# Basic Energy Sciences

## Funding Profile by Subprogram

(dollars in thousands)

| | FY 2005 Current Appropriation | FY 2006 Original Appropriation | FY 2006 Adjustments | FY 2006 Current Appropriation | FY 2007 Request |
|---|---|---|---|---|---|
| Basic Energy Sciences | | | | | |
| Research | | | | | |
| Materials Sciences and Engineering | 621,226 | 746,143 | -8,428[ab] | 737,715 | 1,004,212 |
| Chemical Sciences, Geosciences, and Energy Biosciences | 232,365 | 221,801 | -1,251[ab] | 220,550 | 268,499 |
| Total, Research | 853,591 | 967,944 | -9,679 | 958,265 | 1,272,711 |
| Construction | 230,025 | 178,073 | -1,781[a] | 176,292 | 148,269 |
| Total, Basic Energy Sciences | 1,083,616[c] | 1,146,017 | -11,460 | 1,134,557 | 1,420,980 |

**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 of 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 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.

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,

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[a] Reflects a rescission in accordance with P.L. 109-148, the Emergency Supplemental Appropriations Act to address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006, as follows: Materials Sciences and Engineering (-$7,461,000); Chemical Sciences, Geosciences, and Energy Biosciences (-$2,218,000); and Construction (-$1,780,000).
[b] Reflects a reallocation of funding in accordance with H.Rpt. 109-86, the report for the House-passed Energy and Water Development Appropriations Act, 2006, as follows: Materials Sciences and Engineering (-$967,000); Chemical Sciences, Geosciences, and Energy Biosciences (+$967,000).
[c] Total is reduced by $8,898,000 for a rescission in accordance with P.L. 108-447, the Consolidated Appropriations Act, 2005; $18,764,000, which was transferred to the SBIR program; and $2,252,000, which was transferred to the STTR program.

and safety of energy generation, conversion, transmission, and use. For example, research on toughened ceramics will result 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 photo conversion 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 Program Goals**

The Department's Strategic Plan identifies four strategic goals (one each for defense, energy, science, and environmental aspects of the mission) plus seven general goals that tie to the strategic goals. The BES program supports the following goal:

Science Strategic Goal
General Goal 5, World-Class Scientific Research Capacity: Provide world-class scientific research capacity needed to: ensure the success of Department missions in national and energy security; advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; or provide world-class research facilities for the Nation's science enterprise.

The BES program has one program goal which contributes to General Goal 5 in the "goal cascade:"

Program Goal 5.22.00.00: 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 Program Goal 5.22.00.00 (Advance the Basic Science for Energy Independence)**

Within the Basic Energy Sciences program, the Materials Science and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram contribute to Program Goal 5.22.00.00 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 (10-year) goals in scientific advancement that the BES program is committed to and that progress can be measured against.

- 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 Program Goal 5.22.00.00 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 micro characterization 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 is also establishing a suite of Nanoscale Science Research Centers that will change 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 contribute 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 General and Program Goal

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Goal 5, World-Class Scientific Research Capacity | | | |
| Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence (Basic Energy Science) | 1,083,616 | 1,134,557 | 1,420,980 |

## Annual Performance Results and Targets

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence | | | | | |
| Materials Sciences and Engineering | | | | | |
| N/A | 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: Demonstrate measurement of spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm.[a] | Improve Spatial Resolution: Demonstrate measurement of 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 | 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: Demonstrate measurement of x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse (>$10^8$ photons/pulse).[a] | Improve temporal resolution: Demonstrate measurement of x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse (>$10^8$ photons/pulse).[a] |
| Chemical Sciences, Geosciences, and Energy Biosciences | | | | | |
| N/A | 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] | Improve Simulation: Perform a three-dimensional combustion reacting flow simulation involving more than 30 reacting species and 20 million grid points. | Improve Simulation: Beginning in FY 2007, increasing the size of the simulation will no longer provide useful new information. Thus, this measure is being discontinued. |
| Materials Sciences and Engineering | | | | | |
| 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. [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] | 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. |

