocation has led to termination of a facility and the remaining BES operating facilities operations will be nearly flat funded with FY 2007. The impact of the flat funding of the x-ray and neutron scattering facilities is likely to result in reduced hours of operation at these facilities by as much as 20%. This reduction in hours of operation will permit the remaining facilities to resume maintenance activities and upgrades—which have been deferred since FY 2006. In FY 2009, operation of these scientific user facilities is funded at a level that will permit optimal service to users. FY 2009 marks the first year of sole BES support for SLAC linac operations, which transitioned from HEP to BES funding in FY 2006 through FY 2008.

Additional funds are provided in FY 2009 for full operation of the SLAC linac and for enhanced beamline 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. 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 $5,000,000. 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. Of the total FY 2009 operations budget, $617,788,000 is provided for operating expenses, $67,369,000 is provided for capital equipment, $32,643,000 is provided for AIP, and $1,447,000 is provided for GPP.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Facilities			
Advanced Light Source, LBNL	48,797	47,367	51,049
Advanced Photon Source, ANL	105,000	105,000	116,514
National Synchrotron Light Source, BNL	36,900	36,900	40,149
National Synchrotron Light Source-II, BNL	22,000	20,000	10,000
Stanford Synchrotron Radiation Laboratory, SLAC	30,725	30,825	33,028
High Flux Isotope Reactor, ORNL	55,705	54,511	58,780
Intense Pulsed Neutron Source, ANL	15,500	8,000	4,000
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,500	10,500	11,155
Spallation Neutron Source, ORNL	165,500	164,640	177,640
Center for Nanophase Materials Sciences, ORNL	18,115	18,000	19,975
Center for Integrated Nanotechnologies, SNL/LANL	17,864	18,100	20,100
Molecular Foundry, LBNL	19,056	18,250	20,150
Center for Nanoscale Materials, ANL	18,019	18,526	20,857
Center for Functional Nanomaterials, BNL	—	18,250	20,150
Linac Coherent Light Source (LCLS), SLAC	13,000	15,500	19,000
Linac for LCLS, SLAC	37,550	61,500	96,700

The following table shows the hours of operation and numbers of users for the major scientific user facilities—the synchrotron radiation sources and the neutron scattering facilities. Optimal hours represent the total number of hours the facilities can operate for users, which excludes routine maintenance, machine research, operator training, accelerator physics, etc. In addition, scheduled upgrades and known shutdowns for the specified fiscal year are taken into consideration. A difference between optimal hours and scheduled hours reflects a reduction in operating hours due to funding limitations. Scheduled hours for FY 2007 represent the actual number of hours delivered to users. NSLS and SSRL delivered unscheduled hours to users in FY 2007 resulting in a total greater than Optimal Hours estimates.

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Estimate
All Facilities			
Optimal Hours	29,070	35,800	34,000
Scheduled Hours	27,551	28,580	31,800
Unscheduled Downtime	6%	<10%	<10%
Number of Users	9,079	8,510	9,800

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Estimate
Advanced Light Source			
Optimal Hours	4,200	5,600	5,600
Scheduled Hours	3,916	5,000	5,400
Unscheduled Downtime	12%	<10%	<10%
Number of Users	1,748	1,900	2,100
Advanced Photon Source			
Optimal Hours	5,000	5,000	5,000
Scheduled Hours	4,751	4,380	4,800
Unscheduled Downtime	2%	<10%	<10%
Number of Users	3,420	3,000	3,500
National Synchrotron Light Source			
Optimal Hours	5,400	5,400	5,400
Scheduled Hours	5,971	4,900	5,200
Unscheduled Downtime	3%	<10%	<10%
Number of Users	2,219	2,000	2,100
Stanford Synchrotron Radiation Laboratory			
Optimal Hours	5,400	5,400	5,400
Scheduled Hours	5,424	4,500	5,000
Unscheduled Downtime	2%	<10%	<10%
Number of Users	1,151	1,100	1,300
High Flux Isotope Reactor			
Optimal Hours	1,200	4,500	4,500
Scheduled Hours	1,178	3,100	3,900
Unscheduled Downtime	0%	<10%	<10%
Number of Users	72	130	450

				(dollars in thousands)		
				FY 2007	FY 2008	FY 2009
	FY 2007 Actual	FY 2008 Estimate	FY 2009 Estimate			
Intense Pulsed Neutron Source						
Optimal Hours	3,600	3,600	—			
Scheduled Hours	2,965	1,000	—			
Unscheduled Downtime	3%	<10%	—			
Number of Users	173	80	—			
Manuel Lujan, Jr. Neutron Scattering Center						
Optimal Hours	3,600	3,600	3,600			
Scheduled Hours	2,806	3,000	3,500			
Unscheduled Downtime	<19%	<10%	<10%			
Number of Users	272	260	280			
Spallation Neutron Source						
Optimal Hours	670	2,700	4,500			
Scheduled Hours	540	2,700	4,000			
Unscheduled Downtime	19%	<10%	<10%			
Number of Users	24	40	70			
SBIR/STTR				**—**	**24,340**	**26,939**

