Basic Energy Sciences

Funding Profile by Subprogram

	(dollars in thousands)		
	FY 2006 Current Appropriation	FY 2007 Request	FY 2008 Request
Basic Energy Sciences			
Research			
Materials Sciences and Engineering	726,895	1,004,212	1,093,219
Chemical Sciences, Geosciences, and Energy Biosciences	206,961	268,499	283,956
Total, Research	933,856	1,272,711	1,377,175
Construction	176,292	148,269	121,322
Total, Basic Energy Sciences	1,110,148[a]	1,420,980	1,498,497
Stanford Linear Accelerator Center (SLAC) Linac Operations (non-add) [b]	(29,400)	(40,000)	(61,500)
Basic Energy Sciences, excluding SLAC Linac Operations (non-add)[b]	(1,080,748)	(1,380,980)	(1,436,997)

Public Law Authorizations:
Public Law 95-91, "Department of Energy Organization Act", 1977
Public Law 103-62, "Government Performance and Results Act of 1993"
Public Law 108-153, "21st Century Nanotechnology Research and Development Act", 2003
Public Law 109-58, "Energy Policy Act of 2005"

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 aspects of biosciences.

Benefits

BES delivers the knowledge needed to support the President's National Energy Plan for improving the quality of life for all Americans. In addition, BES works cooperatively with other agencies and the programs of the National Nuclear Security Administration to discover knowledge and develop tools to strengthen national security. As part of its mission, the BES program plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

---

[a] Total is reduced by $11,460,000 for a rescission in accordance with P.L. 109-148, the Emergency Supplemental Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006; $21,794,000, which was transferred to the SBIR program; and $2,615,000, which was transferred to the STTR program.

[b] The SLAC linear accelerator (linac) supports operations of the B-Factory (funded by High Energy Physics (HEP)) and will also support operations of the Linac Coherent Light Source (currently under construction and funded by BES). With the completion of B-Factory operations in FY 2008, SC has been transitioning funding of the SLAC linac from HEP to BES, with FY 2008 representing the third and final year of joint funding with HEP. BES totals without SLAC linac funding are presented to display program growth exclusive of this functional transfer.

Basic research supported by the BES program touches virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. Research in materials sciences and engineering leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety of energy generation, conversion, transmission, 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 contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation and seismic imaging for reservoir definition. Finally, research in the molecular and biochemical nature of photosynthesis aids the development of solar photo-energy conversion and biomass 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 Strategic Goals 3.1, Scientific Breakthroughs and 3.2, Foundations of Science

Within the Basic Energy Sciences program, the Materials Science and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram contribute to Strategic Goals 3.1 and 3.2 by producing seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, geosciences, and energy biosciences. These subprograms build leading research programs that provide world-class, peer-reviewed research results cognizant of both DOE mission needs and new scientific opportunities. Scientific discoveries at the frontiers of these disciplines impact energy resources, production, conversion, efficiency, and the mitigation of the adverse impacts of energy production and use—discoveries that will accelerate progress toward energy independence, economic growth, and a sustainable environment.

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.

The Materials Science and Engineering subprogram also contributes to Strategic Goals 3.1 and 3.2 by managing BES facility operations and construction to the highest standards of overall performance, using merit evaluation with independent peer review. The synchrotron radiation light sources, neutron scattering facilities, and electron-beam microcharacterization centers reveal the atomic details of metals and alloys; glasses and ceramics; semiconductors and superconductors; polymers and biomaterials; proteins and enzymes; catalysts, molecular sieves, and filters; and materials under extremes of temperature, pressure, strain, and stress. Researchers are now able to make new materials and study their atomic formation as it happens using these new probes. Once the province of specialists, mostly physicists, these facilities are now used by thousands of researchers annually from all disciplines. The Materials Science and Engineering subprogram has established a suite of Nanoscale Science Research Centers that are changing the way materials research is done by providing the ability to fabricate complex structures using chemical, biological, and other synthesis techniques; characterize them; assemble them; and integrate them into devices—and do it all in one place. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram contributes to this goal by managing the Combustion Research Facility at Sandia National Laboratories in Livermore, California, an internationally recognized facility for advanced characterization techniques and for the study of combustion science and technology.

Funding by Strategic and GPRA Unit Program Goal

(dollars in thousands)

	FY 2006	FY 2007	FY 2008
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	1,110,148	1,420,980	1,498,497

Annual Performance Results and Targets

FY 2003 Results	FY 2004 Results	FY 2005 Results	FY 2006 Results	FY 2007 Targets	FY 2008 Targets
GPRA Unit Program Goal 3.1/2.50.00 (Advance the Basic Science for Energy Independence)					
Materials Sciences and Engineering					
N/A	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]	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]
N/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]	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. [Met Goal]	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]	Maintain and operate the scientific user facilities to achieve an average at least 90% of the total scheduled operating time.	Maintain and operate the scientific user facilities to achieve an average at least 90% of the total scheduled operating time.
Chemical Sciences, Geosciences, and Energy Biosciences					
N/A	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 is discontinued.	

[a] No further improvement is expected in FY 2007 and FY 2008 for these measures since the current suite of instruments has met their maximum performance level. This target is a measure of SC's intent to maintain the maximum level of performance for users of the current SC facilities until the next generation of instruments and facilities becomes available.

FY 2003 Results	FY 2004 Results	FY 2005 Results	FY 2006 Results	FY 2007 Targets	FY 2008 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. [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: +1.3% 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]	Meet the cost and timetables within 10% of the baselines given in the construction project datasheets for all ongoing construction projects.	Meet the cost and timetables within 10% of the baselines given in the construction project datasheets for all ongoing construction projects.

Means and Strategies

The Basic Energy Sciences program will use various means and strategies to achieve its GPRA Unit Program goals. However, various external factors may impact the ability to achieve these goals.

The BES program will support fundamental, innovative, peer-reviewed research to create new knowledge in areas important to the BES mission, i.e., in materials sciences and engineering, chemical sciences, geosciences, and biosciences. BES also plays a critical role in constructing and operating a wide array of scientific user facilities for the nation's researchers. All research projects 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: (1) changing mission needs as described by the DOE and SC mission statements and strategic plans; (2) scientific opportunities as determined, in part, by scientific workshops and proposals received by researchers; (3) 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; (4) unanticipated failures in critical components of scientific user facilities or major research programs; and (5) 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 and with other federal agencies (e.g., National Science Foundation, National Aeronautics and Space Administration, Department of Agriculture, Department of Interior, and National Institutes of Health). 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 2008 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 2008. 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. To better explain our scientific performance measures, the Office of Science developed a website (http://www.sc.doe.gov/measures) that answers questions such as "What does this measure mean?" and "Why is it important?" 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.

OMB has previously provided BES with three recommendations to further improve performance:

- Follow up on recommendations of past expert reviews and use new reviews to assess progress toward long-term programmatic goals.
- Improve performance reporting at BES user facilities to better reflect the instrumentation and staffing issues most directly connected to scientific output.
- Produce a plan for managing and operating the High Flux Isotope Reactor (HFIR) that explicitly addresses the reliability problems while ensuring public health and safety.

In response to OMB's past recommendations BES has:

- Continued to use an external assessment process to review its funding management practices and the quality, relevance, and performance of the research that it funds. The most recent review found the Materials Sciences and Engineering Division to be well managed and supporting a research portfolio with excellent national and international standing.
- Formally charged BESAC to assess progress toward the long term goals of the BES program as part of the regular BESAC Committee of Visitors reviews of BES program areas.
- Established new measures to assess effective utilization of its major user facilities and continued efforts to improve performance reporting of its facilities.
- Conducted two peer reviews of the HFIR in May 2006. The first addressed progress toward the completion and installation of the cold source. The second addressed the operations of the reactor and the scientific program. The second review also examined issues of reliability. Both reviews considered the facility in the context of the larger neutron scattering program at the Oak Ridge National Laboratory (ORNL). A report summarizing the results of HFIR reviews and actions to correct operational deficiencies was provided to OMB by DOE on September 21, 2006.

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.

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, efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2006, the program funded research in more than 175 academic institutions located in 47 states and in 13 DOE laboratories located in 9 states. BES supports a large extramural research program, with approximately 35% 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. During this 30-year period, the basic research supported by the BES program has touched virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. The basic knowledge derived from fundamental research has resulted in a vast array of advances, including:

- high-energy and high-power lithium and lithium ion batteries and thin-film rechargeable miniaturized batteries;
- thermoacoustic refrigeration devices that cool without moving parts and without the use of freons;
- compound semiconductors, leading to the world's highest efficiency photovoltaic solar cells;
- catalysts for the production of new polymers (annually, a multibillion dollar industry) and for a host of other products and energy-efficient processes;
- high-strength, lightweight magnets for sensors and for small motors used in power steering and other vehicle functions;
- strong, ductile alloys for use in high-temperature applications;
- nonbrittle ceramics for use in hammers, high-speed cutting tools, engine turbines, and other applications requiring lightweight and/or high-temperature materials;
- new steels, improved aluminum alloys, magnet materials, and other alloys;
- polymer materials for rechargeable batteries, car bumpers, food wrappings, flat-panel displays, wear-resistant plastic parts, and polymer-coated particles in lubricating oils; and
- processes for extraction of radioactive and hazardous metal ions from solutions for nuclear fuel purification/reprocessing and for cleanup of radioactive wastes.

These advances came by exploiting the results of basic research that sought answers to the most fundamental questions in materials sciences, chemistry, and the other disciplines supported by BES.

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 with properties that are not found in nature. This understanding comes in large measure from synchrotron x-ray and neutron scattering sources, electron microscopes, and other atomic probes as well as terascale computers. 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 facilities and coordinated programs that transcend what individuals alone can do. The program in nanoscale science, including the formation of Nanoscale Science Research Centers, continues that philosophy.

How We Work

To ensure that the most scientifically promising research is supported, the BES program engages in long-range planning and prioritization; regular, external, independent review of the supported research to ensure quality and relevance; and evaluation of program performance through establishment and subsequent measurement against goals and objectives. These activities rely heavily on input from external sources including workshops and meetings of the scientific community, advice from the federally chartered Basic Energy Sciences Advisory Committee (BESAC), intra-DOE and Interagency Working Groups, and reports from other groups such as the National Academy of Sciences. To accomplish its mission, the BES program supports research in both universities and DOE laboratories; plans, constructs, and operates world-class scientific user facilities; and maintains a strong infrastructure to support research in areas of core competencies. Some of the details of how BES works are given in the sections below.

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 BESAC report, “Basic Research Needs to Assure a Secure Energy Future,” which describes 10 themes and 37 specific research directions for increased emphasis. This report will help the program map its research activities for many years to come.

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 substantive issues, including those associated with mature facilities. For example, the reviews clearly highlighted the change that occurred as the light sources 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 light sources experienced a quadrupling of the number of users in the decade of the 1990s. This success and its consequent growing pains were delineated by our reviews. The outcomes of these reviews helped develop new models of operation for existing light sources and neutron scattering facilities as well as the new Spallation Neutron Source, which was completed in FY 2006.

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.

Program Reviews

All research projects supported by the BES program undergo regular peer review and merit evaluation based on procedures set down in 10 CFR Part 605 for the extramural grant program and in an analogous process for the laboratory programs (http://www.science.doe.gov/bes/labreview.html). These peer review and merit evaluation procedures are described within documents found at http://www.science.doe.gov/bes/peerreview.html. These evaluations assess:

- Scientific and/or technical merit or the educational benefits of the project;
- Appropriateness of the proposed method or approach;
- Competency of personnel and adequacy of proposed resources;
- Reasonableness and appropriateness of the proposed budget; and
- Other appropriate factors, established and set forth by SC in a notice of availability or in a specific solicitation.

In addition, on a rotating schedule, BESAC reviews the major elements of the BES program using Committees of Visitors (COVs). COVs are charged with assessing the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document proposal actions; the quality of the resulting portfolio, specifically the breadth and depth of portfolio elements and the national and international standing of the elements; and progress toward the long-term PART goals. The first three reviews assessed the chemistry activities (FY 2002), the materials sciences and engineering activities (FY 2003), and the activities associated with the management of the light sources, the neutron sources, and the new Nanoscale Science Research Centers (FY 2004). This COV review cycle began again in FY 2005, so that all elements of the BES program are reviewed every three years.

Planning and Priority Setting

Because the BES program supports research covering a wide range of scientific disciplines as well as a large number of major scientific user facilities, planning is an ongoing activity. Many long-range planning exercises for elements of the BES program are performed under the auspices of BESAC. Prioritization within each of these program elements is achieved via such studies. Prioritization across the entirety of the BES program is more complex than that for a homogeneous program where a single planning exercise results in a prioritization.

Inputs to prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, 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 the hydrogen economy, basic research for effective solar energy utilization, and basic research for nuclear fuel cycles) or for which BES represents the sole U.S. steward of the field (e.g., heavy-element chemistry). Construction of new user facilities such as the Spallation Neutron Source, the Linac Coherent Light Source, the Nanoscale Science Research Centers, or upgrades or replacements to existing facilities such as the High Flux Isotope Reactor, the Stanford Synchrotron Radiation Laboratory, and the National Synchrotron Light Source-II follow from input from BESAC and from broad, national strategies that include the input from multiple federal agencies.

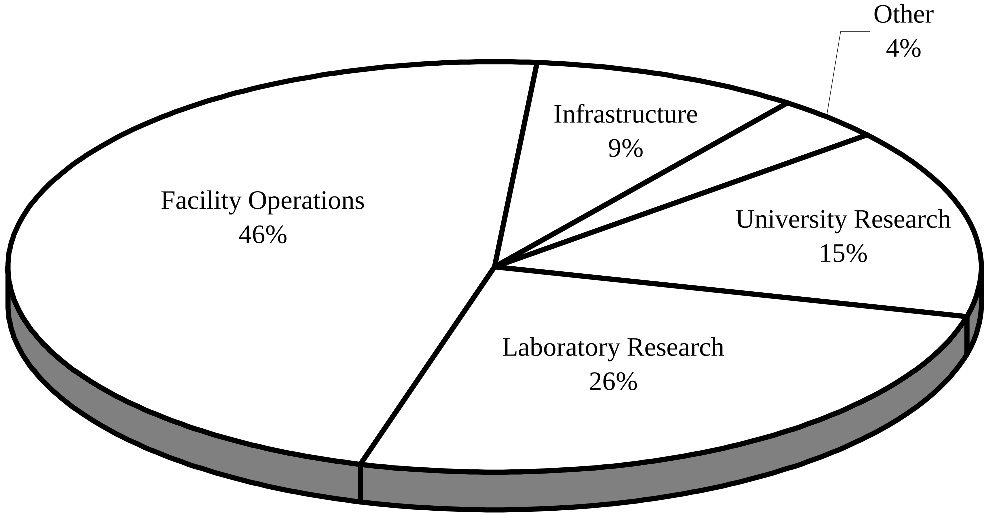
The FY 2008 budget request continues priorities established in the past few years. The Spallation Neutron Source enters its second year of full operation after construction from FY 1999 to FY 2006. A significant investment in the area of nanoscale science includes the operation of new Nanoscale Science Research Centers at Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory (LBNL), Argonne National Laboratory (ANL) and Sandia National Laboratories (SNL)/Los Alamos National Laboratory (LANL), and Brookhaven National Laboratory (BNL). Construction funding is provided for the Linac Coherent Light Source (LCLS), a fourth generation light source that will provide orders of magnitude higher intensities of coherent x-ray light than do current synchrotron radiation light sources. The LCLS will be a facility for groundbreaking research in the physical and life sciences owing to its femtosecond pulses of extremely high peak brightness x-ray beams. It will be the first such facility in the world. R&D funding is provided for upgrades on next-generation x-ray synchrotron sources. Project Engineering Design and R&D funding are provided for the National Synchrotron Light Source-II (NSLS-II) project, which sets a new standard for storage-ring-based light sources. The NSLS-II would be the first light source that combines nanometer spatial resolution with high brightness, coherence, and beam stability, thus enabling routine nanometer-scale characterization of materials. Construction funding is provided for the User Support Building at the Advanced Light Source to provide laboratory and instrument set-up space for the users of the light source.