[a] No further improvement is expected in FY 2006–FY 2011 as compared to the level of achievement for FY 2005. Performance levels for resolution (temporal and spatial) have reached the maximum for the current suite of available instruments. 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 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Construction | | | | | |
| Cost and timetables were maintained within 10% of the baselines given in the construction project data sheets 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 data sheets 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 data sheets 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 data sheets for all construction projects ongoing during the year (Results: +0.2% cost variance and -2.5% schedule variance). [Met Goal] | Meet the cost and timetables within 10% of the baselines given in the construction project data sheets for all ongoing construction projects. | Meet the cost and timetables within 10% of the baselines given in the construction project data sheets for all ongoing construction projects. |

**Means and Strategies**

The Basic Energy Sciences program will use various means and strategies to achieve its 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 proposal pressure and scientific workshops; (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 closely coordinated with the activities of 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 implemented a tool to evaluate selected programs. PART was developed by 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 by which programs can assess their activities differently than by traditional reviews. The BES program has incorporated feedback from OMB and has taken the necessary steps to continue to improve performance.

In the FY 2005 PART review, OMB gave the BES program a very high 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 found that BES has developed a limited number of adequate performance measures which are continued for FY 2007. 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 Report.

OMB developed PARTWeb for the FY 2007 Budget—a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the website http://ExpectMore.gov and will improve public access to PART assessments and follow up actions. For 2006, there are three continuing actions and one new action for Basic Energy Sciences.

- Following up on recommendations of past expert reviews, and using new reviews to assess progress toward long-term programmatic goals.
- The Department will work to include the long-term goals of each program in grant solicitations, and will improve performance reporting by grantees and contractors.
- Improving performance reporting at its user facilities to better reflect the instrumentation and staffing issues most directly connected to scientific output.
- New action—producing a detailed corporate solution for managing and operating the High Flux Isotope Reactor that explicitly addresses the reliability problems while ensuring public health and safety.

In response, BES will continue to use the Committees of Visitors to review progress toward the long term goals of the program and will continue efforts to improve performance reporting. A review of the management and operations of the High Flux Isotope Reactor has been scheduled in 2006 that will address reliability, safety, and health issues. The solution to the reliability problem will be contained in the Basic Energy Sciences report of the review results.

**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 Act of 1992.

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, and efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2005, the program funded research in more than 190 academic institutions located in 48 states and in 13 Department of Energy (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 and characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples. 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, 8,000 researchers from universities, national laboratories, and industrial laboratories perform experiments at these facilities. 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 micro batteries;
- thermo acoustic 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 we work are given in the sections below.

**Advisory and Consultative Activities**

Charges are provided to BESAC by 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/production/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 (1) 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) and (2) specially empanelled subcommittees of BESAC. These subcommittees have reviewed the synchrotron radiation light sources, the neutron scattering facilities, and the electron-beam micro characterization facilities. The reports of these reviews are available on the BES website (http://www.science.doe.gov/bes/BESAC/reports.html). Regardless of whether a review is by an independent committee charged by a BES program manager or by a BESAC subcommittee charged by the Director of the Office of Science, the review has standard elements. 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 now under construction.

Facilities that are in design or construction are reviewed according to procedures set down in DOE Order 413.3 “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 Spallation Neutron Source, the Linac Coherent Light Source, or the Nanoscale Science Research Centers), 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:

(1) Scientific and/or technical merit or the educational benefits of the project;
(2) Appropriateness of the proposed method or approach;
(3) Competency of personnel and adequacy of proposed resources;
(4) Reasonableness and appropriateness of the proposed budget; and
(5) 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.