In FY 2007, $20,699,000 and $2,484,000 were transferred to the SBIR and STTR programs, respectively. The FY 2008 and FY 2009 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

	FY 2007	FY 2008	FY 2009
Total, Materials Sciences and Engineering	**879,323**	**954,060**	**1,125,579**

Explanation of Funding Changes

	FY 2009 vs. FY 2008 ($000)
Experimental Condensed Matter Physics	
Increases are provided for mid-scale instrumentation ($+2,500,000); hydrogen economy ($+3,350,000); and solar energy conversion ($+3,939,000).	+9,789

	FY 2009 vs. FY 2008 ($000)
Theoretical Condensed Matter Physics	
Increases are provided for emergent behavior ($+1,500,000); electric energy storage ($+2,000,000); hydrogen economy ($+2,938,000); solar energy conversion ($+1,920,000); and nanoscale phenomena for energy applications ($+2,000,000).	+10,358
Mechanical Behavior and Radiation Effects	
Increases are provided to enhance core research in high-temperature mechanical behavior and radiation effects in materials under extreme environments ($+1,000,000) and to fund new basic research to develop a new generation of robust materials for utilization in high-temperature and irradiation-probe environments for advanced nuclear energy systems ($+8,492,000).	+9,492
Physical Behavior of Materials	
Increases are provided for new research to develop new concepts underpinning electrolyte development ($+1,500,000); hydrogen economy ($+700,000); solar energy conversion ($+3,379,000); and nanoscale behavior in materials for energy applications ($+2,000,000).	+7,579
Neutron and X-ray Scattering	
Decrease is due to transfer of support for the HFIR user program to the SNS facility operations budget; the SNS and HFIR user programs will be operated jointly ($-8,500,000). Increases are provided to determine electrode and electrolyte structure in electrical energy storage devices at various states of charge and discharge, cycle life, and operating conditions and to develop new concepts using x-ray and neutron scattering tools for in-situ characterization of electrochemical reactions in electrical energy storage systems ($+3,000,000); mid-scale instrumentation ($+10,600,000); ultrafast science ($+4,000,000); hydrogen economy ($+2,300,000); and support scattering research for materials under extreme conditions ($+1,758,000).	+13,158
Electron and Scanning Probe Microscopies	
Increases are provided to support new research to fund basic research to develop new concepts based on electron scattering and scanning probe techniques for in-situ characterization of electrochemical reactions in electrical energy storage systems ($+1,500,000); ultrafast science ($+1,000,000); mid-scale instrumentation ($+2,000,000); hydrogen economy ($+100,000); solar energy conversion ($+3,876,000); nanoscale electrons and scanning probes development ($+2,000,000); and enhance core research in developing novel electron and scanning probes for materials characterization under extreme conditions ($+1,000,000).	+11,476
Experimental Program to Stimulate Competitive Research (EPSCoR)	
The FY 2009 Request will allow EPSCoR to continue at a level consistent with the FY 2007 Appropriation and the FY 2008 Request.	-6,440

	FY 2009 vs. FY 2008 ($000)
Synthesis and Processing Science	
Increases are provided to fund new basic research in applying novel design rules for synthesizing nanostructured materials and assemblies for electrical energy storage ($+1,500,000); emergent behavior ($+1,000,000); hydrogen economy ($+3,000,000); solar energy conversion ($+1,439,000); and novel design in nanoscale synthesis ($+2,000,000).	+8,939
Materials Chemistry and Biomolecular Materials	
Increases is provided to support new basic research for electrical energy storage to further expand the materials design and synthesis efforts in developing novel electrolytes, nanostructured electrode architectures, and new electrochemical couples ($+7,469,000); mid-scale instrumentation ($+1,500,000); hydrogen economy ($+2,938,000); solar energy conversion ($+3,973,000); and nanoscale tools for developing mid-scale synthesis and characterization ($+2,000,000).	+17,880
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.	+3,067
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.	+7,287
Nanoscale Science Research Centers Other Project Costs	
Decrease in funding due to completion of the Nanoscale Science Research Centers.	-500
Spallation Neutron Source Instrumentation I	
Scheduled increase for the Major Item of Equipment which will provide instrumentation for the Spallation Neutron Source.	+144
Spallation Neutron Source Instrumentation II	
Scheduled increase for the Major Item of Equipment which will provide instrumentation for the Spallation Neutron Source.	+1,000
Linac Coherent Light Source Ultrafast Science Instruments (LUSI)	
Scheduled increase for the Major Item of Equipment for the Linac Coherent Light Source Ultrafast Science Instruments.	+9,000