Finally, funding is provided to renovate a two-story wing of the Central Laboratory building at the Stanford Linear Accelerator Center (SLAC) for a new research initiative—the Photon Ultrafast Laser Science and Engineering (PULSE) Center. The PULSE Center, together with LCLS, the Stanford Synchrotron Radiation Laboratory, and research programs in materials and chemical sciences, create a robust and diverse photon sciences research program at SLAC.

How We Spend Our Budget

The BES program has three major program elements: research, facility operations, and construction and laboratory infrastructure support. Of that part of the program that supports research, approximately one-third goes to support work in universities, with most of the remainder going to support work in DOE laboratories. The facility operations budget has grown relative to the research budget over the past decade, reflecting the commissioning of new and upgraded facilities as well as the increased importance of these facilities in enabling the research of thousands of researchers across the nation. Project Engineering Design (PED) and construction funding remain significant budget components in FY 2008 for the Linac Coherent Light Source, the National Synchrotron Light Source-II, and the Advanced Light Source User Support Building.

Basic Energy Sciences Budget Allocation
FY 2008



Research

The BES program is one of the nation's largest supporters of fundamental research. Research is supported in both DOE laboratories and universities. While peer review of all research ensures outstanding quality and relevance, each of the two research sectors has unique characteristics and strengths.

National Laboratory Research: Research sited at DOE laboratories often takes advantage of the premier scientific user facilities for x-ray, neutron, and electron beam scattering at the laboratories as well as other specialized facilities, such as hot cells, which are not typically found at universities. Mission-critical research is also sited at DOE laboratories when it is outside of the mainstream of research supported at universities, e.g., heavy-element chemistry or combustion chemistry. Research sited at DOE laboratories is very often collocated with and sometimes cofunded with research activities of the DOE technology offices, providing a synergism not available in universities. Finally, research that requires strong interdisciplinary interactions, large teams of closely collaborating researchers, or a large technical support staff is also well suited to DOE laboratories.

University Research: Universities provide access to the nation's largest scientific talent pool and to the next generation of scientists. Development of the workforce through the support of faculty, graduate students working toward a doctoral degree, and postdoctoral associates developing their research and management skills is a high priority. The R&D workforce developed under this program provides new scientific talent in areas of fundamental research. Furthermore, engaging faculty and students in the work of the BES program develops a broad appreciation for the basic research needs associated with the program.

Collaborations between National Laboratory Research and University Research: Historically, collaborations between the two research sectors have been strong, particularly in areas where both sectors derive significant benefits. Examples include the use of the major BES facilities by university and industry researchers and the contribution of these researchers to new instrument concepts and to instrument fabrication at the facilities. The Nanoscale Science Research Centers and new activities in ultrafast science and basic research for the hydrogen economy are expected to both strengthen and broaden these partnerships.

Significant Program Shifts

In FY 2008, there are a number of significant program milestone increases and decreases, including the following in the area of construction, Major Items of Equipment, and facility operations:

- Construction of the Spallation Neutron Source (SNS) was officially completed on June 5, 2006, ahead of schedule, under budget, and meeting all technical milestones. Over the next two to three years, the facility will continue to fabricate and commission instruments and will increase power to full levels. Two Major Items of Equipment will permit the fabrication of approximately nine to ten additional instruments for the SNS, thus nearly completing the initial suite of 24 instruments that can be accommodated in the high-power target station.
- All five Nanoscale Science Research Centers will be operational in FY 2008: the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Molecular Foundry at Lawrence Berkeley National Laboratory, the Center for Nanoscale Materials at Argonne National Laboratory, the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory, and the Center for Functional Nanomaterials at Brookhaven National Laboratory.
- The Linac Coherent Light Source will continue construction at the planned levels. Funding is provided separately for design and fabrication of instruments for the facility. Funding is also provided to partially support operation of the Stanford Linear Accelerator Center (SLAC) linac. This marks the third year of the transition of linac funding from the High Energy Physics Program to the Basic Energy Sciences Program.
- Support is provided for PED ($45,000,000) and Other Project Costs ($20,000,000) for the National Synchrotron Light Source-II (NSLS-II), which is proposed to be built as a replacement for NSLS to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. NSLS-II would provide the world's finest capabilities for x-ray imaging.
- Support is provided for construction of the Advanced Light Source User Support Building ($17,200,000), which will provide space for experimental setup of equipment prior to use at the Advanced Light Source, space to accommodate a long beam line that will extend from the floor of the Advanced Light Source into the User Support Building, and temporary office space and conference rooms for users.
- Support is provided for PED ($950,000) and Construction ($6,450,000) for renovation of a two-story wing of the SLAC Central Laboratory building to house offices and laser laboratories for the Photon Ultrafast Laser Science and Engineering (PULSE) Center.

In FY 2008, there are shifts in the nanoscale science and engineering research activities contributing to the BES investments in research at the nanoscale and an overall increase in funding. All five planned Nanoscale Science Research Centers are in operation. Overall, the total investment for these Nanoscale Science Research Centers increases due to cost-of-living increases in the facility operations budget. Funding for research at the nanoscale increases owing to increases in funding for activities related to the hydrogen economy and for general funding increases in research at the nanoscale. The table below provides a summary of nanoscale science research funding within BES. In addition to this funding, a new request of $3,000,000 is identified in the Biological and Environmental Research (BER) program for research relevant to environmental and ecological aspects of nanomaterials. This work will be coordinated between BER and BES.

Nanoscale Science Research Funding

	(dollars in thousands)				
	TEC	TPC	FY 2006	FY 2007	FY 2008
Materials Sciences and Engineering					
Research			67,982	108,542	122,330
Major Item of Equipment, Center for Nanophase Materials, ANL			14,000	—	—
Facility Operations					
Center for Functional Nanomaterials, BNL			—	—	19,934
Center for Integrated Nanotechnologies, SNL/A & LANL			11,500	19,190	19,934
Center for Nanophase Materials Sciences, ORNL			17,800	19,190	19,934
Center for Nanophase Materials, ANL			3,500	19,190	19,934
Molecular Foundry, LBNL			8,000	19,190	19,934
Chemical Sciences, Geosciences, and Energy Biosciences					
Research			28,769	49,109	57,085
Construction					
Center for Functional Nanomaterials, BNL	79,700	81,000	36,187	18,864	366
Center for Integrated Nanotechnologies, SNL/A & LANL	73,754	75,754	4,580	247	—
Molecular Foundry, LBNL	83,604	84,904	9,510	257	—
Total			201,828	253,779	279,451

In FY 2008, $59,500,000 is requested for basic research activities to realize the potential of a hydrogen economy. The research program is based on the BES workshop report "Basic Research Needs for the Hydrogen Economy" that can be found at http://www.science.doe.gov/production/bes/hydrogen.pdf. The 2003 report highlights the gap between our present capabilities for hydrogen production, storage, and use and those required for a competitive hydrogen economy. To be economically competitive with the present fossil fuel economy, the cost of fuel cells must be lowered by a factor of five and the cost of producing hydrogen must be lowered by a factor of four. Moreover, the performance and reliability of hydrogen technology for transportation and other uses must be improved dramatically. Simple incremental advances in the present state-of-the-art cannot bridge this gap. Narrowing the gap significantly will require a comprehensive, long-range program of innovative high-risk/high-payoff basic research that is intimately coupled to and coordinated with applied programs. The objective of such a program must not be evolutionary advances but rather revolutionary breakthroughs in understanding and in controlling the chemical and physical interactions of hydrogen with materials. Detailed findings and research directions identified during the workshop are presented in the report.

In response to the BES solicitation on Basic Research for the Hydrogen Fuel Initiative for FY 2005 funding, 668 qualified preapplications were received in five submission categories: novel materials for hydrogen storage; membranes for separation, purification, and ion transport; design of catalysts at the nanoscale; solar hydrogen production; and bio-inspired materials and processes. Three of the five focus areas—novel storage materials, membranes, and design of catalysts at the nanoscale—accounted for about 75% of the submissions. Following a review, principal investigators on about 40% of the preapplications were invited to submit full applications; 227 full applications were received and were peer reviewed according to the guidelines in 10 CFR 605; 70 awards were made in late FY 2005. BES involved staff from the Office of Energy Efficiency and Renewable Energy (EERE) in the preapplication review process to ensure basic research relevance to technology program goals. Furthermore, BES has begun participation in EERE's annual program review meeting to promote information sharing. In FY 2006, BES organized parallel sessions at that meeting for the BES principal investigators. The research topic of hydrogen storage was emphasized. A total of $21,473,000 in new funding related to the hydrogen economy was awarded in FY 2005 as a result of this solicitation. An additional $17,500,000 in FY 2007 and an additional $9,500,000 in FY 2008 will be used to fund new proposals based on new solicitations.

President's Hydrogen Initiative

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Materials Sciences and Engineering Research	15,472	28,075	33,420
Chemical Sciences, Geosciences, and Energy Biosciences	17,028	21,925	26,080
Total Hydrogen Initiative	32,500	50,000	59,500

Stanford Linear Accelerator Center, Linac Operations

For decades, SLAC has been one of the world's leading research laboratories in the design, construction, and operation of state-of-the-art electron accelerators and related experimental facilities for use in high-energy physics and synchrotron radiation research. With the advent of the Linac Coherent Light Source (LCLS) project, the role that SLAC plays in x-ray science has greatly expanded. Indeed, after the planned shutdown of the B-factory at the end of FY 2008, the SLAC linac will be dedicated to the world's first x-ray free electron laser. The potential applications of this new experimental tool are legion: nanotechnology, solid-state physics, biology, energy production, medicine, electronics, and fields that do not yet exist. Recognizing the importance of the SLAC linac to the BES program, the Office of Science has been transitioning support for the SLAC linac from HEP to BES, with FY 2008 marking the third and final year of split funding.

BES funding for SLAC Linac operations is shown on the "Linac for LCLS, SLAC" line within Materials Science and Engineering/Facilities Operations activity. The following tables identify the SLAC linac funding amounts within BES and overall.

SLAC Linac Operations Funding within BES

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Materials Science and Engineering/Facility Operations			
Linac for LCLS, SLAC	29,400	40,000	61,500
Other BES Facility Operations	423,733	604,885	637,024
Total, Materials Science and Engineering/Facility Operations	453,133	644,885	698,524

Total SLAC Linac Operations Funding

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Basic Energy Sciences	29,400	40,000	61,500
High Energy Physics	56,100	52,100	32,500
Total, SLAC Linac Operations	85,500	92,100	94,000

Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) program is a set of coordinated investments across all Office of Science mission areas with the goal of achieving breakthrough scientific advances via computer simulation that were impossible using theoretical or laboratory studies alone. Advances in high-end computing technology, together with innovative algorithms and software, are being exploited as intrinsic tools for scientific discovery. SciDAC has also pioneered an effective model of multidisciplinary collaboration among discipline-specific scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can productively exploit terascale computing and networking resources.

The SciDAC program in BES consists of two activities: (1) characterizing chemically reacting flows as exemplified by combustion and (2) achieving scalability in the first-principles calculation of molecular properties, including chemical reaction rates. In the characterization of chemically reacting flows, the scientific problem is one of multiple scales from the molecular scale (where the physical descriptions are discrete in nature) to the laboratory scale (where the physical descriptions are continuous). A collaboration involving Sandia National Laboratories and four universities successfully implemented a fully parallel direct numerical simulation that incorporated a widely used program for solving the species profiles for combustion systems involving dozens of species and hundreds of reactions. In achieving scalability in the first-principles calculation of molecular properties, progress has been made on several fronts, but perhaps the most encouraging is work dealing with electron correlation, a problem responsible for the poor scaling of quantum chemistry codes. A novel method for incorporating correlation directly into quantum mechanical descriptions of atoms and molecules is now being incorporated into a massively parallel computer code.

Scientific Facilities Utilization

The BES program request supports the scientific user facilities. Research communities that have benefited from these facilities include materials sciences, condensed matter physics, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, medical research, and industrial technology development. More detailed descriptions of the specific facilities and their funding are given in the subprogram narratives and in the sections entitled Site Description and Major User Facilities.

Two tables follow: The first shows the hours of operation and numbers of users for the major scientific user facilities—the synchrotron radiation sources and the neutron scattering facilities. The second 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 have met or are on schedule to meet all Level 0 and Level 1 Milestones, which are shown in the table.

Synchrotron Light Source and Neutron Scattering Facility Operations

	FY 2006 Actual	FY 2007 Estimate	FY 2008 Estimate
All Facilities			
Optimal Hours[a]	31,300	32,700	32,700
Scheduled Hours[b]	29,595	32,700	32,700
Unscheduled Downtime	11.5%	<10%	<10%
Number of Users	9,211	9,660	10,020
Advanced Light Source			
Optimal Hours[a]	5,600	5,600	5,600
Scheduled Hours[b]	6,109[c]	5,600	5,600
Unscheduled Downtime	2.5%	<10%	<10%
Number of Users	2,158	2,100	2,200
Advanced Photon Source			
Optimal Hours[a]	5,000	5,000	5,000
Scheduled Hours[b]	4,876	5,000	5,000
Unscheduled Downtime	2.5%	<10%	<10%
Number of Users	3,274	3,300	3,500
National Synchrotron Light Source			
Optimal Hours[a]	5,400	5,400	5,400
Scheduled Hours[b]	5,880[d]	5,400	5,400
Unscheduled Downtime	4.2%	<10%	<10%
Number of Users	2,105	2,300	2,300

[a] 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.
[b] Scheduled hours for FY 2006 represent the actual number of hours delivered to users
[c] Actual hours exceed optimal hours in FY 2006 because planned downtime for maintenance and upgrades was deferred into FY 2007. FY 2007 actual hours will reflect the downtime for upgrades.
[d] Hours delivered to users exceeded optimal hours because maintenance downtime was less than expected due to a low number of faults and no major installations in FY 2006.

	FY 2006 Actual	FY 2007 Estimate	FY 2008 Estimate
Stanford Synchrotron Radiation Laboratory			
Optimal Hours[a]	5,000	5,000	5,000
Scheduled Hours[b]	4,821	5,000	5,000
Unscheduled Downtime	3.8%	<10%	<10%
Number of Users	1,124	1,200	1,300
High Flux Isotope Reactor			
Optimal Hours[a]	2,400	4,500	4,500
Scheduled Hours[b]	556	4,500	4,500
Unscheduled Downtime	89.5%	<10%	<10%
Number of Users	42	220	220
Intense Pulsed Neutron Source			
Optimal Hours[a]	3,600	3,600	3,600
Scheduled Hours[b]	3,575	3,600	3,600
Unscheduled Downtime	3.2%	<10%	<10%
Number of Users	211	240	200
Manuel Lujan, Jr. Neutron Scattering Center			
Optimal Hours[a]	4,300	3,600	3,600
Scheduled Hours[b]	3,778	3,600	3,600
Unscheduled Downtime	16.8%	<10%	<10%
Number of Users	297	300	300
Spallation Neutron Source[c]			

Cost and Schedule Variance

	FY 2006 Actual	FY 2007 Estimate	FY 2008 Estimate
Spallation Neutron Source, ORNL			
Cost Variance	+1.25%		
Schedule Variance	-0.35%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Ring Beam Available to Target	N/A	N/A
	Approve Critical Decision 4 – Start of Operations		

[a] 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.
[b] Scheduled hours for FY 2006 represent the actual number of hours delivered to users.
[c] For the Spallation Neutron Source, there is an inadequate basis for making a reliable estimate at this time.