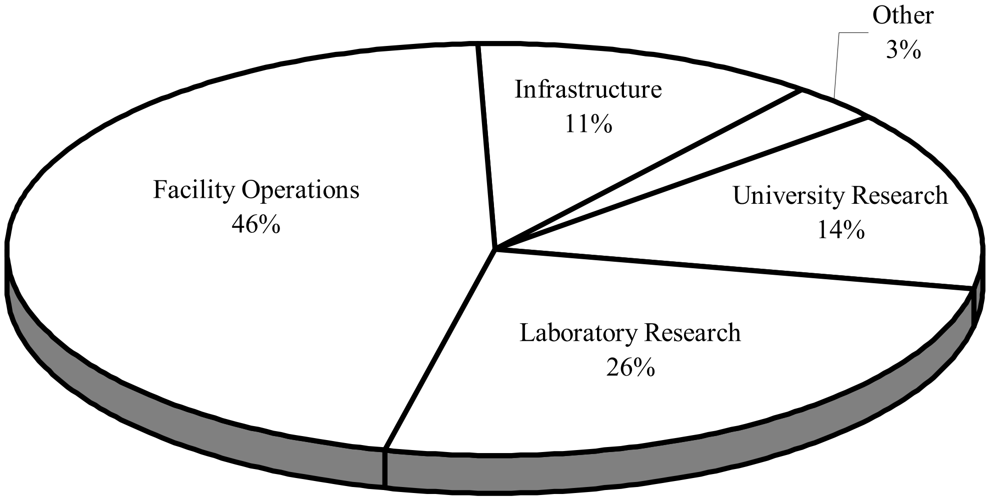
Inputs to our prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, these considerations have led to: increased investments in science at the nanoscale to take advantage of 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 and basic research for effective solar energy utilization) 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 National Academy of Sciences studies and from broad, national strategies that include the input from multiple federal agencies.

The FY 2007 budget request continues priorities established in the past few years. The Spallation Neutron Source will enter its first 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, Lawrence Berkeley National Laboratory, Argonne National Laboratory and Sandia National Laboratories/Los Alamos National Laboratory. Construction funding is provided for the Nanoscale Science Research Center at Brookhaven National Laboratory. Project Engineering Design and construction funding also are provided for the Linac Coherent Light Source (LCLS), a 4$^{th}$ 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 and spallation neutron sources.

**How We Spend Our Budget**

The BES program has three major program elements: research, facility operations, and construction and laboratory infrastructure support. Approximately 35% of the research funding 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 2007 for the Linac Coherent Light Source, the Nanoscale Science Research Center at Brookhaven National Laboratory, and the National Synchrotron Light Source-II. The FY 2007 Request also includes construction funding for the Advanced Light Source (ALS) User Support Building at the Lawrence Berkeley National Laboratory.

## Basic Energy Sciences Budget Allocation
## FY 2007




### 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 2007, there are a number of significant program milestones and increases, including the following in the area of construction and Major Items of Equipment:

- Construction of the Spallation Neutron Source (SNS) will be completed during the 3rd quarter of FY 2006. Over the next two to three years, the facility will continue to fabricate and commission instruments, funded both as part of the SNS project and from other sources including non-DOE sources, and will increase power to full levels. A new Major Item of Equipment is funded in FY 2007 that will allow the fabrication of approximately four to five additional instruments for the SNS, thus nearly completing the initial suite of 24 instruments that can be accommodated in the high-power target station ($10,000,000).
- Four Nanoscale Science Research Centers will be fully operational in FY 2007: 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, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory. A fifth Center, the Center for Functional Nanomaterials at Brookhaven National Laboratory, will receive final year construction funding.
- The Linac Coherent Light Source will continue Project Engineering Design (PED) and construction at the planned levels. Funding is provided separately for preconceptual design and fabrication of instruments for the facility. Funding is also provided to partially support operation of the SLAC linac. This marks the second year of the transition to LCLS operations at SLAC.
- Support is provided for PED ($20,000,000) and Other Project Costs ($25,000,000) for the National Synchrotron Light Source-II (NSLS-II), which will be built as a replacement for NSLS-I, 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 will provide the world's finest capabilities for x-ray imaging.
- Support is provided for PED for the Advanced Light Source User Support Building ($3,000,000), which will provide space for experimental set up 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.