	FY 2009 vs. FY 2008 ($000)
Transmission Electron Aberration Corrected Microscope (TEAM)	
Decrease for the Major Item of Equipment for the Transmission Electron Aberration Corrected Microscope due to the completion of the project.	-6,687
Total, Materials Sciences and Engineering Research	**+95,542**
Facilities Operations	
▪ **Operation of National User Facilities**	
Increase for the Advanced Light Source to support accelerator operations and users.	+3,682
Increase for Advanced Photon Source to support accelerator operations and users.	+11,514
Increase for National Synchrotron Light Source to support accelerator operations and users.	+3,249
Decrease for National Synchrotron Light Source-II – Other Project Costs per the project schedule.	-10,000
Increase for the Stanford Synchrotron Radiation Laboratory to support accelerator operations and users.	+2,203
Increase for High Flux Isotope Reactor to support reactor operations.	+4,269
Decrease for the Intense Pulsed Neutron Source to maintain the facility in a safe storage condition.	-4,000
Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and users at approximately the FY 2008 level.	+655
Increase for Spallation Neutron Source. The increase includes an increase for operations ($+4,500,000) and also the transfer of funds previously funded in X-ray and Neutron Scattering for the now joint SNS-HFIR user program. ($+8,500,000).	+13,000
Increase for the Center for Nanophase Materials to support operations and users.	+1,975
Increase for the Center for Integrated Nanotechnologies to support operations and users.	+2,000
Increase for the Molecular Foundry to support operations and users.	+1,900
Increase for the Center to Nanoscale Materials to support operations and users.	+2,331
Increase for the Center for Functional Nanomaterials to support operations and users.	+1,900
Increase for Linac Coherent Light Source Other Project Costs per the project schedule ($+1,500,000) and increase to begin operations of the LCLS portion of the Linac that has been commissioned ($+2,000,000).	+3,500

	FY 2009 vs. FY 2008 ($000)
Increase for Stanford Linear Accelerator Center for the first year of full BES support of the linac operations.	+35,200
Total, Facilities Operations	**+73,378**
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expense.	+2,599
Total Funding Change, Materials Sciences and Engineering	**+171,519**

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Chemical Sciences, Geosciences, and Energy Biosciences			
Chemical Sciences, Geosciences, and Energy Biosciences Research	209,380	209,905	289,513
Facilities Operations	7,648	7,000	—
SBIR/STTR	—	5,672	7,600
Total, Chemical Sciences, Geosciences, and Energy Biosciences	217,028	222,577	297,113

Description

This subprogram supports experimental and theoretical 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; 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, photoelectrochemistry, 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, the themes are 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 sequestration.

Selected FY 2007 Research Accomplishments

- *Ultrafast laser probes reveal unexpected quantum behavior in nature's photosynthetic apparatus.* Evolutionary development over 3 billion years has allowed nature to perfect the design rules for converting sunlight into chemical energy. The photosynthetic apparatus allows plants to absorb sunlight, transform its energy into reactive electrons, and then transfer the electrons to molecular reaction centers for conversion into chemical energy—with nearly 100% efficiency. Researchers have found that the speed of energy transfer is the key to this efficiency and are now using laser and x-ray techniques to probe the electron transfer mechanism on an ultrafast time scale (10^{-15} seconds). A wavelike energy transfer from the photon absorption site to the first electron transfer site is followed by a rapid "hand-off" of the electron from one molecule to another until the reaction center is reached. This result is surprising—this type of coherent energy transfer, which is uniquely quantum mechanical, was not anticipated in such a complex molecular system—and reveals yet another nuance in the mechanism of photosynthesis.
- *Artificial systems to create chemical fuels from sunlight and water*. Light-driven splitting of water to form molecular hydrogen and oxygen is a complex process that requires the net transfer of several electrons: two electrons to make hydrogen and four electrons to make oxygen. Inspired by improved understanding of the structure and function of the natural photosynthetic reaction center, researchers have created molecular assemblies with novel architectures that gather electrons in close proximity when illuminated by sunlight and that catalyze multi-electron transfer with several metal atoms. One particularly effective artificial assembly that produces hydrogen gas contains a dimer of two ruthenium atoms. Other ruthenium complexes, in which the metal atoms are arranged with exact spacing, catalyze the extraction of the four electrons to evolve oxygen with a high degree of stability. In order to make a durable artificial system, however, positively charged protons must be moved at the same time to compensate for the movement of negatively charged electrons. In both the natural and artificial systems, a water molecule that is precisely positioned by the calcium atom can better release a proton in conjunction with oxygen evolution. These new assemblies catalyze several key steps in water splitting and provide guidance for the synthesis of more effective and durable systems that produce fuel from water and sunlight.
- *Advanced probes of the complex chemistry of combustion*. Efficient combustion of hydrocarbon fuels maximizes energy output while minimizing formation and release of unwanted emissions such as fine particles of carbon soot. Recently, an integrated theoretical and experimental effort has clarified the basic chemical reactions that transform fuels into small aromatic compounds—the initial, critical step in soot particle formation. Using quantum chemistry and reaction rate theory, reaction rates and product yields were calculated for the many different aromatic products of a prototypical reaction. Complementary experiments at the Advanced Light Source employing a novel kinetics reactor coupled with vacuum ultraviolet (VUV) photoionization and mass spectrometric detection have provided the first direct, time-resolved measurements of the isomer distribution of the products

formed in the propargyl association reaction. The experimental and computational results are in good agreement and set the stage for further targeted studies of other reactions that are critical to incipient soot formation.