	FY 2006 Actual	FY 2007 Estimate	FY 2008 Estimate
Linac Coherent Light Source, SLAC			
Cost Variance	-4.03%		
Schedule Variance	-2.72%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 3b – Start Construction	None	None
Center for Nanophase Materials Sciences, ORNL			
Cost Variance	+0.01%		
Schedule Variance	-1.03%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 4b – Start Full Operations	N/A	N/A
Center for Integrated Nanotechnologies, SNL/LANL			
Cost Variance	+0.72%		
Schedule Variance	-0.61%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 4a – Start Initial Operations	Approve Critical Decision 4b – Start of Full Operations	N/A
The Molecular Foundry, LBNL			
Cost Variance	-0.24%		
Schedule Variance	-0.87%		
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
Center for Nanoscale Materials, ANL			
Cost Variance	+2.01%		
Schedule Variance	-4.26%		
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
Center for Functional Nanomaterials, BNL			
Cost Variance	-2.97%		
Schedule Variance	-8.64%		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	Approve Critical Decision 4a – Start of Initial Operations	Approve Critical Decision 4b – Start of Full Operations

	FY 2006 Actual	FY 2007 Estimate	FY 2008 Estimate
Instrumentation for Spallation Neutron Source I, ORNL			
Cost Variance	+1.35%		
Schedule Variance	-2.21%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 2 for Instruments #4-5 – Performance Baseline Approve Critical Decision 3 for Instrument #3 – Start Construction Approve Critical Decision 3 for Instruments #4-5 – Start Construction	none	Approve Critical Decision 4 – Start of Operations for Instruments #1-2
Transmission Electron Aberration Corrected Microscopy (TEAM), LBNL			
Cost Variance	[a]		
Schedule Variance	[a]		
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	Approve Critical Decision 4a – Start of Operation TEAM 0.5
Advanced Light Source User Support Building, LBNL			
Cost Variance	[a]		
Schedule Variance	[a]		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	Approve Critical Decision 1 – Alternative Selection/Cost Range Approve Critical Decision 2 – Performance Baseline Approve Critical Decision 3 – Start of Construction	None

Construction and Infrastructure

- **Linac Coherent Light Source (LCLS) Project**

  Most x-ray experiments performed at synchrotron radiation light sources produce static pictures of materials averaged over relatively long times. However, the electrons and atoms in molecules, crystal lattices, polymers, biomaterials, and all other materials are in constant motion. Merely

[a] Performance Baseline approved 1st Quarter, FY 2007.

measuring atomic "form" will not tell us all there is to know about molecular "function." We need to perform experiments that provide us with information on the motions of atoms in materials as well as their equilibrium positions. This will give us insight as never before possible into catalysis, chemical processes, protein folding, and molecular assembly.

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source and that has pulse lengths measured in femtoseconds—the timescale of electronic and atomic motions. The advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons have revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be even more dramatic.

The LCLS Project will provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Å (Angstrom) range. The characteristics of the light from the LCLS will open new realms of scientific inquiry and applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. Optical devices beyond the undulator manipulate the direction, size, energy, and duration of the x-ray beam and carry it to whatever experiment is under way. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

FY 2008 budget authority of $51,356,000 is requested. The estimated Total Project Cost is $379,000,000. Additional information on the LCLS Project is provided in the LCLS construction project datasheet, project number 05-R-320.

- **National Synchrotron Light Source – II (NSLS-II) Project**

The NSLS-II is a proposed 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 would 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.

The NSLS-II would have the best storage-ring-based synchrotron light source in the world, but, more importantly, the NSLS-II would be transformational in that it can open new regimes of scientific discovery and investigation. The ability to probe materials with 1 nm or better spatial resolution and to analyze their dynamics with 0.1 meV energy resolution will be truly revolutionary. For example, it should be possible to investigate the atomic and electronic structure and chemical composition of nanometer-scale objects under realistic in-situ device operating conditions. It should also be possible to investigate processes that change the energy or spin state of electrons, such as their interaction with the atomic lattice or other electrons or spins. These processes form the foundation of many diverse phenomena, such as photosynthesis and spin-based quantum computing, and the ability to study them with high spatial resolution would be unprecedented.

In FY 2008, budget authority is requested to continue Project Engineering and Design ($45,000,000) and for R&D activities ($20,000,000) to address technical risks in four key areas—energy resolution, spatial resolution, superconducting undulators, and superconducting storage ring magnets. These R&D activities will be carried out at Brookhaven National Laboratory and by researchers elsewhere as needed. Additional information on the NSLS-II Project is provided in the NSLS-II Project Engineering and Design datasheet, project number 07-SC-06.

- **Advanced Light Source (ALS) User Support Building Project**

  The ALS User Support Building to be located at the Lawrence Berkeley National Laboratory will provide high-quality user support space in sufficient quantity to accommodate the very rapid growth in the number of ALS users and to accommodate projected future expansion. Efficient use of the experimental beamlines at the ALS requires adjacent space for setting up experimental apparatus before moving the apparatus into place on the experimental floor. By the end of FY 2005, almost 40 beamlines were in simultaneous and nearly continuous operation for the use of 2,000 scientists and students. All available floor space for staging experiments is now occupied with operating beamlines, necessitating shutdown of beamlines and work stoppage when the experimental apparatus is built, when it is commissioned, and when it is moved into place at the beamline. Such use of beam time is unacceptable for advanced, state-of-the art instrumentation. In addition to being too small, the current user support space does not meet seismic building codes. Structural upgrades have been evaluated and would not be cost effective. The User Support Building will provide staging areas for ALS experiments, space for a long beamline that will extend from the floor of the ALS into the User Support Building, and temporary office space for visiting users. FY 2008 budget authority of $17,200,000 is requested for construction using a design-build approach that is based on private sector best practices. Additional information on the ALS User Support Building Project is provided in the User Support Building datasheet, project number 08-SC-01.

- **Photon Ultrafast Science and Engineering (PULSE) Center**

  The PULSE Center is a new research activity at SLAC that builds on existing SLAC core competencies in the atomic physics, chemistry, condensed matter physics, and biology. The PULSE Center will focus on ultrafast structural and electronic dynamics in materials sciences, the generation of attosecond laser pulses, single-molecule imaging, and the origin of efficient light harvesting and solar energy conversion in molecular systems.

  The PULSE Center will be located in the Central Laboratory building (B040), a mixed use building consisting of three joined structures: a three-story wing joined to a two-story wing by a one story section. 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 program needs. Roughly 33% of the space will be used for offices, 50% for lab space, and 17% for conference/meeting rooms. In FY 2008, budget authority is requested to initiate Project Engineering and Design ($950,000) and construction renovation ($6,450,000) activities. Additional information is provided in the Photon Ultrafast Laser Science and Engineering Building Renovation datasheet, project number 08-SC-11.

General Plant Projects (GPP) and General Purpose Equipment (GPE)

BES provides funding for GPP and GPE for Argonne National Laboratory, Ames Laboratory, and Oak Ridge National Laboratory.

Workforce Development

The BES program supports development of the R&D workforce through support of undergraduate researchers, graduate students working toward doctoral degrees, and postdoctoral associates developing their research and management skills. The R&D workforce developed under this program provides new scientific talent in areas of fundamental research and also provides talent for a wide variety of technical and industrial areas that require the problem solving abilities, computing skills, and technical skills developed through education and experience in fundamental research. In addition, the BES scientific user facilities provide outstanding hands-on research experience to many young scientists. Thousands of students and post-doctoral investigators are among the researchers who conduct experiments at BES-supported facilities each year. The work that these young investigators perform at BES facilities is supported by a wide variety of sponsors including BES, other Departmental research programs, other federal agencies, and private institutions.

	FY 2006	FY 2007 estimate	FY 2008 estimate
# University Grants	810	1,000	1,080
Average Size	$150,000	$150,000	$150,000
# Permanent Ph.D.s (FTEs)	3,900	4,830	5,220
# Postdoctoral Associates (FTEs)	1,140	1,380	1,480
# Graduate Students (FTEs)	1,810	2,170	2,350

External Independent Reviews

The costs of conducting External Independent Reviews (EIRs) for Capital Asset Projects greater than $100,000,000 within SC are funded by SC. Examples of EIRs include conducting Performance Baseline EIRs prior to Critical Decision-2 (CD-2) to verify the accuracy of cost and schedule baseline estimates and conducting Construction/Execution Readiness EIRs, which are done for all Major System projects prior to CD-3. These funds, which are managed by the Office of Engineering and Construction Management, are exclusively used for EIRs directly related to these projects funded within SC. Beginning in FY 2007, the EIR business line will be financed via the Working Capital Fund to achieve parity on how EIRs are funded and to standardize the administration of these critical activities.

Materials Sciences and Engineering

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Materials Sciences and Engineering			
Materials Sciences and Engineering Research	273,762	335,099	368,398
Facilities Operations	453,133	644,885	698,524
SBIR/STTR	—	24,228	26,297
Total, Materials Sciences and Engineering	726,895	1,004,212	1,093,219

Description

This subprogram extends the frontiers of materials sciences and engineering to expand the scientific foundations for the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. The subprogram also plans, constructs, and operates the major x-ray scattering and neutron scattering scientific user facilities and the Nanoscale Science Research Centers.

Included within the $368,398,000 research component of this subprogram for FY 2008 are facility-related activities such as R&D for new and upgraded facilities, accelerator and detector research, and all BES FY 2008 Major Items of Equipment. These activities total $56,211,000.

Benefits

Ultimately, the research leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. For example, the fuel economy in automobiles is directly proportional to the weight of the automobile, and fundamental research on strength of materials has led to stronger, lighter materials, which directly affects fuel economy. The efficiency of a combustion engine is limited by the temperature and strength of materials, and fundamental research on alloys and ceramics has led to the development of materials that retain their strength at high temperatures. Research in semiconductor physics has led to substantial increases in the efficiency of photovoltaic materials for solar energy conversion. Fundamental research in condensed matter physics and ceramics has underpinned the development of practical high-temperature superconducting wires for more efficient transmission of electric power.

Supporting Information

The subprogram supports basic research to understand the atomistic basis of materials properties and behavior and how to make materials perform better at acceptable cost through new methods of synthesis and processing. Basic research is supported in magnetic materials, semiconductors, superconductors, metals, ceramics, alloys, polymers, metallic glasses, ceramic matrix composites, catalytic materials, surface science, corrosion, neutron and x-ray scattering, chemical and physical properties, electron beam microcharacterization, nanotechnology, and new instrumentation. This subprogram, a premier sponsor of condensed matter and materials physics in the U.S., is the primary supporter of the BES user facilities.

Selected FY 2006 Research Accomplishments

- *Nanofluidic transistor*. Imagine a valve to precisely control the flow of liquids but with dimensions so tiny that only one molecule at a time can pass through it. Controlled flow of ions in a liquid was recently demonstrated through very small nanochannels barely large enough to pass large molecules. Named “nanofluidic transistors,” the nanochannel assembly functions in a way similar to ordinary transistors where the flow of electrons can be regulated by applying a voltage. Demonstrations were carried out on a 35-nanometer channel constructed between two silicon dioxide plates; the channel was filled with water and potassium chloride salt. The flow of potassium ions could be completely stopped by applying an electric current across the channel. The regulation of the flow (or current) of charged molecules was also demonstrated. This exciting discovery now makes possible detection and separation of individual molecules in a fluid. Among the important implications of this discovery are advanced nanoscale chemical analysis with extreme sensitivity and the capability of sorting individual molecules.
- *Unexpected spontaneous reversal of magnetization in nanoscaled structures*. New and unexpected magnetic phenomena have been discovered in ultrathin bilayers of ferromagnetic and antiferromagnetic films. Ferromagnetic materials (e.g., iron) have a positive magnetization due to the alignment of the magnetic moments. Antiferromagnet materials (e.g., nickel oxide) have no net magnetization due to the anti-parallel alignment of the magnetic moments. In bulk magnetic materials, regions of aligned magnetic moments, termed magnetic domains, are expected to align with an external applied magnetic field. The magnetic strength is determined by the degree of alignment of the magnetic domains. In contrast to naturally occurring bulk magnetic materials, an ultrathin ferromagnetic layer in close contact with an antiferromagnetic layer will spontaneously align *opposite* to the applied magnetic field upon cooling. The close proximity of the two different layers also results in an increase in magnetic strength. The ability to control and detect the magnetic alignment in ultrathin magnetic materials could lead to new concepts in computer data storage design. The fundamental understanding of the unexpected phenomena may also influence future research and development of magnetic based biological and chemical sensors.
- *Nano-electronic hydrodynamics and turbulence*. Electrons moving across a nanometer-sized wire have been found to behave hydrodynamically, i.e., like a liquid flowing from one bucket to another through a small opening. This behavior is exactly contrary to expectations from a quantum mechanical prediction, and it has prompted theoretical predictions of new phenomena. Most striking is the prediction of possible turbulent electrical transport with eddy currents in nanoscale conductors that could seriously limit current flow. Such turbulent currents could then lead to extremely high electronic temperatures due to the “friction” of the electrons as they move against each other, resulting in potential premature failure at much reduced current flow. Experiments are being carried out to test these theoretical developments.
- *Using bioinspired methods to synthesize and assemble materials*. Biological systems are renowned for synthesizing inorganic materials under mild conditions and assembling them into exquisitely shaped structures with high precision and control. Recently, by emulating the underlying chemistry and approaches of biology, several inorganic materials have been synthesized under mild conditions (room temperature, neutral pH, etc.), with a potential for significant energy savings in their large-scale manufacture. Some of the materials synthesized include semiconducting titanium dioxide, gallium oxide, and zinc oxide for solar energy conversion; ferroelectric barium titanate nanoparticles for energy storage; magnetite nanoparticles for ultra-high density magnetic information storage; and nanocrystalline palladium for hydrogen storage. Furthermore, by exploiting the ability of biological

macromolecules (e.g., DNA, proteins, viruses) to self-assemble into large, well-defined structures and to nucleate the growth of inorganic materials, researchers have shown that complex electronic circuit elements and large ordered arrays of nanoparticles can be assembled with a precision that far exceeds the current top-down fabrication capabilities.

- *Unveiling the superconductor mystery*. Understanding the phenomena of superconductivity and its mechanism has been among the most challenging issues facing the condensed matter and materials physics communities. The mystery of superconductivity is being tackled by a concerted effort, coupling synthesis and characterization with theory, modeling, and simulation. The recent discovery of superconductivity in actinide- and boron-containing materials indicates superconductivity may exist in many material systems yet to be discovered. The search for new materials is augmented by sophisticated techniques to modify the electronic properties of known superconducting materials, both chemically and electrically. Advances in new characterization tools, including proximal probes, have made possible the discovery of new phenomena, including competing phases within the superconducting phase. First principles calculations assisted by generalized density functional theory enabled accurate predictions of the electronic structure of superconducting materials. When coupled to an electron pairing mechanism, numerical models are being developed to predict the superconducting transition temperature as a first step towards a priori design of new superconductors.

Selected FY 2006 Facility Accomplishments

- The Advanced Light Source (ALS) at LBNL

  Experiments begin on new femtosecond X-ray beamline. Experiments using ultrafast soft x-rays began in FY 2006 on Beamline 6.0.1.2. High-resolution x-ray spectroscopy and diffraction at photon energies from 150–1800 eV are now possible using the new, high-brightness, in-vacuum-undulator beamline, which increases the flux by a factor of 1000 relative to its predecessor. Beamline 6.0.1, a complementary hard x-ray beamline using the same insertion device and extending the photon energy available to users from 2.2–10 keV, was also installed, and its commissioning was begun. In the first measurements, soft x-ray pulses of 200-femtosecond duration were used to study phase transitions in vanadium oxide.

- The Advanced Photon Source (APS) at ANL

  Record nanofocusing with an innovative lens design. A new device, the Multilayer Laue Lens, developed at Argonne National Laboratory jointly between the APS and the Center for Nanoscale Materials, has set a world's record for line size resolution produced with a hard x-ray beam. The wafer from which the device was made won a 2005 R&D 100 award, given to the world's top 100 scientific and technological innovations. Enhancements to the device have now increased its ability to focus the x-rays with an energy level of 19.5 keV to less than 20 nanometers. Using the lens, researchers will be able to visualize three-dimensional electronic circuit boards to find circuit errors, map impurities in biological or environmental samples at the nanometer scale, or analyze samples inside high-pressure or high-temperature cells because hard x-rays, unlike soft x-rays, are able to penetrate container walls. This device has potential for a multitude of uses, including possible incorporation at the nanoprobe beamline at APS associated with the Center for Nanoscale Materials facility.

- The National Synchrotron Light Source (NSLS) at BNL

  Novel undulator design developed and installed. A custom-designed, cryogenic-ready, in-vacuum, miniature-gap hybrid undulator has been installed in the X25 straight section of the NSLS x-ray ring. The new radiation source, the first of its kind, will be an order of magnitude brighter than the original wiggler. By cooling the magnet array, this insertion device can have a higher magnetic field and a higher radiation resistance, resulting in a larger photon energy tuning range. Consequently, unlike previous miniature-gap undulators in use at the NSLS, this new undulator will be continuously tunable from 2 to 20 keV by employing all harmonics up through the 9th. This upgrade will provide significant benefits to the macromolecular crystallography program at the NSLS. This technology will be useful to all medium-energy storage rings in the world.