There also are a number of increases in research. In FY 2007, the Office of Science will support expanded efforts in basic research related to transformational energy technologies. This derives from the BESAC workshop report "Basic Research Needs to Assure a Secure Energy Future." Within BES, there are increases to ongoing basic research for effective solar energy utilization, for the hydrogen economy, and for work underpinning advanced nuclear energy power. These are described briefly below. BES not only asks its communities of scientists to provide the scientific foundations to overcome short-term "showstoppers" in energy technologies such as these three, BES also asks researchers to reach far beyond today's problems in order to provide the basis for long-term solutions to what is probably society's greatest challenge—a secure, abundant, and clean energy supply. To that end, there also are increases in research for grand challenge science questions and for new technique development. Grand challenge science includes the study of the fundamental phases of matter and phase transitions; quasiparticles; interactions of strong and weak forces in molecular bonding; "communication" among electrons, atoms, molecules, cells, and organisms; the harnessing of properties of elementary particles, atoms, and molecules to create fundamentally new ways to store, manipulate, and transmit information; and organizing principles at the nanoscopic and mesoscopic scales, intermediate between atomic and macroscopic dimensions. This will be a topic of a forthcoming BESAC workshop.

Briefly, additional research funding is provided in the following areas:

- Basic research for the hydrogen economy. Research to realize the potential of a hydrogen economy will be increased from $32,500,000 to $50,000,000. The research program is based on the BES workshop report "Basic Research Needs for the Hydrogen Economy." The results of the FY 2005 solicitation are described later in this document.
- Basic research for effective solar energy utilization (+$34,115,000). Investments will be focused in three areas: solar-to-electric, solar-to-fuels, and solar-to-thermal conversions. Each of the three generic approaches to exploiting the solar resource has untapped capability well beyond its present usage. Many of the proposed research directions identified in the 2005 BES workshop report "Basic Research Needs for Solar Energy Utilization" concern important cross-cutting issues such as (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties (e.g., polycrystalline materials versus expensive single crystal materials or plastics and polymers instead of metals and semiconductors); (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar energy conversion infrastructure, such as transparent conductors and robust, inexpensive thermal management materials. Powerful new methods of nanoscale fabrication, characterization, and simulation—using tools that were not available as little as five years ago—create new opportunities for understanding and manipulating the molecular and electronic pathways of solar energy conversion.
- Basic research for advanced nuclear energy systems (+$12,432,000). Basic research related to advanced fuel cycles is needed in areas such as (1) control and predictive capability of processes driven by small energy differences, e.g., aggregation and precipitation; (2) fundamental principles to guide ligand design; (3) investigation of new separations approaches based on magnetic and electronic differences; (4) development of environmentally benign separations processes, which produce no secondary wastes and consume no chemicals; and (5) development of modeling of separations processes to optimize waste minimization and minimize opportunities for diversion of nuclear materials (i.e. optimize proliferation resistance). Basic research also is needed in areas of materials for advanced reactors and waste forms for spent fuels from the new generation of reactors. This requires understanding and predicting the properties and behaviors of materials over long time scales and multiple length scales—from atoms to bulk materials. The efficiency, safe operating lifetime, and overall performance of fission energy systems is limited by the load-bearing capacity of structural materials under the maximum temperatures and hostile corrosive, applied stress, and radiation environmental parameters under which they must perform. New generation fission systems require structural materials possessing a combination of properties that will enable them to sustain their performance under such hostile parameters for durations of the order of 100 years.
- Complex systems or emergent behavior (+$5,000,000). Emergent behaviors arise from the collective, cooperative behavior of individual components of a system. Current understanding of emergent behaviors is very limited. The challenge of understanding how emergent behavior results from the complexity of competing interactions is among the most compelling of our time, spanning

physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magneto resistance, random field magnets, and spin liquids and glasses. Investments will encompass experimental, theoretical, and computational approaches capable of interrogating systems at comparable physical and time scales to gain direct insight into the mechanisms underpinning the cooperative behavior. Unlocking the mysteries of these systems will lay the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties.