- *Remarkable new insights into chemical bonding.* The search for model transition-metal oxide catalysts has led to the discovery of a new kind of bonding involving the 5d atomic orbitals on a triangular shaped cluster of tantalum atoms. The 5d orbitals combine to form a previously unknown type of delocalized molecular bond that may be important for other transition metal compounds. Using exquisitely sensitive experimental tools, coupled with computational chemistry, the discovery of subtle differences in bonding was recognized as the origin of different reaction pathways of thorium and uranium ions as they react to form organometallic complexes in solution. Such insights also led to the design of a new tweezer-like molecule, which has now been synthesized and shown to achieve selective separation chemistry of radioactive species.

- *New chemical imaging capability using neutron scattering.* Researchers are using neutron scattering techniques to probe chemically modified interfaces that are important in geochemistry, biochemistry, catalysis science, and separations membranes. BASIS, a newly commissioned backscattering spectrometer end station at the Spallation Neutron Source, takes advantage of increased flux and a significant increase in energy resolution to investigate oxide hydration layers and probe the dynamics of the interactions of water with metals, minerals, and other chemically important substrates. Coupling these observations with computational molecular dynamics simulations recently revealed new dynamical behavior of water in hydration layers on metals and minerals. Neutron scattering is also being used to probe the dynamics of organic molecules tethered to silica surfaces and to probe the differences in interfacial interactions between hydrocarbons and surfaces.

Detailed Program Justification

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Chemical Sciences, Geosciences, and Energy Biosciences Research	**209,380**	**209,905**	**289,513**
▪ **Atomic, Molecular, and Optical Science**	**18,112**	**18,112**	**23,659**

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.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

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 2009, emphasis will continue on the development of new ultrafast x-ray and optical probes; theories for the interpretation of ultrafast measurements; use of optical fields to control quantum mechanical processes; and atomic and molecular interactions at ultracold temperatures. In FY 2009, there are increases for coherent control of quantum systems ($+1,047,000), ultrafast science ($+2,000,000), chemical imaging ($+500,000), mid-scale instrumentation ($+500,000), and nanoscale science associated with complex systems ($+1,500,000).

▪ **Chemical Physics Research**	**33,877**	**34,777**	**52,764**

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 activity has a gas-phase chemical physics portion and a condensed phase and interfacial molecular science portion. 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 and theory 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 provided an impressive challenge to 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 2009, there will be an increased focus on experimental and theoretical research aimed at developing predictive models for clean and efficient combustion of biofuels and alternative fossil fuels in modern engines. 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 2009, there are increases for gas-phase chemical physics focused on combustion of alternative transportation fuels ($+392,000); ultrafast science ($+1,000,000); chemical imaging ($+750,000); mid-scale instrumentation ($+500,000); emergent behavior in condensed phase systems ($+1,000,000); nanoscale interfacial systems ($+1,500,000); solar energy conversion ($+1,697,000); and interfacial chemical physics relevant to electrical energy storage, including studies of electrode-electrolyte interfaces, charge transfer, and transport ($+3,969,000). Also in FY 2009, there is an increase due to the transfer of the Combustion Research Facility from Facility Operations to Chemical Physics Research ($+7,179,000). The CRF has been transferred to the research portion of the budget in recognition of its role as a research operation with visitor access via collaboration with staff scientists rather than a user facility.

	FY 2007	FY 2008	FY 2009
▪ **Solar Photochemistry**	**30,603**	**30,603**	**39,569**

This activity was formerly named Photochemistry and Radiation Research. The 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 the future molecular optoelectronic device development.

In FY 2009, continued emphasis will be placed on studies of semiconductor/polymer interfaces, multiple charge generation within semiconductor nanoparticles, and dye-sensitized solar cells. Research will be extended in inorganic/organic donor-acceptor molecular assemblies and in the use of nanoscale materials in solar photocatalytic generation of chemical fuels. In FY 2009, there are increases for ultrafast science ($+1,000,000); solar energy conversion, including solar photo-electrochemistry and solar photoconversion using solid-state organic systems ($+4,686,000); research related to the hydrogen economy, including solar hydrogen production ($+1,280,000); and enhanced experimental and theoretical studies of photo-electrochemical and interfacial charge transfer processes in electrical energy storage ($+2,000,000).

	FY 2007	FY 2008	FY 2009
▪ **Photosynthetic Systems**	**14,750**	**14,750**	**19,926**

This activity was formerly named Molecular Mechanisms of Natural Solar Energy Conversion. The 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. Accentuated 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 2009, 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 2009, there are increases for chemical imaging ($+750,000); emergent behavior in biological systems ($+500,000); and 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 ($+3,926,000).

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
▪ **Physical Biosciences**	**14,175**	**14,175**	**15,675**

This activity was formerly named Metabolic Regulation of Energy Production. The 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, particularly improved biochemical pathways for biofuel production, next generation energy conversion/storage devices, and efficient and environmentally friendly and sustainable catalysts.

In FY 2009, continued emphasis will be placed on probing organizational principles of biological energy transduction and chemical storage systems using advanced molecular imaging and x-ray or neutron methods for structural determination. Research will probe structure-function relationships in biochemical systems and visualize biochemical activity at the molecular level in living cells. In FY 2009, there is an increase for the application of physical characterization tools to biochemical systems ($+1,500,000).