- The Stanford Synchrotron Radiation Laboratory (SSRL) at SLAC

  Operation at high current of 500 mA. The SPEAR3 accelerator reached its design current of 500 mA for the first time during a special run last year. Under similar test conditions, a selected beam line (BL 6) was subsequently operated successfully at 500 mA to test the performance of newly designed optical components, including the liquid-nitrogen-cooled double crystal monochromator. The success of this test paves the way for commissioning the other beam lines. The SPEAR3 accelerator received permission to operate routinely at 500 mA following an extensive accelerator readiness review. Authorization for operating beam lines for users at 500 mA is expected during the FY 2007 user run, when selected time periods will be allocated to commission, characterize, and operate beam lines at high current. SSRL is planning to operate full time with high current in FY 2008.

- The Spallation Neutron Source (SNS) at ORNL

  Commissioning and initial instrument results. Construction and commissioning of the Spallation Neutron Source, an accelerator-based neutron source that will provide the most intense pulsed neutron beams in the world for scientific research and industrial development, was completed, and the facility began operations in late FY 2006. The backscattering spectrometer that is part of the initial suite of instruments has unprecedented dynamic range and an energy resolution of better than 3×10^{-6} electron volts. Initial operation of this hardware involved test measurements of excitations in picoline (a hydrocarbon), which confirmed the performance of the instrument.

Detailed Justification

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Materials Sciences and Engineering Research	**273,762**	**335,099**	**368,398**
▪ **Structure and Composition of Materials**	**19,385**	**22,245**	**24,245**

This activity supports basic research on the structure and composition of materials including research on the arrangement and identity of atoms and molecules in materials and the development of quantitative characterization techniques, theories, and models describing how atoms and molecules are arranged. Also sought are the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces, and precipitates.

The properties of materials used in all areas of energy technology 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. This dependence occurs because the spatial and chemical inhomogeneities in materials (e.g., dislocations, grain boundaries, magnetic domain walls, and precipitates) determine and control critical behaviors such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, surface/catalytic reactivity, superconducting parameters, magnetic behavior, corrosion susceptibility, etc.

Capital equipment is provided for items such as new electron microscopes and improvements to existing instruments.

In FY 2008, funding will continue on advanced instruments with capabilities to characterize and interpret atomic configurations and packing arrangements at the nanoscale with improved resolution and accuracy, including the ability to determine composition, bonding, and physical properties of materials. Within this funding, there is an increase to support new research to develop ultrafast electron scattering probes as companion tools to ultrafast photon probes ($+2,000,000). The main emphasis will be on characterization of transient nonequilibrium nanoscale structures.

	FY 2006	FY 2007	FY 2008
▪ **Mechanical Behavior and Radiation Effects**	**11,766**	**18,195**	**20,195**

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials. Work supported includes the behavior of materials under repeated or cyclic stress, under high rates of stress application as in impact loading, and over a range of temperatures corresponding to the stress and temperature conditions in energy conversion systems. The objective is to achieve an atomic-level understanding of the relationship between mechanical behavior and defects in materials, including defect formation, growth, migration, and propagation. This research aims to build on this atomic-level understanding to develop predictive models for the design of materials having superior mechanical behavior. The focus of basic research in radiation effects is to achieve an atomic-level fundamental understanding of mechanisms of radiation damage and to learn how to design radiation-tolerant materials. Concerns include radiation induced embrittlement and radiation assisted stress-corrosion cracking. Other goals include achieving an atomic level understanding of amorphization mechanisms (transition from crystalline to a non-crystalline phase) and the modification of surface behavior by techniques such as ion implantation.

This program contributes to DOE missions in the areas of fossil energy, fusion energy, nuclear energy, transportation systems, industrial technologies, defense programs, radioactive waste storage, energy efficiency, and environment management. This research helps understand load-bearing capability, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility or deformability of materials that is critical to their ease of fabrication, and radiation effects including understanding and modeling of radiation damage and surface modification using ion implantation. This activity relates to energy production and conversion through the need for failure resistant materials that perform reliably in the hostile and demanding environments of energy production and use. This program contributes to understanding mechanical properties of materials and aspects of nuclear technologies ranging from radioactive waste storage to extending the lifetime of nuclear facilities.

Capital equipment is provided for items such as in-situ high-temperature furnaces and characterization instrumentation.

In FY 2008, funding will continue support for research on understanding the mechanisms that are related to both the deformation and degradation of materials. Specific emphasis will be on nanoscale mechanics, and in particular the complex mechanical interactions of fundamental building blocks in directed self assembly. The program also supports the development of new theoretical and experimental tools to probe the deformation and degradation behaviors at the nanoscale. Within this funding, there is an increase to enhance core research activities in high temperature mechanical behavior and radiation effects in materials under extreme environments ($+2,000,000).

	FY 2006	FY 2007	FY 2008
▪ **Physical Behavior of Materials**	**23,298**	**29,756**	**34,193**

This activity supports basic research at the atomic and molecular level to understand, predict, and control physical behavior and functional properties of materials by developing models for the response of materials to environmental stimuli such as temperature, electromagnetic fields, chemical environments, and proximity of surfaces or interfaces. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the superconducting properties for high-temperature superconductors; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures encountered in energy conversion processes; and diffusion and transport of ions in ceramic electrolytes for improved performance in batteries and fuel cells.

Research underpins the missions of DOE by developing the basic science necessary for improving the reliability of materials in mechanical and electrical applications and for improving the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, hostile chemical environments, etc.), understanding how their behavior is linked to their surroundings and treatment history is important.

Capital equipment is provided for items such as spectroscopic instruments, instruments for electronic and magnetic property measurement, and analytical instruments for chemical and electrochemical analysis.

In FY 2008, major activities will include basic research for solar to electricity conversion. Areas of emphasis include polycrystalline, nanocrystalline, and organic materials to replace expensive single crystals; innovative design of interpenetrating photoconversion materials networks to improve charge separation and collection efficiency; and the development of novel processes to obtain extremely high conversion efficiencies at modest cost. With the anticipated vigorous development of new types of nanoscale materials, new opportunities will emerge to dramatically improve solar energy conversion efficiency. Within this funding, there is an increase to initiate new research activities in inorganic and organic light emitting materials ($+2,000,000). Special emphasis will be on novel materials or concepts, including nanophotonics and other nanoscale material assemblies and architectures. An additional increase will fund new solar-to-electricity and solar-to-fuels conversion research ($+2,437,000).

	FY 2006	FY 2007	FY 2008
▪ **Synthesis and Processing Science**	**15,357**	**21,022**	**24,522**

This activity supports basic research to understand and develop innovative ways to make materials with desired structure, properties, or behavior. Examples of activities in synthesis and processing include the growth of single crystals of controlled orientation, purity, and perfection; the formation of thin films of controlled structure and orientation by various techniques; atomic and molecular self assembly to create and explore new materials; nanostructured materials including those that mimic the structure of natural materials; the preparation and control of powder or particulate matter for consolidation into bulk form by many alternative processes; sol-gel processes; the welding and joining of materials including dissimilar materials or materials with substantial differences in their coefficients of thermal expansion; plasma, laser, and charged particle beam surface modification and materials synthesis; and myriad issues in process science. This activity also includes development of in-situ measurement techniques and capabilities to quantitatively determine variations in the energetics and kinetics of growth and formation processes on atomic or nanometer length scales.

This activity includes the operation ($727,000) 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 that are not otherwise available to academic, governmental, and industrial research communities to be used for research purposes.

This activity underpins many of the DOE technology programs, and appropriate linkages have been established in the areas of light weight metallic alloys; structural ceramics; high-temperature superconductors; and industrial materials, such as intermetallic alloys.

Capital equipment includes controlled crystal growth apparatus, furnaces, lasers, chemical vapor and molecular beam epitaxial processing equipment, plasma and ion sources, and deposition equipment.

In FY 2008, funding will include continued support for research on nanoscale synthesis and processing. Major emphasis will be on providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations to probe the atomistic basis of the emergent behavior. Research on emergent behavior will have a significant impact on developing new materials and devices for energy applications, including spin-based electronics and multifunctional sensors. Within this funding, there are increases to support new research activities on novel approaches to the design, discovery and synthesis of materials for hydrogen storage ($+1,500,000). Key emphasis will be on tailoring the atomic and molecular structure and chemical arrangements to maximize the storage capacity while maintaining optimal kinetic characteristics for practical charge and discharge functions. New research activities will also be initiated in the design and synthesis of nanoscale materials ($+2,000,000).

	FY 2006	FY 2007	FY 2008
▪ **Engineering Research**	**2,006**	**1,000**	**—**

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 are terminated because of competing priorities.

	FY 2006	FY 2007	FY 2008
▪ **Neutron and X-ray Scattering**	**44,313**	**62,055**	**63,355**

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures of

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008

materials as well as the relationship of these structures and excitations to the physical properties of materials. The increasing complexity of such energy-relevant materials as nanoscale catalysts, superconductors, semiconductors, and magnets requires ever more sophisticated neutron and x-ray scattering techniques to extract useful knowledge and develop new theories for the behavior of these materials. Both ordered and disordered materials are of interest, as are strongly correlated electron systems, surface and interface phenomena, and behavior under environmental variables such as temperature, pressure, and magnetic field. X-ray and neutron scattering, together with the electron scattering supported under Structure and Composition of Materials and Electron-beam Microcharacterization Facilities, are the primary tools for characterizing the atomic, electronic, and magnetic structures of materials.

Research in the areas of nanostructured materials and novel hydrogen storage media will be continued using the structural and chemical information garnered from x-ray and especially neutron scattering. Structural studies on carbon-based hydrogen storage media-such as nanotubes, nanohorns, fullerenes, and nanoscale hydrides-also will be performed to reveal the site of hydrogen incorporation and the mechanisms of hydrogen storage. The knowledge and technique developed in this activity have broad applicability in developing new materials for efficient and environmentally acceptable energy technologies.

Capital equipment is provided for items such as detectors, monochromators, mirrors, and beamline instrumentation at all of the facilities.

In FY 2008, activities will be initiated in photon-based ultrafast materials science research to characterize the physical, lattice, and electronic structures of highly correlated electron systems ($+1,300,000).

▪ **Experimental Condensed Matter Physics**	**37,279**	**47,480**	**50,480**

This activity supports condensed matter physics with emphases in electronic structure, surfaces, interfaces, and new materials. Research includes measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This activity includes the design and synthesis of new materials with new and improved properties. These materials include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The development of new techniques and instruments, including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy, is a major component of this activity. Measurements are made under extreme conditions of temperature, pressure, and magnetic field.

This research is aimed at a fundamental understanding of the behavior of materials that underpin DOE technologies. This activity supports research in photovoltaics, superconductivity, magnetic materials, thermoelectrics, and optical materials that underpin various technology programs in Energy Efficiency and Renewable Energy (EERE). Research in superconductivity and photovoltaics is coordinated with the solar technologies program in EERE. In addition, this activity supports the strategically important information technology and electronics industries in the fields of semiconductor physics, electronics, and spintronics research.

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

Capital equipment is provided for crystal growth equipment, scanning tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets, and computers.

In FY 2008, major activities will continue in the development of nanomaterials for both energy conversion and hydrogen energy storage, 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, photovoltaics, thermal management, super-strong lightweight materials, hydrogen storage, and electrical power transmission. Within this funding, there is an increase to enhance key core research activities in low dimensional materials and other strongly correlated electron systems ($+3,000,000).

	FY 2006	FY 2007	FY 2008
▪ **Condensed Matter Theory**	**23,198**	**27,408**	**31,753**

This activity supports basic research in theory, modeling, and simulations of the condensed matters, and it complements the Experimental Condensed Matter Physics activity. A current major thrust is in nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not well understood. For the simplest semiconductor systems, carbon nanotubes, and similar “elementary” systems, there has been considerable progress. However, progress in establishing the theoretical framework for more complex materials and hybrid structures has been limited. Computer simulations will play a major role in understanding materials at the nanometer scale and in the development “by design” of new nanoscale materials and devices. The greatest challenges and opportunities are in the transition regions where nanoscale phenomena are just beginning to emerge from the macroscopic and microscale regimes.

The Computational Materials Sciences Network supports cooperative research teams for studies requiring numerous researchers with diverse expertise ($1,730,000). Examples include fracture mechanics—understanding ductile and brittle behavior; microstructural evolution in which microstructural effects on the mechanics of materials; magnetic materials across all length scales; excited state electronic structure and response functions; and strongly correlated electron systems. The knowledge and computational tools developed in this activity have broad applicability on programs supported by Energy Efficiency and Renewable Energy and National Nuclear Security Administration.

Capital equipment will be provided for items such as computer workstations, beamline instruments, ion implantation, and analytical instruments.

In FY 2008, major activities will include theoretical and computational approaches capable of interrogating systems to gain direct insight on the mechanisms underpinning the cooperative behavior of complex systems. Unlocking the mysteries of these systems will provide the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties. Within this funding, there is an increase to support new theory, modeling and simulation activities to characterize and understand key mechanisms governing the interactions of hydrogen with materials for high-capacity solid-state hydrogen storage ($+2,345,000). Major emphasis for hydrogen research will be on establishing the theoretical

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

framework via multi-time and multi-spatial scale approaches to predict and guide the design of solid-state hydrogen storage materials for transportation and stationary applications. New activities will be initiated to understand new electron pairing mechanisms to guide the future design of bulk and nano-architectured complex oxides with strongly correlated electron behavior ($+2,000,000).

	FY 2006	FY 2007	FY 2008
▪ **Materials Chemistry**	**42,040**	**49,748**	**54,467**

This activity supports basic research on the design, synthesis, characterization, and properties of novel materials and structures. The portfolio emphasizes solid-state chemistry, surface chemistry, and interfacial chemistry. It includes investigation of novel materials such as low-dimensional solids, self-assembled monolayers, electrocatalysts, cluster and nanocrystal-based materials, conducting and electroluminescent polymers, organic superconductors and magnets, complex fluids, hybrid materials, biomolecular materials and solid-state neutron detectors. There is a continued interest in the synthesis of new complex materials with nanoscale structural control and unique material properties that originate at the nanoscale. Significant research opportunities also exist at the biology/materials science interface. A wide variety of experimental techniques are employed to characterize these materials, including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance and x-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as surface force apparatus in combination with various spectroscopies.

The research in this activity underpins many energy-related technological areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, sensors and electronics, and materials aspects of environmental chemistry. The development of synthetic membranes using biological approaches may yield materials for advanced separations and energy storage.

Capital equipment is provided for such items as advanced nuclear magnetic resonance and magnetic resonance imaging instrumentation and novel atomic force microscopes.

In FY 2008, major activities will include solar-to-fuels conversion research, with an emphasis on tailoring the absorption and charge separation via the control of photon and electron motion in materials. Such activities will 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. Within this funding, there is an increase to support new research activities for developing bio-inspired approaches to solar hydrogen production and bio-mimetic catalysis for hydrogen storage and fuel cell needs ($+1,500,000). The emphasis will be on tailoring the absorption and charge separation via the control of photon and electron motion in materials and taking full advantage of the nanotechnology/biotechnology revolutions to enable exquisite design of materials and the mimicking of natural function. Additional activities will be initiated for the design and synthesis of biomolecular organic materials for electronic applications ($+2,000,000) and for new basic research for electrical energy storage ($+1,219,000).

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	**7,280**	**8,000**	**8,240**

This activity supports basic research spanning the complete range of activities within the Department 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, New Hampshire, Nevada, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Tennessee (graduated from program in April 2006), Vermont, West Virginia, Wyoming, the Commonwealth of Puerto Rico, and the U.S. Virgin Islands. The work supported by the EPSCoR program includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy physics, and nuclear physics, fusion energy sciences, and the basic sciences underpinning fossil energy, energy efficiency, and renewable energy. In FY 2008, funding is increased for EPSCoR research activities ($+240,000). The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

Alabama	685	258	128
Alaska	—	—	—
Arkansas	135	139	—
Delaware	—	—	—
Hawaii	—	—	—
Idaho	375	375	375
Kansas	135	—	—
Kentucky	—	—	—
Louisiana	462	375	375
Maine	—	—	—
Mississippi	132	—	—
Montana	455	133	131
Nebraska	265	269	140
Nevada	740	105	468
New Hampshire[a]	—	—	—
New Mexico	135	—	—
North Dakota	923	—	350
Oklahoma	350	350	350
Rhode Island	—	—	—
Puerto Rico	375	—	—
South Carolina	660	525	525

[a] Became eligible in FY 2006.