- Ultrafast science (+$10,000,000). Ultrafast science deals with physical phenomena that occur in the range of one-trillionth of a second (one picosecond) to less than one-quadrillionth of a second (one femtosecond). These phenomena are typically probed using extremely short pulses of coherent light from conventional lasers or free electron lasers such as the Linac Coherent Light Source. Ultrafast technology has applications across the fields of atomic and molecular physics, chemistry and chemical biology, coherent control of chemical reactions, materials sciences, magnetic- and electric-field phenomena, optics, and laser engineering. Examples include the making and breaking of molecular bonds and the observation of the elusive chemical transition state. New investments in ultrafast science will focus on research applications of x-ray sources associated with BES facilities and beamlines: the Linac Coherent Light Source; the femtosecond "slicing" beamline at the Advanced Light Source; and the short pulse development at the Advanced Photon Source. Investments will also be made in the development and applications of laser-driven, table-top x-ray sources, including the use of high-harmonic generation to create bursts of x-rays on the even shorter than the femtosecond time scale.
- Mid-scale instrumentation (+$10,000,000). Scientific progress is predicated on observations of new phenomena, which often involve the building of better tools. There is a significant national need for mid-scale instruments that serve multiple users yet which are not as large as the synchrotron and neutron sources. High priority mid-scale instrumentation needs include end stations at the synchrotron light sources and neutron scattering facilities; laser systems for ultrafast or high-energy-density studies; micro- and atomic-scale characterization tools such as electron microcharacterization and scanning probe microscopy; high-field magnets; and facilities for providing large crystals and other unique materials for researchers throughout the Nation.
- Chemical imaging (+$5,000,000). Investments will develop and apply new methods to measure the chemical behavior of individual molecules and reactions, with high resolution in both space and time in order to elucidate fundamental principles of chemical processes at the nanoscale level. The research will build on current single-molecule spectroscopies and microscopies by adding simultaneous time-dependent characterization of evolving chemical processes, ultimately with femtosecond time resolution.

Additional information on these activities is in the relevant Construction Project Data Sheets and throughout the detailed narrative justifications.

In FY 2007, there are significant shifts in the nanoscale science and engineering research activities contributing to the BES investments in research at the nanoscale and a substantial overall increase in funding. Four of the five planned Nanoscale Science Research Centers are in their first full year of operation, with only one Center still in construction. Overall, the total investment for these Nanoscale Science Research Centers decreases by about 10 percent owing to the planned decrease in construction funding. Funding for research at the nanoscale increases very significantly owing to increases in funding for activities related to the hydrogen economy, solar energy conversion, advanced nuclear energy systems, fundamental studies of materials at the nanoscale, and instrumentation for characterizing materials at the nanoscale.

## Nanoscale Science Research Funding

(dollars in thousands)