▪ **Catalysis Science**	**39,711**	**39,711**	**56,927**

This activity was formerly named Catalysis and Chemical Transformation. The activity develops the fundamental scientific principles enabling rational catalysts 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, hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structures 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 2009, 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 feedstocks will be explored. Increased emphasis will be placed on the use of modern 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 2009, there are increases for ultrafast science ($+1,000,000); chemical imaging of operating catalytic systems ($+750,000); mid-scale instrumentation ($+500,000); solar energy conversion, including photo-catalysis ($+2,838,000); research related to enhanced hydrogen production and use ($+5,128,000), nanoscale catalyst development ($+1,000,000); and experimental and theoretical studies of electrocatalytic processes relevant to electrical energy storage, especially those involving novel electrolytes and ionic liquids ($+6,000,000).

	FY 2007	FY 2008	FY 2009
▪ **Separations and Analysis**	**15,860**	**15,860**	**28,338**

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. An analysis is an essential component of every chemical process from manufacture through safety as well as risk assessment and environmental protection.

	(dollars in thousands)	
FY 2007	FY 2008	FY 2009

In FY 2009, 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 2009, there are increases for advanced chemical separations ($+254,000); analytical chemical imaging ($+1,750,000); mid-scale instrumentation ($+500,000); emergent behavior ($+1,000,000); solar energy conversion ($+1,696,000); research related to the hydrogen economy, including enhanced membrane research ($+2,278,000); and research in membrane and interphase charge transfer and charge transport for electrical energy storage, especially through nanoscale ion channels and their functionalized counterparts ($+5,000,000).

	FY 2007	FY 2008	FY 2009
▪ **Heavy Element Chemistry**	**9,427**	**9,427**	**18,789**

This activity supports research in the chemistry of the heavy elements, including actinides and fission products. The unique molecular bonding of the heavy elements, driven by the active participation of 5f electrons, 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 the environments associated with the storage of radioactive wastes.

In FY 2009, funding will support 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 2009, there are increases for enhanced efforts on actinide chemistry under extreme conditions ($+370,000); mid-scale instrumentation ($+500,000); and enhanced efforts in actinide chemistry and separations science related to advanced nuclear energy systems, especially those aspects related to future reactor or separations design ($+8,492,000).

	FY 2007	FY 2008	FY 2009
▪ **Geosciences Research**	**21,392**	**21,392**	**28,918**

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 the 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 2009, funding will continue to support research in areas that impact DOE mission areas. Of particular interest are 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 2009, there are increases for experimental and theoretical geochemical studies of complex subsurface fluids ($+526,000); nanoscale geochemistry ($+1,000,000); mid-scale instrumentation ($+500,000); chemical imaging ($+500,000); and research in solid earth geophysics and geochemistry for understanding the stability and transformations of deep underground carbon sequestration ($+5,000,000).

	FY 2007	FY 2008	FY 2009
▪ **Chemical Energy and Chemical Engineering**	**375**	**—**	**—**

This activity supported research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes. In FY 2008, remaining chemical energy and chemical engineering research activities were terminated because of competing priorities.

	FY 2007	FY 2008	FY 2009
▪ **General Plant Projects (GPP)**	**9,884**	**9,884**	**705**

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. 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 Facilities Operations justification in the Materials Sciences and Engineering subprogram. The total estimated cost of each GPP project will not exceed $5,000,000.

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

	FY 2007	FY 2008	FY 2009
	(dollars in thousands)		
▪ **General Purpose Equipment (GPE)**	**1,214**	**1,214**	**4,243**

GPE funding is provided for Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the BES stewardship responsibilities for these laboratories for GPE that supports multipurpose research. Infrastructure funding is requested to maintain, modernize, and upgrade the ORNL, ANL, and Ames sites and facilities to correct deficiencies due to aging, changing technology, and inadequate past investments.

Facility Operations	**7,648**	**7,000**	**—**

Beginning in FY 2009, the Combustion Research Facility (CRF) will be budgeted under Chemical Physics Research. The CRF was previously budgeted for as a facility under Facility Operations, but it has been transferred to the research portion of the budget in recognition of its role as a research operation with visitor access via collaboration with staff scientists rather than a user facility.

Facilities

Combustion Research Facility	7,648	7,000	—
SBIR/STTR	**—**	**5,672**	**7,600**

In FY 2007, $5,078,000 and $609,000 were transferred to the SBIR and STTR programs, respectively. The FY 2008 and FY 2009 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**217,028**	**222,577**	**297,113**

Explanation of Funding Changes

	FY 2009 vs. FY 2008 ($000)
Atomic, Molecular and Optical Science	
Increases are provided for coherent control of quantum systems ($+1,047,000); ultrafast science ($+2,000,000); chemical imaging ($+500,000); mid-scale instrumentation ($+500,000); and nanoscale science associated with complex systems ($+1,500,000).	+5,547
Chemical Physics Research	
Increases are provided for gas-phase chemical physics focused on combustion of alternative transportation fuels ($+392,000); ultrafast science ($+1,000,000); chemical imaging ($+750,000); mid-scale instrumentation ($+500,000); emergent behavior in condensed phase systems ($+1,000,000); nanoscale interfacial systems ($+1,500,000); solar energy conversion ($+1,697,000); and interfacial chemical physics relevant to electrical energy storage, including studies of electrode-electrolyte interfaces, charge transfer and transport $+3,969,000). Also in FY 2009, includes transfer of the Combustion Research Facility (CRF) from Facility Operations($+7,179,000). The CRF	