	FY 2006	FY 2007	FY 2008
	(dollars in thousands)		
South Dakota	125	—	—
Tennessee	140	140	140
Vermont	—	—	—
U.S. Virgin Islands	—	—	—
West Virginia	855	135	495
Wyoming	140	140	—
Technical Support	193	110	110
Other[a]	—	4,946	4,653

	FY 2006	FY 2007	FY 2008
▪ **Electron-beam Microcharacterization**	**7,790**	**7,945**	**8,183**

This activity, which was previously budgeted in Structure and Composition of Materials, supports three electron-beam microcharacterization user centers: the Electron Microscopy Center for Materials Research at Argonne National Laboratory, the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory, and the Shared Research Equipment Program at Oak Ridge National Laboratory. These centers contain a variety of highly 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. Understanding and control of materials at this level is critical to developing materials for and understanding principles of photovoltaic energy conversion, hydrogen production, storage, and utilization, catalysis, corrosion, response of materials in high-temperature, radioactive, or other extreme environments, and many other situations that have direct bearing on energy, environmental, and security issues.

Electron probes are ideal 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 certain cases, just one. Furthermore, the use of these charged particles allows electromagnetic control and lensing of electron beams, resulting in spatial resolution that can approach single atomic separations or better.

Capital equipment is provided for instruments such as scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, related surface characterization apparatus and scanning probe microscopes, and auxiliary tools such as spectrometers, detectors, and advanced sample preparation equipment.

In FY 2008, additional funds are provided for continued user operations, scientific research of the staff, and development of new instruments or techniques at the electron beam microcharacterization user centers ($+238,000).

[a] Uncommitted funds in FY 2007 and FY 2008 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
▪ **Accelerator and Detector Research**	**1,522**	**3,000**	**8,985**

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Research seeks to achieve a fundamental understanding beyond the traditional accelerator science and technology to develop new concepts for synchrotron radiation and spallation neutron sources. Research includes studies of the creation and transport of ultra-high brightness electron beams to drive Self Amplified Spontaneous Emission (SASE) Free Electron Lasers (FELs) such as the LCLS. Collective electron effects such as micro-bunch instabilities from coherent synchrotron and edge radiation are key areas of interest, as they can degrade the beam brightness. In the area of neutron science, there is research to develop improved high-intensity, low-emittance proton sources to achieve high-power spallation sources. More efficient proton sources can increase the reliability and lifetime due to lower radiofrequency (RF) power requirements.

This work is closely aligned and coordinated with activities in the High Energy Physics, Nuclear Physics, and Advanced Scientific Computing Research programs within the Office of Science. Coordination with other agencies, notably NSF, will continue in areas such as R&D on energy-recovery linacs and on the development of x-ray detectors. To exploit fully the fluxes delivered by synchrotron radiation facilities and the SNS, new detectors capable of acquiring data several orders of magnitude faster than present detectors are required. Improved detectors are especially important in the study of multi-length scale systems such as protein-membrane interactions as well as nucleation and crystallization in nanophase materials. They will also enable real-time kinetic studies and studies of weak scattering samples.

Capital equipment provided for these studies includes lasers for photoionization and laser wake field studies, RF hardware, data acquisition equipment, and optical equipment such as polarizers and beam splitters, interferometers, and specialized cameras.

In FY 2008, activities in novel accelerator and source concepts as well as detector research will continue. An increase is provided to continue the growth of this activity ($+5,985,000). This activity recognizes the importance of fundamental research in accelerator and detector science to the Basic Energy Sciences Program, which now supports the largest collection of synchrotron light sources and neutron scattering facilities of any organization worldwide.

▪ **General Plant Projects (GPP)**	**1,250**	**737**	**737**

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems as part of the BES stewardship responsibilities. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed $5,000,000.

▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**	**2,000**	**—**	**—**

Capital Equipment funding for new and upgraded instrumentation has been completed.

▪ **Nanoscale Science Research Centers**	**993**	**500**	**500**

Funding is provided for Other Project Costs for Nanoscale Science Research Centers.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
▪ **The Center for Nanoscale Materials**	**14,000**	**—**	**—**

Funding was completed in FY 2006 for the Major Item of Equipment, with a total estimated cost of $36,000,000, for instrumentation for the Center for Nanoscale Materials at Argonne National Laboratory. The instrumentation will be contained in a new building, which was constructed by the State of Illinois at a cost of $36,000,000 and that is dedicated to the Center operations. The building is appended to the Advanced Photon Source. Included within the Center's instrument suite will be an x-ray nanoprobe beamline at the Advanced Photon Source. This beamline will permit nondestructive examination of magnetic, electronic, and photonic materials important both for basic science and as foundations for future nanotechnologies.

▪ **Spallation Neutron Source Instrumentation I**	**12,579**	**10,500**	**11,856**

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. The instrument concepts for the Major Item of Equipment project were competitively selected using a peer review process, and the instruments will be installed at the SNS on a phased schedule between FY 2007–2011. An additional Major Item of Equipment, SING II, will fund four additional instruments at the SNS.

▪ **Spallation Neutron Source Instrumentation II**	**—**	**10,000**	**10,000**

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 for the Spallation Neutron Source that will be installed at the SNS. The instrument concepts for the Major Item of Equipment project will be competitively selected using a peer review process. The project will 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 External Independent Reviews. It is anticipated that these instruments will be installed at the SNS on a phased schedule beginning in about FY 2010.

▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)**	**1,500**	**—**	**—**

Funding was completed in FY 2006 for research leading to Critical Decision 0 for a Major Item of Equipment for instruments for the Linac Coherent Light Source.

▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)**	**—**	**10,000**	**10,000**

Funds are provided for a Major Item of Equipment with a total estimated cost in the range of $50,000,000 to $60,000,000 and a total project cost in the range of $54,000,000 to $64,000,000 for four instruments for the Linac Coherent Light Source that will be installed after the LCLS line item project is completed in FY 2009. These instruments, together with the instrument contained within the LCLS project, address all but one of the science thrust areas in the LCLS First Experiments report. The technical concepts for the four instruments have been developed in consultation with the scientific community through a series of workshops, conferences, and focused review committees. Instrument designs for the Major Item of Equipment project will be competitively selected using a peer review process. The project will be managed by the Stanford Linear Accelerator Center. The TEC will be narrowed to a cost and schedule performance baseline following completion of Title I

	FY 2006	FY 2007	FY 2008

design and External Independent Reviews. It is anticipated that these four instruments will be installed at the LCLS on a phased schedule between FY 2009–2012. When completed, the LCLS will provide accommodations for six instrument stations, four of which will be used by the instruments in this Major Item of Equipment.

▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	**6,206**	**5,508**	**6,687**

Funds are provided for a Major Item of Equipment with a total estimated cost of $11,600,000 and a total project cost of $27,087,000. The funding amounts displayed include equipment funding and other project costs which are a significant portion of the total project cost. Equipment funding included is $2,000,000 in FY 2006, $3,500,000 in FY 2007, and $6,100,000 in FY 2008. The TEAM project will construct an aberration-corrected electron microscope and make this capability available to the materials and nanoscience communities. The projected improvement in spatial resolution, contrast, sensitivity, and the flexibility of design of electron optical instruments will provide unprecedented opportunities to observe directly the atomic-scale order, electronic structure, and dynamics of individual nanoscale structures. The TEAM instrument will serve as a platform for future aberration-corrected instruments optimized for different purposes, such as wide-gap in-situ experimentation, ultimate spectroscopy, ultrafast high-resolution imaging, synthesis, field-free high resolution magnetic imaging, diffraction and spectroscopy, and other extremes of temporal, spectral, spatial or environmental conditions.

Facilities Operations	**453,133**	**644,885**	**698,524**

The operations of the scientific user facilities are funded at a level that will permit service to users at the FY 2007 level or better. Studies conducted by BES in FY 2004 and FY 2005 for the synchrotron light sources concluded that the number and quality of instruments and the level of staff employed to serve the user community were not entirely adequate to provide the perceived optimal utilization of these facilities. These studies will be discussed in greater detail in the forthcoming 2007 Office of Science and Technology Policy Interagency Working Group Report on U.S. Synchrotron Radiation Light Sources. This Interagency Working Group was tasked with investigating the status, needs, associated policy matters, and interagency coordination issues required for maximizing the scientific impact and efficient operation of existing sources. The investigations included aspects of planning, development, operations, and termination of such facilities and related programs, as well as potential research needs for development of next-generation sources. In FY 2008, additional funds will be applied to these needs at all of the synchrotron light sources. In addition, funds are provided to partially support operation of the SLAC linac previously fully funded by the High Energy Physics (HEP) program. This marks the third year of a transition of support for SLAC linac operations from HEP to BES. FY 2008 funding is requested for National Synchrotron Light Source-II Other Project Costs for R&D activities to reduce technical risk, including equipment funds for instrumentation required to test prototype components. The Combustion Research Facility is funded in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram at a level that will permit service to users at about the FY 2007 level. The facility operations budget request, presented in a consolidated manner later in this budget, 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 that are supported in the Materials Sciences and Engineering subprogram. General plant project

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008

(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 included in the Materials Sciences and Engineering subprogram is provided below. Of the total operations budget, $608,332,000 goes to operating expenses, $62,315,000 to capital equipment, $26,451,000 to AIP, and $1,426,000 to GPP. The four operating Nanoscale Science Research Centers will have been peer reviewed by early 2007, so the FY 2008 budget is the last one that will show equal operations allocations. Execution of the FY 2008 budget will take into account the review results.

Facilities

Facility	FY 2006	FY 2007	FY 2008
Advanced Light Source, LBNL	41,853	49,802	53,152
Advanced Photon Source, ANL	95,640	108,604	115,908
National Synchrotron Light Source, BNL	36,196	40,763	43,505
National Synchrotron Light Source-II	1,900	25,000	20,000
Stanford Synchrotron Radiation Laboratory, SLAC	25,925	35,836	38,413
High Flux Isotope Reactor, ORNL	57,418	51,598	54,598
Intense Pulsed Neutron Source, ANL	15,500	18,531	18,531
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,000	10,582	10,992
Spallation Neutron Source, ORNL	95,001	171,409	166,755
Center for Nanophase Materials Sciences, ORNL	17,800	19,190	19,934
Center for Integrated Nanotechnologies, SNL/LANL	11,500	19,190	19,934
Molecular Foundry, LBNL	8,000	19,190	19,934
Center for Nanoscale Materials, ANL	3,500	19,190	19,934
Center for Functional Nanomaterials, BNL	—	—	19,934
Linac Coherent Light Source (LCLS), SLAC	3,500	16,000	15,500
Linac for LCLS, SLAC	29,400	40,000	61,500

	FY 2006	FY 2007	FY 2008
SBIR/STTR	**—**	**24,228**	**26,297**

In FY 2006, $16,914,000 and $2,030,000 were transferred to the SBIR and STTR programs, respectively. The FY 2007 and FY 2008 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

	FY 2006	FY 2007	FY 2008
Total, Materials Sciences and Engineering	**726,895**	**1,004,212**	**1,093,219**

Explanation of Funding Changes

	FY 2008 vs. FY 2007 ($000)
Materials Sciences and Engineering Research	
▪ **Structure and Composition of Materials**	
Increases are provided to support new research to develop electron scattering probes as companion tools to ultrafast photon probes.	+2,000
▪ **Mechanical Behavior and Radiation Effects**	
Increase is provided to enhance core research activities in high-temperature mechanical behavior and radiation effects in materials under extreme environments.	+2,000
▪ **Physical Behavior of Materials**	
Increase is provided for new research activities in inorganic and organic light emitting materials ($+2,000,000) and in new solar-to-electricity and solar-to-fuels conversion research ($+2,437,000).	+4,437
▪ **Synthesis and Processing Science**	
Increases are provided to support research activities on novel approaches to the design, discovery and synthesis of materials for hydrogen storage ($+1,500,000) and for the design and synthesis of nanoscale materials ($+2,000,000).	+3,500
▪ **Engineering Research**	
Activities are terminated.	-1,000
▪ **Neutron and X-ray Scattering**	
Increase is provided for research in photon-based ultrafast materials science to characterize physical, lattice and electronic structures of highly correlated electron systems.	+1,300
▪ **Experimental Condensed Matter Physics**	
Increase is provided to enhance key core research activities and other strongly correlated electron systems.	+3,000
▪ **Condensed Matter Theory**	
Increases are provided to support new theory, modeling and simulation activities to characterize and understand key mechanisms governing the interactions of hydrogen with materials for high capacity solid-state hydrogen storage ($+2,345,000) and to understand new electron pairing mechanisms to guide the future design of bulk and nano-architectured complex oxides with strongly correlated electron behavior ($+2,000,000).	+4,345

	FY 2008 vs. FY 2007 ($000)
▪ **Materials Chemistry**	
Increases are to support new research activities for developing bio-inspired approaches to solar hydrogen production and bio-mimetic catalysis for hydrogen storage and fuel cell needs ($+1,500,000), for the design and synthesis of biomolecular organic electronic materials ($+2,000,000), and for basic research for electrical energy storage ($+1,219,000).	+4,719
▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**	
Increase is provided for additional EPSCoR research activities.	+240
▪ **Electron-beam Microcharacterization**	
Increase is provided for continued user operations and development of new instruments and techniques.	+238
▪ **Accelerator and Detector Research**	
Increase is provided to continue the growth of this activity to support the next generation of accelerator-based facilities including energy recovery linacs.	+5,985
▪ **Spallation Neutron Source Instrumentation I**	
Scheduled increase for the Major Item of Equipment for instrumentation for the Spallation Neutron Source.	+1,356
▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	
Scheduled increase for the Major Item of Equipment for the Transmission Electron Aberration Corrected Microscope.	+1,179
Total, Materials Sciences and Engineering Research	**+33,299**
Facilities Operations	
▪ **Operation of National User Facilities**	
Increase for the Advanced Light Source to support accelerator operations and users above the FY 2007 level.	+3,350
Increase for Advanced Photon Source to support accelerator operations and users above the FY 2007 level.	+7,304
Increase for National Synchrotron Light Source to support accelerator operations and users above the FY2007 level.	+2,742
Decrease for National Synchrotron Light Source-II – Other Project Costs per FY 2007 project datasheet.	-5,000

	FY 2008 vs. FY 2007 ($000)
Increase for the Stanford Synchrotron Radiation Laboratory to support accelerator operations and users above the FY 2007 level and for Other Project Costs associated with the Photon Ultrafast Laser Science and Engineering (PULSE) Building Renovation ($100,000).	+2,577
Increase for High Flux Isotope Reactor to support reactor operations.	+3,000
Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and users at the FY 2007 level.	+410
Decrease for Spallation Neutron Source. The decrease includes an overall increase for operations and a decrease reflecting the funding ($-8,000,000) for the one-time purchase of heavy water in FY 2007.	-4,654
Increase for the Center for Nanophase Materials Sciences for continued operations.	+744
Increase for Center for Integrated Nanotechnologies for continued operations.	+744
Increase for Molecular Foundry for continued operations.	+744
Increase for Center for Nanoscale Materials for continued operations.	+744
Increase for Center for Functional Nanomaterials to begin first year of operation.	+19,934
Decrease for Linac Coherent Light Source Other Project Costs per FY 2007 project datasheet.	-500
Increase for Stanford Linear Accelerator Center in support of the linac operations.	+21,500
Total, Facilities Operations	**+53,639**
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expense.	+2,069
Total Funding Change, Materials Sciences and Engineering	**+89,007**

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Chemical Sciences, Geosciences, and Energy Biosciences			
Chemical Sciences, Geosciences, and Energy Biosciences Research	200,710	255,113	269,876
Facilities Operations	6,251	6,805	7,069
SBIR/STTR	—	6,581	7,011
Total, Chemical Sciences, Geosciences, and Energy Biosciences	206,961	268,499	283,956

Description

This subprogram provides support for basic research in atomic, molecular and optical science; chemical physics; photochemistry; radiation chemistry; physical chemistry; inorganic chemistry; organic chemistry; analytical chemistry; separation science; heavy element chemistry; geochemistry; geophysics; and physical biosciences.