| | TEC | TPC | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|---|---|
| Materials Sciences and Engineering | | | | | |
| Research | | | 65,307 | 70,328 | 108,542 |
| Major Item of Equipment, Center for Nanophase Materials (ANL) | | | 12,000 | 14,000 | — |
| Facility Operations | | | | | |
| Center for Functional Nanomaterials (BNL) | | | — | — | — |
| Center for Integrated Nanotechnologies (SNL/A & LANL) | | | — | 11,900 | 19,190 |
| ORNL, Center for Nanophase Materials Sciences | | | — | 17,800 | 19,190 |
| Center for Nanophase Materials (ANL) | | | — | 3,500 | 19,190 |
| Molecular Foundry (LBNL) | | | — | 8,100 | 19,190 |
| Chemical Sciences, Geosciences, and Biosciences | | | | | |
| Research | | | 27,645 | 26,914 | 49,109 |
| Project Engineering Design and Construction | | | | | |
| PED– All sites | | 21,318 | 1,996 | — | — |
| Construction | | | | | |
| Center for Functional Nanomaterials (BNL) | 79,700 | 81,000 | 18,317 | 36,187 | 18,864 |
| Center for Integrated Nanotechnologies (SNL/A & LANL) | 73,754 | 75,754 | 30,650 | 4,580 | 247 |
| ORNL, Center for Nanophase Materials Sciences | 63,740 | 64,740 | 17,669 | — | — |
| Molecular Foundry (LBNL) | 83,604 | 84,904 | 31,828 | 9,510 | 257 |
| Total | | | 205,412 | 202,819 | 253,779 |

In FY 2007, $50,000,000 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 enormous 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 by the three panels 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: (1) novel materials for hydrogen storage, (2) membranes for separation, purification, and ion transport, (3) design of catalysts at the nanoscale, (4) solar hydrogen production, and (5) 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 EERE in the preapplication review process to ensure basic research relevance to technology program goals. Furthermore, BES will participate in EERE's annual program review meeting to promote information sharing and, beginning in FY 2006, will organize parallel sessions at that meeting for the BES principal investigators. 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. The additional $17,500,000 in FY 2007 will be used to augment awards made in FY 2005 and to fund additional proposals based on a new solicitation.

## President's Hydrogen Initiative

(dollars in thousands)

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| Materials Sciences and Engineering Research | 14,761 | 16,600 | 28,075 |
| Chemical Sciences, Geosciences, and Biosciences | 14,422 | 15,900 | 21,925 |
| Total Hydrogen Initiative | 29,183 | 32,500 | 50,000 |

### 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. The power of computers and networks is increasing exponentially. 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 new 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 program is bringing computation and simulation to parity with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate modeling and prediction, plasma physics, particle physics, accelerator design, astrophysics, chemically reacting flows, and computational nanoscience.

The SciDAC program in BES consists of two major 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. The method of choice for the complete characterization of combustion at all scales is direct numerical simulation. A collaboration involving Sandia National Laboratories and four universities successfully implemented a fully parallel implementation of 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 in dealing with the problem of 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 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 percents. 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 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| All Facilities | | | |
| Optimal Hours[a] | 30,700 | 31,300 | 32,700 |
| Scheduled Hours[b] | 28,129 | 30,610 | 32,700 |
| Unscheduled Downtime | 7.9% | <10% | <10% |
| Number of Users | 9,042 | 8,050 | 9,660 |
| Advanced Light Source | | | |
| Optimal Hours[a] | 5,600 | 5,600 | 5,600 |
| Scheduled Hours[b] | 5,344 | 5,520 | 5,600 |
| Unscheduled Downtime | 3.6% | <10% | <10% |
| Number of Users | 2,003 | 1,770 | 2,100 |
| Advanced Photon Source | | | |
| Optimal Hours[a] | 5,000 | 5,000 | 5,000 |
| Scheduled Hours[b] | 4,931 | 4,900 | 5,000 |

[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 2005 show actual number of hours delivered to users.