	FY 2009 vs. FY 2008 ($000)
was previously budgeted for as a facility under Facility Operations, but it has been transferred to the research portion of the budget in recognition of its role as a research operation with visitor access via collaboration with staff scientists rather than a user facility.	+17,987
Solar Photochemistry	
Increases are provided for ultrafast science ($+1,000,000); solar energy conversion ($+4,686,000); hydrogen ($+1,280,000); and enhanced experimental and theoretical studies of photo-electrochemical and interfacial charge transfer processes in electrical energy storage ($+2,000,000).	+8,966
Photosynthetic Systems	
Increases are provided for chemical imaging ($+750,000); emergent behavior in biological systems ($+500,000); and solar energy conversion ($+3,926,000).	+5,176
Physical Biosciences	
Increase is provided for the application of physical characterization tools to biochemical systems.	+1,500
Catalysis Science	
Increases are provided for ultrafast science ($+1,000,000); chemical imaging of operating catalytic systems ($+750,000); mid-scale instrumentation ($+500,000); solar energy conversion ($+2,838,000); research related to enhanced hydrogen production and use ($+5,128,000); nanoscale catalyst development ($+1,000,000); and experimental and theoretical studies of electrocatalytic processes relevant to electrical energy storage, especially those involving novel electrolytes and ionic liquids ($+6,000,000).	+17,216
Separations and Analysis	
Increases are provided for advanced chemical separations ($+254,000); analytical chemical imaging ($+1,750,000); mid-scale instrumentation ($+500,000); emergent behavior ($+1,000,000); solar energy conversion ($+1,696,000); research related to hydrogen economy ($+2,278,000); and research in membrane and interphase charge transfer and charge transport for electrical energy storage, especially through nanoscale ion channels and their functionalized counterparts ($+5,000,000).	+12,478
Heavy Element Chemistry	
Increases are provided for enhanced efforts in actinide chemistry under extreme conditions ($+370,000); mid-scale instrumentation ($+500,000); and enhanced efforts in actinide chemistry and separations science related to advanced nuclear energy systems, especially those aspects related to future reactor or separations design ($+8,492,000).	+9,362

	FY 2009 vs. FY 2008 ($000)
Geosciences Research	
Increases are provided for research in solid earth geophysics and geochemistry for understanding the stability and transformations of deep underground carbon sequestration ($+5,000,000); experimental and theoretical geochemical studies of complex subsurface fluids ($+526,000); nanoscale geochemistry ($+1,000,000); mid-scale instrumentation ($+500,000); and chemical imaging ($+500,000).	+7,526
General Plant Projects (GPP)	
Decrease in general plant projects due to transfer of non-programmatic GPP funds to the Science Laboratory Infrastructure program to support the SC Infrastructure Modernization Initiative.	-9,179
General Purpose Equipment (GPE)	
Increase for GPE provided for enhanced infrastructure at Ames, ANL, and ORNL.	+3,029
Total, Chemical Sciences, Geosciences and Energy Biosciences Research	**+79,608**
Facility Operations	
Funding for the CRF is transferred from Facility Operations to Research. The CRF was previously budgeted for as a facility under Facility Operations, but it has been transferred to the research portion of the budget in recognition of its role as a research operation with visitor access via collaboration with staff scientists rather than a user facility.	-7,000
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in operating expenses.	+1,928
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	**+74,536**

Construction

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Construction			
Advanced Light Source User Support Building, LBNL	1,500	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	3,000	29,727	93,273
Linac Coherent Light Source, SLAC	101,161	50,889	36,967
Center for Functional Nanomaterials, BNL	18,864	363	—
The Molecular Foundry, LBNL	257	—	—
Center for Integrated Nanotechnologies, SNL/LANL	247	—	—
Total, Construction	125,029	93,265	145,468

Description

Construction is needed to support the research in the subprograms in the BES program. 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.

The following table shows cost and schedule variance. Note: Cost Variance is the difference between the value of the physical work performed and the actual cost expended. A negative result is unfavorable and indicates the potential for a cost overrun. Schedule variance is the difference between the value of the physical work performed and the value of the work planned. A negative result is unfavorable and indicates that the project is behind schedule. Variance data are shown as percentages. They are shown against the project’s performance measurement baseline that includes cost and schedule contingency and are as of the end of each fiscal year. All projects, except those identified in a footnote, have met or are on schedule to meet all Level 0 and Level 1 Milestones, which are shown in the table.