Included within the $269,876,000 research component of this subprogram is support for General Plant Projects and General Purpose Equipment totaling $15,790,000.

Benefits

Ultimately, research in chemical sciences leads to the development of such advances as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for clean and efficient production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in geosciences contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance. Research in biosciences provides the foundation for new biological, biomimetic, and bioinspired paths to solar energy conversion; fuels and chemical feedstock production; chemical catalysis; and materials synthesis.

Supporting Information

This research seeks to understand chemical reactivity through studies of the interactions of atoms, molecules, and ions with photons and electrons; the making and breaking of chemical bonds in the gas phase, in solutions, at interfaces, and on surfaces; and energy transfer processes within and between molecules. In geosciences, support is provided for mineral-fluid interactions; rock, fluid, and fracture physical properties; and new methods and techniques for geosciences imaging from the atomic scale to the kilometer scale. In the area of biosciences, support is provided for molecular-level studies on solar energy capture through natural photosynthesis; the mechanisms and regulation of carbon fixation and carbon energy storage; the synthesis, degradation, and molecular interconversions of complex hydrocarbons and carbohydrates; and the study of novel biosystems and their potential for materials synthesis, chemical catalysis, and materials synthesized at the nanoscale.

This subprogram is the nation's sole support for heavy-element chemistry, and it is the nation's primary support for homogeneous and heterogeneous catalysis, photochemistry, radiation chemistry, separations and analysis, and gas-phase chemical dynamics.

Selected FY 2006 Research Accomplishments

- *Measuring the ultrafast motion within a molecule using its own electrons*. Modern ultrafast lasers make it possible, in principle, to follow in real time the motions of the atoms that comprise a molecule. However, optical lasers are only indirect probes of atomic motion. This problem will be alleviated with the advent of the world's first x-ray free-electron laser, the Linac Coherent Light Source (LCLS), since x-rays allow direct tracking of atomic positions. Until the LCLS is available, optical laser pulses can be used in clever ways to track atomic motion in molecules. In one recently demonstrated example, the molecule's own electrons are used as the probe of atomic motion in a highly excited molecule. The electric field from an intense, optical laser pulse initially pulls electrons away from the molecule and then accelerates them back toward it. The highly energetic electrons scatter from the molecule. Rather than measure the scattered electrons, as might be done in an electron diffraction experiment, the new method exploits another phenomenon that is particularly sensitive to atomic motion. When the electrons re-collide with the molecule, they emit x-ray radiation in a process known as high-harmonic generation (HHG), and it is these x-rays that are detected. The wavelength of the re-colliding electrons is comparable to distances between atoms in a molecule; thus, the HHG x-rays emitted are highly sensitive to atomic motion within the molecule. This new method shows great promise as a way of imaging energetic molecules undergoing ultrafast structural transformations, including the fundamental action of all of chemistry, and the making and breaking of chemical bonds.
- *Sunlight-driven transformation of carbon dioxide into methanol*. The first step in the chemical transformation of carbon dioxide into a transportable fuel such as methanol involves the interaction of light with a catalyst in a process known as photocatalysis. It has long been known that the photocatalytic formation of methanol from carbon dioxide can be initiated by high-energy ultraviolet radiation. Recent work has demonstrated that the critical first reaction that splits carbon dioxide into carbon monoxide and a free oxygen atom can also be triggered with visible light. This advance makes it feasible to consider harnessing sunlight to drive the photocatalytic production of methanol from carbon dioxide. The key to the new advance is to perform the initial photocatalytic reaction on the walls of the nanometer-sized channels of a porous silica solid through the excitation by visible light of a bimetallic catalyst. The energy from the absorption of light causes an electron to transfer from one metal in the catalyst to the other and subsequently activates the gaseous carbon dioxide to eliminate an oxygen atom to yield the carbon monoxide product. Various combinations of metals are now being explored with the goal of designing a complete and sustainable system to produce methanol.
- *Catalytic synthesis of alternative fuels and chemicals*. Current manufacturing technologies for fuels and chemicals are often inefficient. The need to dramatically improve efficiency in fuel and chemical production is motivating the search for new chemical pathways using new catalysts tailored to guide chemical reactions with precision toward a selected product without wasteful sub-products. Recent approaches enlist different catalysts to cooperate in parallel to transform molecular intermediates. Sometimes referred to as tandem catalysis, this approach can potentially yield ultrahigh selectivity. An example is the venerable Fisher-Tropsch production of diesel fuel from carbon monoxide and hydrogen. Model catalysts for this polymerization reaction are typically unselective and yield a mixture of hydrocarbons or alcohols with carbon-chain lengths varying over a wide range. For

minimum energy consumption and maximum yield, the ideal process should provide a very narrow carbon-chain range. Two recent advances may rejuvenate the Fisher-Tropsch process: the discovery of efficient metathesis catalysts, which led to the Nobel Prize in Chemistry for 2006, and the selective activation of carbon-hydrogen bonds. Two catalysts are necessary to carry out these two very different functions simultaneously on the same growing polymers. The carbon-hydrogen activation catalyst limits the yield of low-end hydrocarbons, and the metathesis polymerization catalyst simultaneously controls the high-end hydrocarbons. This can potentially lead to an ideal diesel-oil without the need for energy-intensive separations. This new tandem catalysis application is being followed intensely by researchers worldwide for its potential to revolutionize the science of alternative fuels and chemicals synthesis.

- *Carrier multiplication: a possible revolutionary step toward highly efficient solar cells*. In a normal solar cell, a single photon from the sun is converted into a single carrier of electrical current (an electron-hole pair) in a bulk crystal material called a semiconductor. This process is inherently inefficient because much of the energy of the solar photon is wasted as excess heat in the semiconductor. Recent experiments on the interaction of photons with nanocrystalline samples of semiconductors have demonstrated a remarkable effect, known as carrier multiplication, in which a single photon creates multiple charge carriers. Recent work has demonstrated that as many as seven charge carriers can be created with a single photon and that the process is universal, i.e., it occurs in all types of nanocrystalline semiconductors. These new results suggest that nanoscale confinement plays an important role in the carrier multiplication mechanism, which is now thought to be an instantaneous excitation of multiple electrons by a single photon. Critical issues must be addressed before an operational solar cell based on carrier multiplication can be created, such as separating and harvesting the charge carriers to create electrical current. However, present estimates of the conversion efficiency for a solar cell based on carrier multiplication are as high as 50 percent, which is about twice that of the best solar cell in current operation. Doubling solar cell conversion efficiency would represent a revolutionary advance in our ability to harness renewable energy from the sun.

- *Visualizing chemistry: the promise of advanced chemical imaging*. The emerging possibility of "chemical imaging" is transforming the way scientists follow the chemical transformation of molecules on surfaces, within cells, or immersed in other complex environments. Chemical imaging is the term given to a set of experimental techniques that use photon beams, electron beams, or proximal electromechanical probes to track molecules in two- or three-dimensional space and real time, while keeping track of chemical identity and even molecular structure. In the ideal limit, chemical imaging means nanometer spatial resolution, femtosecond temporal resolution, and "fingerprint" recognition of the molecular mass and structure. As a recent example, researchers are using focused laser beams (space and time information) coupled with mass spectrometry (chemical identification), to track specific metabolites in functioning cells. Multiplexing the mass information allows the simultaneous mapping of several species. Understanding the metabolic transformation of important biomolecules in cells is the first step toward influencing them in service of improved biochemical processes. Other examples include the use of chemical imaging to examine single-site catalysts as they influence reactions on surfaces and light-harvesting "antenna molecules" that are key participants in photochemical charge-transfer processes.

Detailed Program Justification

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Chemical Sciences, Geosciences, and Energy Biosciences Research	**200,710**	**255,113**	**269,876**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**15,685**	**19,248**	**21,278**

This activity supports theory and experiments to understand the properties of and interactions among atoms, molecules, ions, electrons, and photons. Included among the research activities are studies to determine the quantum mechanical description of such properties and interactions; interactions of intense electromagnetic fields with atoms and molecules; development and application of novel x-ray light sources; development of new ultrafast optical probes; and ultracold collisions and quantum condensates.

The knowledge and techniques developed in this activity have wide applicability. Results of this research provide new ways to use photons, electrons, and ions to probe matter in the gas and condensed phases. This has enhanced our ability to understand materials of all kinds and enables the full exploitation of the BES synchrotron light sources, electron beam microcharacterization centers, and neutron scattering facilities. Furthermore, by studying energy transfer within isolated molecules, AMO science provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer between molecules and ultimately the making and breaking of chemical bonds.

The AMO Science activity is the sole supporter of synchrotron-based AMO science studies in the U.S., which includes ultrashort x-ray pulse generation and utilization at the ALS and APS. This program is also the principal U.S. supporter of research in the properties and interactions of highly charged atomic ions, which are of direct consequence to fusion plasmas.

Capital equipment is provided for items including lasers and optical equipment, unique ion sources or traps, position sensitive and solid-state detectors, and control and data processing electronics.

In FY 2008, major activities will include the interactions of atoms and molecules with intense laser pulses; the development of new ultrafast optical probes and theories for the interpretation of ultrafast measurements; the use of optical fields to control quantum mechanical processes; the studies of atomic and molecular interactions at ultracold temperatures; and the creation and utilization of quantum condensates that provide strong linkages between atomic and condensed matter physics at the nanoscale. Within this funding, there are increases for nanoscale science associated with complex systems ($+1,500,000) and to maintain advances in ultrafast science ($+530,000).

▪ **Chemical Physics Research**	**30,863**	**37,813**	**41,503**

This activity supports experimental and theoretical investigations of gas phase chemistry and chemistry in the condensed phase and at interfaces. Gas phase chemistry emphasizes the dynamics and rates of chemical reactions characteristic of combustion, with the aim of developing theories and computational tools for use in combustion models and experimental tools for validating these models. The study of chemistry in the condensed phase and at well-characterized surfaces and the reactions of metal and metal oxide clusters lead to the development of theories on the molecular origins of surface-mediated catalysis.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008

This activity also has oversight for the Combustion Research Facility (which is budgeted below in Facilities Operations), a multi-investigator facility for the study of combustion science and technology. In-house BES-supported efforts combine theory, modeling, and experiment including diagnostic development, kinetics, and dynamics. Several innovative non-intrusive diagnostics have been developed to characterize gas-phase processes, including high-resolution optical spectroscopy, time-resolved Fourier-transform infrared spectroscopy, picosecond laser-induced fluorescence, and ion-imaging. Other activities at the Combustion Research Facility involve BES interactions with Fossil Energy, Energy Efficiency and Renewable Energy, and industry.

This activity contributes to DOE missions, since nearly 85% of the nation's energy supply has its origins in combustion and this situation is likely to persist for the foreseeable future. The complexity of combustion—the interaction of fluid dynamics with hundreds of chemical reactions involving dozens of unstable chemical intermediates—has provided an impressive challenge to predictive modeling of combustion processes. Predicted and measured reaction rates will be used in models for the design of new combustion devices with maximum energy efficiency and minimum undesired environmental consequences. The research in chemical dynamics at surfaces is aimed at developing predictive theories for surface mediated chemistry such as that encountered in industrial catalysis or environmental processes. Surface mediated catalysis reduces the energy demands of industrial chemical processes by bypassing energy barriers to chemical reaction. Surface mediated catalysis is used to remove pollutants from combustion emissions.

Capital equipment is provided for such items as picosecond and femtosecond lasers, high-speed detectors, spectrometers, and computational resources.

In FY 2008, there will be an increased emphasis on chemical physics in the condensed phase, including the fundamental understanding of weak, non-covalent interactions and their relationship to chemical and physical properties of macroscopic systems and on electron driven chemical reactions at interfaces relevant to solar energy conversion. Within this funding, there are increases for nanoscale science associated with complex behavior in the condensed phase and at interfaces ($+1,500,000), advances in chemical imaging and ultrafast science ($+971,000), and fundamental aspects of interfacial chemistry, especially at electrode-relevant surfaces, for charge transfer reactions and electrochemical energy storage ($+1,219,000).

▪ **Photochemistry and Radiation Research**	**28,591**	**32,007**	**35,000**

This activity supports fundamental molecular-level research on the capture and conversion of energy in the condensed phase. Fundamental research in solar photochemical energy conversion supports organic and inorganic photochemistry and photocatalysis, photoinduced electron and energy transfer in the condensed phase, photoelectrochemistry, biophysical aspects of photosynthesis, and biomimetic assemblies for artificial photosynthesis. Fundamental research in radiation chemistry supports chemical effects produced by the absorption of energy from ionizing radiation. The radiation chemistry research encompasses heavy ion radiolysis, models for track structure and radiation damage, characterization of reactive intermediates, radiation yields, and radiation-induced chemistry at interfaces. Accelerator-based electron pulse radiolysis methods are employed in studies of highly reactive transient intermediates, and kinetics and mechanisms of chemical reactions in the liquid phase and at liquid/solid interfaces. This activity supports the Notre Dame Radiation

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

Laboratory ($3,298,000), a BES collaborative research center, emphasizing research in radiation chemistry.

Solar photochemical energy conversion is a long-range option for meeting future energy needs. An alternative to semiconductor photovoltaic cells, the attraction of solar photochemical and photoelectrochemical conversion is that fuels, chemicals and electricity may be produced with minimal environmental pollution and with closed renewable energy cycles. Artificial photosynthesis can be coupled to chemical reactions for generation of fuels such as hydrogen, methane, or complex hydrocarbons found in gasoline. The fundamental concepts devised for highly efficient excited-state charge separation in molecule-based biomimetic assemblies should also be applicable in the future development of molecular optoelectronic devices.

Radiation chemistry research supports fundamental chemical effects produced by the absorption of energy from ionizing radiation. This research is important for solving problems in environmental waste management and remediation, the nuclear fuel cycle, and medical diagnosis and radiation therapy.

Capital equipment is provided for such items as pico- and femtosecond lasers, fast Fourier-transform infrared and Raman spectrometers, and upgrades for electron paramagnetic resonance spectroscopy.

In FY 2008, funding will include research to expand our knowledge of the semiconductor/liquid interface, colloidal semiconductors, and dye-sensitized solar cells; inorganic/organic donor-acceptor molecular assemblies and photocatalytic cycles; photosynthetic antennae and the reaction center; the use of nanoscale materials in the photocatalytic generation of hydrogen from water and other fuels from fossil feedstocks; and radiolytic processes at interfaces, radiolytic intermediates in supercritical fluids, and characterization of excited states by dual pulse radiolysis/photolysis experiments. Within this funding, there are increases for enhanced research in solar hydrogen production ($+1,000,000), solar photoelectrochemistry ($+823,000), and solar photoconversion using solid-state organic systems ($+1,170,000).

	FY 2006	FY 2007	FY 2008
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	**11,920**	**18,188**	**19,926**

This activity supports fundamental research to characterize the molecular and chemical mechanisms involved in the conversion of solar energy to chemical energy. Research supported includes the characterization of the chemical processes occurring during photosynthesis, natural catalytic mechanisms involved in the synthesis of chemical fuels, and the chemistry of carbon dioxide fixation. The approaches used include physical, chemical, biochemical, and molecular structure/function analyses. The goal is to provide strategies for the design of non-biological and hybrid processes. This activity complements that in the Biological and Environmental Research program, which focuses on developing a comparative understanding of photosynthetic biological systems and on the genomic, metabolic engineering, and synthetic biology redesign of such natural systems.

Capital equipment is provided for such items as high-speed lasers, high-speed detectors, spectrometers, and computational resources.

	FY 2006	FY 2007	FY 2008

(dollars in thousands)

In FY 2008, funding will support research that focuses on understanding the constituents and molecular-level interactions within natural photosynthetic systems and the detailed molecular processes associated with the absorption of solar energy and the creation of stored chemical energy. Exploiting and mimicking components of natural solar energy conversion will enable future strategies for the bio-inspired design of new energy capture systems. Within this funding, there are increases to maintain advances in both natural and artificial photosynthesis ($+471,000) and for enhanced efforts in understanding defect tolerance and self-repair in natural photosynthetic systems ($+1,267,000).