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Unscheduled Downtime | 1.4% | <10% | <10% |
| Number of Users | 3,215 | 2,640 | 3,300 |
| National Synchrotron Light Source | | | |
| Optimal Hours[a] | 5,500 | 5,400 | 5,400 |
| Scheduled Hours[b] | 5,313 | 5,030 | 5,400 |
| Unscheduled Downtime | 2.4% | <10% | <10% |
| Number of Users | 2,256 | 2,070 | 2,300 |
| Stanford Synchrotron Radiation Laboratory | | | |
| Optimal Hours[a] | 3,700 | 5,000 | 5,000 |
| Scheduled Hours[b] | 3,527 | 4,900 | 5,000 |
| Unscheduled Downtime | 5.0% | <10% | <10% |
| Number of Users | 1,007 | 980 | 1,200 |
| High Flux Isotope Reactor | | | |
| Optimal Hours[a] | 3,400 | 2,400 | 4,500 |
| Scheduled Hours[b] | 2,613 | 2,360 | 4,500 |
| Unscheduled Downtime | 23.2% | <10% | <10% |
| Number of Users | 96 | 100 | 220 |
| Intense Pulsed Neutron Source | | | |
| Optimal Hours[a] | 3,600 | 3,600 | 3,600 |
| Scheduled Hours[b] | 3,462 | 3,600 | 3,600 |
| Unscheduled Downtime | 4.5% | <10% | <10% |
| Number of Users | 244 | 240 | 240 |
| Manuel Lujan, Jr. Neutron Scattering Center | | | |
| Optimal Hours[a] | 3,900 | 4,300 | 3,600 |
| Scheduled Hours[b] | 2,939 | 4,300 | 3,600 |
| Unscheduled Downtime | 23.2% | <10% | <10% |
| Number of Users | 221 | 250 | 300 |
| Spallation Neutron Source[c] | | | |

[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 2005 show 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.

## Cost and Schedule Variance

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Spallation Neutron Source | | | |
| Cost Variance | 0% | | |
| Schedule Variance | -0.3% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Instrument Systems Design Complete<br>Linac Beam Available to Ring | Ring Beam Available to Target<br>Approve Critical Decision 4 – Start of Operations | N/A |
| Linac Coherent Light Source (SLAC) | | | |
| Cost Variance | 0% | | |
| Schedule Variance | -3.9% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 2b – Performance Baseline<br>Approve Critical Decision 3a – Start Long-Lead Procurement | Approve Critical Decision 3b – Start Construction | None |
| Center for Nanophase Materials Sciences (ORNL) | | | |
| Cost Variance | +0.1% | | |
| Schedule Variance | -0.6% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 4a – Start Initial Operations | Approve Critical Decision 4b – Start Full Operations | N/A |
| Center for Integrated Nanotechnologies (SNL/LANL) | | | |
| Cost Variance | -1.2% | | |
| Schedule Variance | -0.3% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | None | Approve Critical Decision 4a – Start Initial Operations | Approve Critical Decision 4b – Start of Full Operations |
| The Molecular Foundry (LBNL) | | | |
| Cost Variance | 0% | | |
| Schedule Variance | +3.9% | | |
| 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 |
| Center for Nanoscale Materials (ANL) | | | |
| Cost Variance | +1.2% | | |
| Schedule Variance | -2.6% | | |
| 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 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Center for Functional Nanomaterials (BNL) | | | |
| Cost Variance............................................ | 0% | | |
| Schedule Variance.................................... | -26.3%[a] | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 3 – Start Construction | None | Approve Critical Decision 4a – Approve Building Occupancy |
| Instrumentation for Spallation Neutron Source I (ORNL) | | | |
| Cost Variance | -3.1% | | |
| Schedule Variance | -5.1% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 2 for Instruments #1-3 – Performance Baseline Approve Critical Decision 3 for Instruments #1-2 – Start Construction | Approve Critical Decision 2 for Instruments #4-5 – Performance Baseline Approve Critical Decision 3 for Instruments #3 – Start Construction | Approve Critical Decision 3 for Instruments #4-5 – Start Construction |

## 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 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

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[a] The significant negative schedule variance for the CFN project is due to the DOE Acquisition Executive's decision to postpone CD-3 approval while BNL extended the procurement process for conventional facilities (CF) to secure a reasonably priced bid. CD-3 was ultimately approved and the CF contract was awarded in late FY 2005. Schedule recovery measures are in place that will ensure that CFN will be completed on time.