Cost and Schedule Variance

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Estimate
Linac Coherent Light Source, SLAC[a]			
Cost Variance	-5.24%		
Schedule Variance	-15.32%		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	None	None
Linac Coherent Light Source Ultrafast Science Instruments, SLAC			
Cost Variance	Not Baselined		
Schedule Variance	Not Baselined		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 1 – Alternate Selection/Cost Range	None Defined	None Defined
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC			
Cost Variance	Not Baselined		
Schedule Variance	Not Baselined		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 0 – Approve Mission Need	None Defined	None Defined
Center for Functional Nanomaterials, BNL			
Cost Variance	6.14%		
Schedule Variance	-1.66%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 4a – Start of Initial Operations	Approve Critical Decision 4b – Start of Full Operations	N/A
National Synchrotron Light Source-II, BNL			
Cost Variance	Not Baselined		
Schedule Variance	Not Baselined		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 1 – Alternate Selection/Cost Range	None Defined	None Defined

[a] Due to the delay and reduced funding related to the FY 2007 Continuing Resolution, the project has been directed to prepare a revised cost and schedule baseline. Currently the project has proposed a CD-4 in 4Q FY 2010. The revised cost and schedule is preliminary until approved by the Deputy Secretary. Office of Science IPR and OECM EIR reviews of the revised cost and schedule baseline were conducted in September and October 2007, respectively. The project has submitted a baseline change proposal/request for action and expects approval in 2Q FY 2008.

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Estimate
Instrumentation for Spallation Neutron Source I, ORNL			
Cost Variance	1.33%		
Schedule Variance	-2.26%		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	Approve Critical Decision 4 – Start of Operations for Instruments #1-2	Approve Critical Decision 4 – Start of Operations for Instrument #3
Instrumentation for Spallation Neutron Source II, ORNL			
Cost Variance	Not Baselined		
Schedule Variance	Not Baselined		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 1 – Alternate Selection/Cost Range	None Defined	None Defined
Transmission Electron Aberration Corrected Microscopy (TEAM), LBNL			
Cost Variance	-0.14%		
Schedule Variance	-1.67%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 2 –Performance Baseline Approve Critical Decision 3 – Start of Construction	Approve Critical Decision 4a – Start of Operation TEAM 0.5	Approve Critical Decision 4b – Start of Operation TEAM 1
Advanced Light Source User Support Building, LBNL			
Cost Variance	2.62%		
Schedule Variance	2.98%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 1 – Alternative Selection/Cost Range Approve Critical Decision 2 – Performance Baseline Approve Critical Decision 3 – Start of Construction	None	None

Detailed Justification

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
Advanced Light Source (ALS) User Support Building, LBNL	**1,500**	**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 2007 PED funding was used to secure a Design-Build contractor to start the preparations of the design documents for the project's critical decisions. In addition, site preparations were completed. FY 2008 funds will be used to complete preparation of the construction solicitation package(s) for USB and perform Title II design services. FY 2009 funds will be used to award construction contract(s) as appropriate and continue the design-build construction projects efforts including Title III construction services. Construction funding for the ALS USB will be completed in FY 2010. This project is using the design-build model for construction, a private-sector best practice for this type of space.

Additional information is provided in the construction project data sheet 08-SC-01.

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 Stanford Linear Accelerator Center. 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 multiprogram 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 funding will be used to begin the PULSE Building Renovation. FY 2009 funding is requested to complete construction. Additional information is provided in the construction project data sheet 08-SC-11.

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. Additional information is provided in the construction project (08-SC-11) data sheet.

National Synchrotron Light Source-II (NSLS-II), BNL	**3,000**	**29,727**	**93,273**

The NSLS-II is proposed as a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It would also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these should enable the study of material properties and functions with a spatial resolution of one nanometer (nm), an energy resolution of 0.1 millielectron volt (meV), and the ultra-high sensitivity required to perform spectroscopy on a single atom. NSLS-II would be the best storage-ring-based synchrotron light source in

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009

the world, but, more importantly, NSLS-II would be transformational in that it can open new regimes of scientific discovery and investigation.

FY 2007 PED funding ($3,000,000) began preliminary design. FY 2008 PED funds will be used to begin final design ($29,727,000). FY 2009 PED funding ($27,273,000) will allow the project to complete final design.

PED funds will assure project feasibility, define the scope, provide estimates of construction costs based on the approved design, develop working drawings and specifications, and provide schedules for construction and procurements. Should a decision to proceed with construction be reached, this design effort will ensure that construction could begin on schedule in FY 2009 ($66,000,000).

Additional information is provided in the construction project data sheet 07-SC-06.

Linac Coherent Light Source, SLAC	**101,161**	**50,889**	**36,967**

The Linac Coherent Light Source (LCLS) Project will provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Ångstrom range. The LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons; the light is coherent or "laser like" enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length to subfemtosecond levels) enabling studies of fast chemical and physical processes.

The FY 2007 funding continued Project Engineering and Design (PED) Title I and Title II design work and construction of the LCLS conventional facilities including the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, Far Experimental Hall, and the renovation of existing buildings at SLAC to provide office space requirements to support LCLS operations. In addition, the assembly and delivery of the undulators and undulator infrastructure to SLAC's Magnetic Measurement Facility was completed. Delivery of the undulators in FY 2007 enables achievement of performance goals in FY 2009.