	FY 2006	FY 2007	FY 2008
▪ **Metabolic Regulation of Energy Production**	**16,859**	**17,601**	**18,056**

This activity supports fundamental research in the molecular processes that regulate chemical reactions important to energy conversion within cells. These studies will provide the basis for designing bioinspired, synthetic systems that achieve desired chemical transformations with high efficiency and specificity. Research supported includes the molecular characterization of key biomolecular components and special assemblies that play an important role in chemical transformations of interest in energy production, transformation, and use. This activity constitutes the fundamental understanding of complex, nanoscale biochemical catalysis.

Capital equipment is provided for such items as lasers, detectors, imaging systems, spectrometers, and computational resources.

In FY 2008, increased emphasis will be placed on understanding interactions that occur within the nanoscale range. An emerging area will be the development of new imaging tools and methods for the in situ observation at high spatial and temporal resolutions. Within this funding, there is an increase for interfacial biochemistry ($+455,000).

	FY 2006	FY 2007	FY 2008
▪ **Catalysis and Chemical Transformation**	**37,225**	**47,459**	**50,927**

This activity supports basic research to understand the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources; and the chemistry of the molecules used to create advanced materials. This activity seeks to develop these principles to enable rational design of catalysts.

Catalytic transformations impact virtually all of the energy missions of the Department. Catalysts are needed for all of the processes required to convert crude petroleum into a clean burning fuel. The production of virtually every chemical-based consumer product requires catalysts. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added chemicals. Environmental impacts from catalytic science can include minimizing unwanted products from production streams and transforming toxic chemicals into benign ones, such as chlorofluorocarbons into environmentally acceptable refrigerants. Research supported by this program also provides the basis and impetus for creating a broad range of new materials, such as mesoporous solids that have improved catalytic properties.

This activity is the nation’s major supporter of catalysis research, and it is the only activity that treats catalysis as a discipline integrating all aspects of homogeneous and heterogeneous catalysis research.

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

Capital equipment is provided for such items as ultrahigh vacuum equipment with various probes of surface structure, Fourier-transform infrared instrumentation, and high-field, solid-state Nuclear Magnetic Resonance (NMR) spectrometers.

In FY 2008, funding will continue to address recommendations of the FY 2002 BESAC-sponsored workshop that described new opportunities afforded by progress in the tools and concepts of nanoscience. The availability of new tools for preparation, characterization, and analysis and the merging of concepts drawn from homogeneous (single phase such as solution) catalysis, heterogeneous (between phases such as gas-surface) catalysis, and biocatalysts provide the potential to pioneer new approaches to catalysis design. New strategies for the rational design of selective oxidation catalysts and catalysts for the production of hydrogen from renewable feedstocks will be explored, and the control of self assembled nanoscale catalyst structures will be studied. Innovative hybrid materials that integrate biomimetic approaches with advances in catalysis will be performed, and the nature of biologically directed mineralization that results in exquisite structural control will be studied. Basic research into the chemistry of inorganic, organic, and inorganic/organic hybrid porous materials with pores in the 1-30 nm range will be undertaken, nano-scale self-assembly of these systems will be studied, and the integration of functional catalytic properties into nanomaterials will be explored. The development of a new generation of fuel-forming catalysts is necessary for integration into both higher-order artificial photosynthetic assemblies and photoelectrochemical devices. Within this funding, there are increases for enhanced catalysis research related to hydrogen production and use ($+1,685,000), for nanoscale catalyst development ($+1,000,000), and for enhanced efforts in biocatalysis and electrocatalysis ($+783,000).

	FY 2006	FY 2007	FY 2008
▪ **Separations and Analyses**	**16,388**	**24,041**	**25,907**

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 entirely new approaches to analysis such as chemical imaging in complex, heterogeneous environments. This activity is the nation's most significant long-term investment in many aspects of separations and analysis, including solvent extraction, ion exchange, and mass spectrometry.

The goal of this activity is to obtain a thorough understanding of the basic chemical and physical principles involved in separations systems and analytical tools so that their utility can be realized.

Work is closely coupled to the Department'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 and to understand and predict the fate of associated contaminants in the environment. Though the cold war legacy is the most obvious of the Department's missions, the economic importance of separation science and technology is huge. For example, distillation processes in the petroleum, chemical, and natural gas industries annually consume the equivalent of 315 million barrels of oil. It has been estimated that separation processes account for more than five percent of the total national energy consumption. Separations are essential to nearly all operations in the processing industries and are also necessary for many analytical procedures. An analysis is an essential component of every chemical process from manufacture through safety and risk assessment and environmental protection.

Capital equipment is provided for such items as computational workstations and inductively coupled plasma torch spectrometers for atomic emission determination.

In FY 2008, funding will include studies at the nanoscale as well as the formation of macroscopic separation systems via self-assembly of nanoscale precursors. This work will build on recent advances in imaging single-molecule interactions and reactions and will expand our knowledge of how molecules interact with pore walls, with one another, and with other molecules to effect separation between molecules. Chemical analysis research will emphasize: (1) the study of hydrogen-separation materials and processes under realistic environmental conditions, rather than in high vacuum; (2) achievement of high temporal resolution, so that changes can be monitored dynamically; and (3) applications of multiple analytical measurements made simultaneously on systems such as fuel cell membranes, which have three percolation networks (proton, electron, and gas). The optimization of the light-harvesting properties of molecules on surfaces and at interfaces requires pushing the analytical means to image these molecules with the requisite spatial and temporal resolution. Within this funding, there are increases for enhanced membrane research for hydrogen ($+1,470,000) and for increased efforts in analytical chemical imaging ($+396,000).

	FY 2006	FY 2007	FY 2008
▪ **Heavy Element Chemistry**	**9,421**	**17,128**	**17,571**

This activity supports research in actinide and fission product chemistry. Areas of interest are synthesis of actinide-containing materials; theoretical methods for, and calculation of, heavy element electronic properties, molecular structure and reactivity; aqueous and non-aqueous coordination chemistry; solution and solid-state bonding and reactivity; measurement of actinide chemical and physical properties; determination of chemical properties of the heaviest actinide and transactinide elements; and studies of the bonding relationship between the actinides, lanthanides, and transition metals.

The heavy element chemistry program, with its genesis in the Manhattan project, has explored the chemical properties of the transuranium and transactinide elements, the latter using techniques developed for isotopes that have half-lives on the order of seconds to tens of seconds. In recent years, the emphasis of the program returned to the chemistry of the lighter transuranium elements and fission products, driven by the necessity to characterize long-lived species found in storage at DOE production sites. Knowledge of the chemical characteristics of actinide and fission-product materials under waste tank conditions is necessary to treat these complex mixtures. Accidental release of actinide and fission product materials to the environment also requires molecular bonding information to predict and mitigate their transport under environmental conditions. This activity is closely coupled to the BES separations and analysis activity.

This activity represents the nation's only funding for basic research in the chemical and physical principles governing actinide and fission product chemistry. The program is primarily at the national laboratories because of the special licenses and facilities needed to obtain and safely handle substantial amounts of radioactive materials. However, research in heavy element chemistry is supported at universities, and collaborations between university and laboratory programs are encouraged. The education of graduate students and postdoctoral researchers is an important responsibility of this activity. Approximately twenty undergraduate students chosen from universities and colleges throughout the U.S. are given introductory lectures in actinide and radiochemistry each summer.

Capital equipment is provided for items used to characterize actinide materials (spectrometers, ion chambers, calorimeters, etc.) and equipment to handle the actinides safely at synchrotron light source experiments.

In FY 2008, funding will continue to include experiment, theory, and modeling to understand the chemical bonding in the heavy elements. Experimental studies will include aqueous and non-aqueous high-pressure chemistry and surface chemistry of these elements. Such studies are essential for the optimization of nuclear fuel cycles. In addition, new beamlines at synchrotron light sources capable of handling samples of these heavy elements will permit detailed spectroscopic studies of specimens under a variety of conditions. The study of the bonding in these heavy elements may also provide new insights into organometallic chemistry, beyond that learned from “standard” organometallic chemistry based on transition metals with d-orbital bonding. Within this funding, there is an increase for enhanced effort in the chemistry of actinides under extreme conditions ($+443,000).

	FY 2006	FY 2007	FY 2008
▪ **Geosciences Research**	**19,897**	**22,345**	**23,918**

The Geosciences activity supports long-term basic research in geochemistry and geophysics. Geochemical research focuses on new paradigms for aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. It seeks fundamental understanding of geochemical processes and reaction rates. Geophysical research focuses on new approaches to understand subsurface physical properties of fluids, rocks, and minerals, and how to determine them from the surface. It seeks fundamental understanding of the physics of wave propagation in complex media. This activity has pioneered the application of x-ray and neutron scattering to geochemical and geophysical studies.

This activity provides the basic research in geosciences that underpins the nation's strategy for understanding and mitigating the terrestrial impacts of energy technologies. The knowledge of subsurface geochemical processes, for instance, is essential to knowing the fate and transport properties of harmful heavy elements from possible nuclear waste releases. Geophysical imaging methods, likewise, are needed to measure and monitor below-ground reservoirs of carbon dioxide resulting from future large-scale carbon sequestration schemes. Finally, an emphasis on multiscale modeling harnesses modern computational power to understand and visualize data as well as to provide predictive capabilities. This activity complements that in the Biological and Environmental Research program, which focuses on the fate, transport, and remediation of DOE-relevant contaminants in the subsurface.

Capital equipment is provided for such items as x-ray and neutron scattering end stations at the BES facilities for environmental samples, and for experimental, field, and computational capabilities.

In FY 2008, funding will continue to provide the majority of individual investigator basic research support for the federal government in areas with the greatest impact on unique DOE missions such as low-temperature, low-pressure geochemical processes in the subsurface. This activity provides the basic research component in solid Earth sciences to the DOE’s energy resources and environmental

	FY 2006	FY 2007	FY 2008

(dollars in thousands)

quality portfolios. Within this funding, there are increases for nanoscale geochemistry ($+1,000,000) and for geochemical imaging ($+573,000).

▪ **Chemical Energy and Chemical Engineering**	**3,958**	**1,817**	**—**

This activity supported research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes.

In FY 2008, consolidate efforts and emphasize other priorities; the remaining research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research will be transferred to other programs or eliminated.

▪ **General Plant Projects (GPP)**	**7,352**	**13,408**	**11,610**

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, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the BES stewardship responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Facilities Operations justification in both the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. The total estimated cost of each GPP project will not exceed $5,000,000.

▪ **General Purpose Equipment (GPE)**	**2,551**	**4,058**	**4,180**

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	**6,251**	**6,805**	**7,069**

The facility operations budget request, which includes operating funds ($6,451,000), capital equipment ($496,000), and GPP ($122,000), is described in a consolidated manner later in this budget. This subprogram funds the Combustion Research Facility. 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.

Facilities

Combustion Research Facility	6,251	6,805	7,069

SBIR/STTR	**—**	**6,581**	**7,011**

In FY 2006, $4,880,000 and $585,000 were transferred to the SBIR and STTR programs, respectively. The FY 2007 and FY 2008 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**206,961**	**268,499**	**283,956**

Explanation of Funding Changes

	FY 2008 vs. FY 2007 ($000)
Chemical Sciences, Geosciences, and Energy Biosciences Research	
▪ **Atomic, Molecular, and Optical (AMO) Science**	
Increases are provided for nanoscale science associated with complex systems ($+1,500,000) and to maintain advances in ultrafast science ($+530,000).	+2,030
▪ **Chemical Physics Research**	
Increases are provided for nanoscale science associated with complex behavior in the condensed phase and at interfaces ($+1,500,000), chemical imaging and ultrafast science ($+971,000), and interfacial chemistry at electrode-relevant surfaces ($+1,219,000).	+3,690
▪ **Photochemistry and Radiation Research**	
Increases are provided for enhanced research in solar hydrogen production ($+1,000,000), solar photoelectrochemistry ($+823,000), and solar photoconversion using solid-state organic systems ($+1,170,000).	+2,993
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	
Increase is provided to maintain advances in both natural and artificial photosynthesis ($+471,000) and enhanced efforts in understanding defect tolerance and self-repair in natural photosynthetic systems ($+1,267,000).	+1,738
▪ **Metabolic Regulation of Energy Production**	
Increase is provided for interfacial biochemistry.	+455
▪ **Catalysis and Chemical Transformation**	
Increases are provided for enhanced catalysis research related to hydrogen production and utilization ($+1,685,000), for nanoscale catalyst development ($+1,000,000), and for enhanced efforts in biocatalysis and electrocatalysis ($+783,000).	+3,468
▪ **Separations and Analyses**	
Increases are provided for enhanced membrane research for hydrogen ($+1,470,000) and for increased efforts in analytical chemical imaging ($+396,000).	+1,866
▪ **Heavy Element Chemistry**	
Increase is provided for the chemistry of actinides under extreme conditions.	+443
▪ **Geosciences Research**	
Increases are provided for nanoscale geochemistry ($+1,000,000) and for geochemical imaging ($+573,000).	+1,573

	FY 2008 vs. FY 2007 ($000)
▪ **Chemical Energy and Chemical Engineering**	
Decrease in Chemical Energy and Chemical Engineering due to termination of program.	-1,817
▪ **General Plant Projects (GPP)**	
Decrease in general plant projects due to completion of prior year projects.	-1,798
▪ **General Purpose Equipment (GPE)**	
Small increase for GPE maintenance of equipment.	+122
Total, Chemical Sciences, Geosciences and Energy Biosciences Research	**+14,763**
Facility Operations	
Increase for the Combustion Research Facility to support operations.	+264
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in operating expenses.	+430
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	**+15,457**

Construction

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Construction			
Spallation Neutron Source, ORNL	41,327	—	—
Project Engineering and Design, Linac Coherent Light Source, SLAC	2,518	161	—
Linac Coherent Light Source, SLAC	82,170	105,740	51,356
Center for Functional Nanomaterials, BNL	36,187	18,864	366
The Molecular Foundry, LBNL	9,510	257	—
Center for Integrated Nanotechnologies, SNL/LANL	4,580	247	—
Project Engineering and Design, National Synchrotron Light Source-II	—	20,000	45,000
Project Engineering and Design, Advanced Light Source User Support Building, LBNL	—	3,000	—
Advanced Light Source User Support Building, LBNL	—	—	17,200
Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	—	—	950
Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	—	—	6,450
Total, Construction	176,292	148,269	121,322

Description

Construction is needed to support the research in each of 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.

Benefits

The new facilities that are in design or under construction—the Linac Coherent Light Source, the Center for Functional Nanomaterials, 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. As described in the Benefits section for the User Facilities, these facilities will provide the nation's 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.

Detailed Justification

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
▪ **Spallation Neutron Source (SNS), ORNL**	**41,327**	**—**	**—**

On June 5, 2006, Deputy Secretary of Energy Clay Sell formally certified the successful completion of the Spallation Neutron Source (SNS) project, located at Oak Ridge National Laboratory (ORNL). The SNS project exceeded its baseline objectives, delivering more technical performance capability than promised, one month ahead of schedule and slightly under budget. In addition, the project achieved an outstanding safety record with no lost workday injuries in over 4.2 million construction work hours.

The SNS project was executed over a period of about 10 years by a DOE multi-laboratory partnership led by the SNS Project Office at ORNL. The SNS project partnership among six DOE laboratories has taken advantage of specialized technical capabilities within the laboratories: Lawrence Berkeley National Laboratory in ion sources; Los Alamos National Laboratory in linear accelerators; Thomas Jefferson National Accelerator Facility in superconducting linear accelerators; Brookhaven National Laboratory in proton storage rings; Argonne National Laboratory in instruments; and Oak Ridge National Laboratory in targets and moderators.

The SNS will become the world's leading research facility for study of the structure and dynamics of materials using neutrons. It will operate as a user facility that will enable researchers from the United States and abroad to study the science of materials that forms the basis for new technologies in telecommunications, manufacturing, transportation, information technology, biotechnology, and health.