Construction funding in FY 2008 will be used to complete most of the LCLS conventional facilities 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. The project has revised the cost and schedule, and the revised baseline was evaluated in late 2007. The revised project baseline was submitted to the Deputy Secretary for approval in 1Q FY 2008. FY 2009 funding is requested to continue technical equipment procurements and installation. Commissioning of the facility will also continue on a phased schedule.

Additional information on the LCLS project is provided in the LCLS construction data sheet, project number 05-R-320.

Center for Functional Nanomaterials, BNL	**18,864**	**363**	**—**

The Center for Functional Nanomaterials (CFN), a BES Nanoscale Science Research Center, will be completed on time and within budget in FY 2008.

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
The Molecular Foundry, LBNL	**257**	**—**	**—**

The Molecular Foundry, a BES Nanoscale Science Research Center, was completed on time and within budget in FY 2007.

Center for Integrated Nanotechnologies, SNL/LANL	**247**	**—**	**—**

The Center for Integrated Nanotechnologies (CINT), a BES Nanoscale Science Research Center, was completed on time and within budget in FY 2007.

Total, Construction	**125,029**	**93,265**	**145,468**

Explanation of Funding Changes

	FY 2009 vs. FY 2008 ($000)
Advanced Light Source (ALS) User Support Building, LBNL	
Increase in funding for construction of the ALS User Support Building, as scheduled.	+6,546
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	
Decrease in funding representing the completion of construction in FY 2009, as scheduled.	-2,663
Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	
Decrease due to completion of PED in FY 2008.	-941
National Synchrotron Light Source-II (NSLS II), BNL	
Decrease in funding to continue Project Engineering and Design ($-2,454,000) and increase to initiate construction ($+66,000,000), as scheduled.	+63,546
Linac Coherent Light Source, SLAC	
Decrease in funding to continue construction of the LCLS project, representing the scheduled ramp down of activities.	-13,922
Center for Functional Nanomaterials, BNL	
Decrease in funding for construction of the Center for Functional Nanomaterials at BNL, representing completion of construction funding.	-363
Total Funding Change, Construction	**+52,203**

Capital Operating Expenses and Construction Summary

Capital Operating Expenses

	(dollars in thousands)		
	FY 2007	FY 2008	FY 2009
General Plant Projects	16,336	10,006	2,152
Accelerator Improvement Projects	16,294	15,411	32,643
Capital Equipment	74,795	74,382	154,317
Total, Capital Operating Expenses	107,425	99,799	189,112

Construction Projects

	(dollars in thousands)					
	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2007	FY 2008	FY 2009	Unappro-priated Balances
08-SC-01 Advanced Light Source User Support Building, LBNL	35,700[a]	—	—	4,954	11,500	17,746
08-SC-10 PED, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	941	—	—	941	—	—
08-SC-11 Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	11,060[b]	—	—	6,391	3,728	—
07-SC-06, National Synchrotron Light Source-II, BNL	791,200	—	3,000	29,727	93,273	665,200
07-SC-12, PED, Advanced Light Source User Support Building, LBNL	1,500	—	1,500	—	—	—
05-R-320 Linac Coherent Light Source, SLAC	352,000[c]	111,930	101,000	50,889	36,967	15,240
05-R-321 Center for Functional Nanomaterials, BNL	79,697[d]	54,505	18,864	363	—	—
04-R-313 The Molecular Foundry, LBNL	83,604[e]	76,132	257	—	—	
03-SC-002, PED, Linac Coherent Light Source, SLAC	35,974	35,813	161	—	—	—

[a] Includes $1,500,000 of PED included in the 07-SC-12 PED, LBNL Advanced Light Source User Support Building datasheet.
[b] Includes $941,000 of PED included in the 08-SC-10 PED, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC datasheet.
[c] Includes 35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source datasheet.
[d] Includes $5,966,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[e] Includes $7,215,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2007	FY 2008	FY 2009	Unappro-priated Balances
03-R-313 Center for Integrated Nanotechnologies, SNL/LANL	73,754[a]	69,348	247	—	—	—
Total, Construction			125,029	93,265	145,468	

Major Items of Equipment *(TEC $2 million or greater)*

(dollars in thousands)

	Total Project Cost (TPC)	Other Project Costs (OPC)	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2007	FY 2008	FY 2009	Completion Date
Spallation Neutron Source Instrumentation I (31MK), ORNL[b]	68,500		68,500	28,744	10,500	11,856	12,000	FY 2011
Transmission Electron Aberration Corrected Microscope (61PC), LBNL	27,087	15,487	11,600	2,000	3,500	6,100	—	FY 2009
Spallation Neutron Source Instrumentation II (71RB), ORNL[c]	40,000–60,000		40,000–60,000	—	500	6,000	7,000	TBD
Linac Coherent Light Source Instrumentation (71RA), SLAC[d]	50,000–60,000		50,000–60,000	—	500	6,000	15,000	TBD
Total, Major Items of Equipment				30,744	15,000	29,956	34,000	

[a] Includes $4,159,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[b] This FY 2003 MIE includes five instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Beam Spectrometer.
[c] 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).
[d] 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).