Briefly, the SNS facility consists of the following: (1) a Front End System, where a pulsed beam of negative hydrogen ions is produced; (2) a Linear Accelerator or Linac System, where the beam is accelerated to an energy of one billion electron volts; (3) a Ring and Transfer System, where the negative ions are converted into protons and then stored in very short, high intensity pulses and then directed onto; (4) a liquid mercury Target System onto which the protons are directed, where neutrons are generated by spallation reactions and then moderated to lower energies; (5) Instrument Systems, which receive the neutrons through beam guides and where experiments are conducted; and (6) Conventional Facilities and site infrastructure, including a Central Laboratory and Office Building. The potential exists for increasing the power and adding a second target station to the SNS.

In May 2006, the first neutrons generated at SNS were used in a spectrometer instrument to study the molecular structure of a material sample. During the months ahead, the facility's proton beam power will be steadily increased, and, by 2008, the design power level of 1.4 megawatts onto the target will be reached. At the same time, the facility's availability to scientific users will also increase to full capacity.

▪ **Project Engineering and Design, Linac Coherent Light Source, SLAC**	**2,518**	**161**	**—**

The purpose of the Linac Coherent Light Source (LCLS) Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons have revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project would provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Å range.

For many years, the Basic Energy Sciences Advisory Committee (BESAC) has been actively involved with the development of such a next-generation light source. In 1997, the BESAC report "DOE Synchrotron Radiation Sources and Science" recommended funding an R&D program in next-generation light sources. In 1999, the BESAC report "Novel, Coherent Light Sources" concluded, "Given currently available knowledge and limited funding resources, the hard x-ray region (8-20 keV or higher) is identified as the most exciting potential area for innovative science. DOE should pursue the development of coherent light source technology in the hard x-ray region as a priority. This technology will most likely take the form of a linac-based free electron laser using self-amplified stimulated emission or some form of seeded stimulated emission…"

The proposed 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 LCLS has considerable potential as a tool for groundbreaking research in the physical and life sciences. LCLS x-rays can be used to create and observe extreme conditions in matter, such as exotic excited states of atoms and warm dense plasmas, previously inaccessible to study. They can be used to directly observe changes in molecular and material structure on the natural time scales of atomic and molecular motions. LCLS x-rays offer an opportunity to image non-periodic molecular structures, such as single or small clusters of biomolecules or nanostructured materials, at atomic or near-atomic resolution. These are only a few examples of breakthrough science that will be enabled by LCLS.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

The proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment.

Funds were appropriated in FY 2006 and requested in FY 2007 for Project Engineering and Design (PED) Title I and Title II design work.

	FY 2006	FY 2007	FY 2008
▪ **Linac Coherent Light Source, SLAC**	**82,170**	**105,740**	**51,356**

Funds appropriated in FY 2005 were used to initiate long-lead procurements. Early acquisition of selected critical path items supported pivotal schedule and technical aspects of the project. These include acquisition of the 120 MeV injector linac, acquisition of the undulator modules and the

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

measurement system needed for verification of undulator performance, and acquisition of main linac magnets and radiofrequency (RF) systems required to produce electron beams meeting the stringent requirements of the LCLS free-electron laser.

Funds appropriated in FY 2006 supported the start of physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall and connecting beam transfer tunnels. In addition, the injector was completed and construction of the downstream linac and electron beam transport to the undulator hall began. Undulator module assembly was started along with construction of x-ray transport/optics/diagnostics systems.

The FY 2007 funding request continued construction of the LCLS conventional facilities including the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Far Experimental Hall. In addition, the assembly and delivery of the undulators and undulator infrastructure to SLAC's Magnetic Measurement Facility continued as did procurements for the x-ray optics, diagnostics, and end stations.

Construction funding requested in FY 2008 is for completion of most of the LCLS conventional facilities and for continued procurement and installation of the technical hardware.

Performance will be measured by meeting the cost and timetables within 10% of the baseline within the construction project datasheet. Additional information on the LCLS Project is provided in the LCLS construction datasheet, project number 05-R-320.

	FY 2006	FY 2007	FY 2008
▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, BNL**	**36,187**	**18,864**	**366**

The Center for Functional Nanomaterials (CFN), a BES Nanoscale Science Research Center, will have as its focus understanding the chemical and physical response of nanomaterials to make functional materials such as sensors, activators, and energy-conversion devices. The facility will use existing facilities such as the NSLS and the Laser Electron Accelerator facility. It will also provide clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. Equipment will include that needed for laboratory and fabrication facilities for e-beam lithography, transmission electron microscopy, scanning probes and surface characterization, material synthesis and fabrication, and spectroscopy.

FY 2005 funding was appropriated for the start of construction; FY 2006 funding continued construction and equipment procurement; and FY 2007 and FY 2008 funding will complete construction of the Center for Functional Nanomaterials at Brookhaven National Laboratory. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project datasheet.

	FY 2006	FY 2007	FY 2008
▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL**	**9,510**	**257**	**—**

The Molecular Foundry, a BES Nanoscale Science Research Center, will focus its research on the interface between soft materials such as those found in living systems and hard materials such as carbon nanotubes, and the integration of these materials into complex functional assemblies. The Molecular Foundry will use existing facilities such as the ALS, the NCEM, and the National Energy Research Scientific Computing Center. The Molecular Foundry will provide laboratories for

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008

materials science, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include clean rooms; controlled environmental rooms; scanning tunneling microscopes; atomic force microscopes; a transmission electron microscope; fluorescence microscopes; mass spectrometers; a DNA synthesizer and sequencer; a nuclear magnetic resonance spectrometer; ultrahigh vacuum scanning-probe microscopes; photo, uv, and e-beam lithography equipment; a peptide synthesizer; advanced preparative and analytical chromatographic equipment; and cell culture facilities.

FY 2004 funding was appropriated for the start of construction, FY 2005 and FY 2006 funding continued construction and equipment procurement, and FY 2007 funding will complete construction. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project datasheet.

	FY 2006	FY 2007	FY 2008
▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, SNL/LANL**	**4,580**	**247**	**—**

The Center for Integrated Nanotechnologies (CINT), a BES Nanoscale Science Research Center, will focus on exploring the path from scientific discovery to the integration of nanostructures into the micro- and macro-worlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. CINT will be jointly administered by Los Alamos National Laboratory (LANL) and Sandia National Laboratories. This Center will make use of a wide range of specialized facilities including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL.

FY 2003 funding was appropriated for the start of construction, FY 2004, FY 2005, and FY 2006 funding continued construction and equipment procurement, and FY 2007 funding will complete construction for the Center for Integrated Nanotechnologies managed jointly by Sandia National Laboratories and Los Alamos National Laboratory. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project datasheet.

	FY 2006	FY 2007	FY 2008
▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS-II)**	**—**	**20,000**	**45,000**

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

FY 2007 funding was requested to begin Project Engineering and Design (PED) Title I and Title II design. PED funds are requested in FY 2008 to complete Title II design.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008

Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project datasheet. Additional information is provided in the construction project datasheet 07-SC-06.

	FY 2006	FY 2007	FY 2008
▪ **Project Engineering and Design, Advanced Light Source (ALS) User Support Building, LBNL**	**—**	**3,000**	**—**

The ALS User Support Building will provide high-quality user support space in sufficient quantity to accommodate the very rapid growth in the number of ALS users and to accommodate projected future expansion. The User Support Building will provide staging areas for ALS experiments, space for a long beamline that will extend from the floor of the ALS into the User Support Building, and temporary office space for visiting users. FY 2007 funding was requested for Project Engineering and Design. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project datasheet.

	FY 2006	FY 2007	FY 2008
▪ **Advanced Light Source (ALS) User Support Building, LBNL**	**—**	**—**	**17,200**

Funds requested in FY 2008 will be used to start civil construction of the ALS User Support Building and perform Title III engineering. This project is using the design-build model for construction, which is a private-sector best practice for this type of space.

	FY 2006	FY 2007	FY 2008
▪ **Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC**	**—**	**—**	**950**

The Stanford Linear Accelerator Center (SLAC) is evolving from a single purpose laboratory focused on high energy physics to a dual purpose facility shifting heavily to photon science with programs in high energy physics and particle astrophysics. This shift in mission emphasis creates the need to upgrade and improve existing office and laboratory space to support the increased level of activities in the photon science mission.

Photon Ultrafast Laser Science and Engineering (PULSE) is the new center for ultrafast science at the Stanford Linear Accelerator Center (SLAC). PULSE represents a major research activity at SLAC that is a key component of the major shift in the emphasis of the laboratory from high energy physics to a multiprogram laboratory with significant activities in photon science. PULSE builds on, and leverages existing strengths in, atomic physics, chemistry, biology, and condensed matter physics. It creates an opportunity to attract outstanding scientific talent, and it will thus help ensure that Stanford University and SLAC are at the forefront of studies of ultrafast phenomena using x-rays and electrons. 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 this building will be renovated to meet the new PULSE program needs. The project scope includes refurbishment of existing offices and four existing laboratories; conversion of space for laser laboratories; and renovation of conference room space. HVAC, electrical and lighting will be modified to meet the needs of the renovated spaces. Roughly 33% of the space will be used for offices, 50% for lab space, and 17% for conference/meeting rooms.

Funds are requested in FY 2008 for PED of the renovation. Additional information is provided in the PED (08-SC-10) and construction project (08-SC-11) datasheets.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
This project will be conducted in accordance with the project management requirements in DOE Order 413.3A and DOE Manual 413.3–1, Program and Project Management for the Acquisition of Capital Assets.			
▪ **Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC**	**—**	**—**	**6,450**
Construction funds for the Photon Ultrafast Laser Science and Engineering Building Renovation described above, are requested in FY 2008 to begin the renovations. Additional information is provided in the PED (08-SC-10) and construction project (08-SC-11) datasheets.			
This project will be conducted in accordance with the project management requirements in DOE Order 413.3A and DOE Manual 413.3–1, Program and Project Management for the Acquisition of Capital Assets.			
Total, Construction	**176,292**	**148,269**	**121,322**

Explanation of Funding Changes

	FY 2008 vs. FY 2007 ($000)
▪ **Project Engineering and Design, Linac Coherent Light Source**	
Decrease in funding for Project Engineering and Design (PED) related to design-only activities for the Linac Coherent Light Source (LCLS) at SLAC, representing completion of activities.	-161
▪ **Linac Coherent Light Source, SLAC**	
Decrease in funding to continue construction for the LCLS project, representing the scheduled ramp down of activities.	-54,384
▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, BNL**	
Decrease in funding for construction of the Center for Functional Nanomaterials at BNL, representing the scheduled ramp down of activities.	-18,498
▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL**	
Decrease in funding for construction of the Molecular Foundry at LBNL, representing the completion of activities.	-257
▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, SNL/LANL**	
Decrease in funding for construction of the Center for Integrated Nanotechnologies at SNL/LANL, representing the completion of activities.	-247

	FY 2008 vs. FY 2007 ($000)
▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS II)**	
Increase in funding to continue Project Engineering and Design.	+25,000
▪ **Project Engineering and Design, Advanced Light Source (ALS) User Support Building, LBNL**	
Decrease in funding representing completion of Project Engineering and Design.	-3,000
▪ **Advanced Light Source (ALS) User Support Building, LBNL**	
Increase in funding for construction of the ALS User Support Building and perform Title III engineering.	+17,200
▪ **Project Engineering and Design, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC**	
Increase to begin design for renovation of SLAC Building 40 to house the PULSE center.	+950
▪ **Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC**	
Increase to begin construction for renovation of SLAC Building 40 to house the PULSE center.	+6,450
Total Funding Change, Construction	**-26,947**

Major User Facilities

Funding Schedule by Activity

Funding for the operation of these facilities is provided in the Materials Sciences and Engineering, and the Chemical Sciences, Geosciences, and Energy Biosciences subprograms.

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Major User Facilities			
Advanced Light Source, LBNL	41,853	49,802	53,152
Advanced Photon Source, ANL	95,640	108,604	115,908
National Synchrotron Light Source, BNL	36,196	40,763	43,505
Stanford Synchrotron Radiation Laboratory, SLAC	25,925	35,836	38,413
Spallation Neutron Source, ORNL	95,001	171,409	166,755
Intense Pulsed Neutron Source, ANL	15,500	18,531	18,531
Manuel Lujan, Jr. Neutron Scattering Center, LANL	10,000	10,582	10,992
High Flux Isotope Reactor, ORNL	57,418	51,598	54,598
Center for Nanophase Materials Sciences, ORNL	17,800	19,190	19,934
Molecular Foundry, LBNL	8,000	19,190	19,934
Center for Integrated Nanotechnologies, SNL/A & LANL	11,500	19,190	19,934
Center for Nanoscale Materials, ANL	3,500	19,190	19,934
Center for Functional Nanomaterials, BNL	—	—	19,934
Combustion Research Facility, SNL/C	6,251	6,805	7,069
Linac Coherent Light Source (LCLS), SLAC	3,500	16,000	15,500
Linac, SLAC	29,400	40,000	61,500
National Synchrotron Light Source-II	1,900	25,000	20,000
Total, Major User Facilities	459,384	651,690	705,593

Description

The BES scientific user facilities provide experimental capabilities that are beyond the scope of those found in laboratories of individual investigators. Synchrotron radiation light sources, high-flux neutron sources, electron beam microcharacterization centers, and other specialized facilities enable scientists to carry out experiments that could not be done elsewhere. These facilities are part of the Department's system of scientific user facilities, the largest of its kind in the world.

Capital Operating Expenses and Construction Summary

Capital Operating Expenses

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
General Plant Projects	11,873	15,624	13,895
Accelerator Improvement Projects	4,449	25,112	26,451
Capital Equipment	69,801	131,657	147,266
Total, Capital Operating Expenses	86,123	172,393	187,612

Construction Projects

	(dollars in thousands)					
	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2006	FY 2007	FY 2008	Unappro-priated Balances
08-SC-01 Advanced Light Source User Support Building, LBNL	30,200[a]	—	—	—	17,200	10,000
08-SC-10, PED, Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	950	—	—	—	950	—
08-SC-11 Photon Ultrafast Laser Science and Engineering Building Renovation, SLAC	11,060[b]	—	—	—	6,450	3,660
07-SC-06, PED, National Synchrotron Light Source-II	75,000	—	—	20,000	45,000	10,000
07-SC-12, PED, Advanced Light Source User Support Building, LBNL	3,000	—	—	3,000	—	—
05-R-320 Linac Coherent Light Source, SLAC	315,000[c]	29,760	82,170	105,740	51,356	10,000
05-R-321 Center for Functional Nanomaterials, BNL	79,700[d]	18,317	36,187	18,864	366	—
04-R-313 The Molecular Foundry, LBNL	83,604[e]	66,622	9,510	257	—	—
03-SC-002, PED, Linac Coherent Light Source, SLAC	35,974	33,295	2,518	161	—	—

[a] Includes $3,000,000 of PED included in the 07-SC-12 PED, LBNL Advanced Light Source User Support Building datasheet.
[b] Includes $950,000 of PED included in the 08-SC-10 PED, Photon Ultrafast and 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 2006	FY 2007	FY 2008	Unappro-priated Balances
03-R-313 Center for Integrated Nanotechnologies, SNL	73,754[a]	64,768	4,580	247	—	—
99-E-334 Spallation Neutron Source, ORNL	1,192,283	1,150,956	41,327	—	—	—
Total, Construction			176,292	148,269	121,322	

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

(dollars in thousands)

	Total Project Cost (TPC)	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2006	FY 2007	FY 2008	Completion Date
Center for Nanoscale Materials (41NG), ANL	72,500[b]	36,000	22,000	14,000	—	—	FY 2006
Spallation Neutron Source Instrumentation I (31MK), ORNL[c]	68,500	68,500	16,165	12,579	10,500	11,856	FY 2007–FY 2011 est.
Transmission Electron Aberration Corrected Microscope (61PC), LBNL	27,087	11,600	—	2,000	3,500	6,100	FY 2009
Spallation Neutron Source Instrumentation II (71RB), ORNL[d]	40,000–60,000	40,000–60,000	—	—	10,000	10,000	TBD
Linac Coherent Light Source Instrumentation (71RA), SLAC[e]	54,000–64,000	50,000–60,000	—	—	10,000	10,000	TBD
Total, Major Items of Equipment			38,165	28,579	34,000	37,956	

[a] Includes $4,159,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[b] This includes $36,000,000 provided by the State of Illinois for construction of the building.
[c] 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.
[d] 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). The FY 2008 Budget Request is for engineering design only.
[e] 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). The FY 2008 Budget Request is for engineering design only.