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 2007 budget authority of $105,740,000 is requested. The estimated Total Project Cost is $379,000,000. Additional information on the LCLS Project is provided in the LCLS construction project data sheet, project number 05-R-320.

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

The NSLS-II, which is under development, will be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of 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 will be the best storage-ring-based synchrotron light source in the world, but, more importantly, NSLS-II will be transformational in that it will 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 will be possible to investigate the atomic and electronic structure and chemical composition of nanometer-scale objects under realistic in-situ device operating conditions. And it will 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 will be unprecedented.

In FY 2007, budget authority is requested to begin Project Engineering and Design and for research and development (R&D) activities 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 Project Engineering Design data sheet, project number 07-SC-06.

Advanced Light Source (ALS) User Support Building Project

The ALS User Support Building to be located at the Lawerence 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 quickly moving the apparatus into place. 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. Additional information on the ALS User Support Building Project is provided in the User Support Building Project Engineering Design data sheet, project number 07-SC-12.

**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 a doctoral degree, 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 an 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 2005 | FY 2006 estimate | FY 2007 estimate |
|---|---|---|---|
| # University Grants | 910 | 810 | 1,000 |
| Average Size | $150,000 | $150,000 | $150,000 |
| # Permanent Ph.D.s (FTEs) | 4,240 | 3,900 | 4,830 |
| # Postdoctoral Associates (FTEs) | 1,220 | 1,140 | 1,380 |
| # Graduate Students (FTEs) | 1,960 | 1,810 | 2,170 |

**External Independent Reviews**

Beginning in FY 2005, the costs of conducting External Independent Reviews (EIRs) for Capital Asset Projects greater than $5,000,000 within SC have been 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 2005 | FY 2006 | FY 2007 |
| Materials Sciences and Engineering | | | |
| Materials Sciences and Engineering Research | 290,400 | 274,220 | 335,099 |
| Facilities Operations | 330,826 | 444,675 | 644,885 |
| SBIR/STTR | — | 18,820 | 24,228 |
| Total, Materials Sciences and Engineering | 621,226 | 737,715 | 1,004,212 |

### 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 $338,099,000 research component of this subprogram for FY 2007 are facility related activities such as R&D for new and upgraded facilities, accelerator and detector research, and all BES FY 2007 Major Items of Equipment. These activities total $50,453,000.

### 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, welding and joining, non-destructive evaluation, electron beam micro characterization, nanotechnology and microsystems, fluid dynamics and heat transfer in materials, nonlinear systems, 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 including new facilities under construction: the Spallation

Neutron Source, the Nanoscale Science Research Centers, the Linac Coherent Light Source, the National Synchrotron Light Source-II, the User Support Building at LBNL, and a number of facility-related Major Items of Equipment.

**Selected FY 2005 Research Accomplishments**

- Synchrotron X-Rays Demonstrate Nanoscale Ferroelectricity. Films only a few atoms thick have been made that retain the controllable electric polarization needed for next generation nanoscale devices. Such ultrathin ferroelectric films have the potential to revolutionize future electronics, sensors, and actuators. Previous studies suggested that, as devices are miniaturized, they lose their ferroelectric character. These studies showed that ferroelectricity persists in films only 6 atoms thick. This landmark success was achieved using a unique instrument to observe thin film growth with high intensity x-rays from the Advanced Photon Source. X-rays reveal in real time the film structure as it grows, atomic layer by atomic layer. The in-situ x-ray techniques developed for this study can now be used to understand the synthesis and environmental interactions of other complex materials, thus addressing a wide range of energy-related challenges.
- A Superconductor that Tolerates Magnetic Fields. One of the biggest obstacles to the practical use of superconductors is the motion of magnetic flux due to an electric current in a superconductor. This motion of magnetic flux reduced the superconducting properties. A large research effort has gone into finding ways to prevent energy loss occurring from the movement of magnetic flux in copper oxide high temperature superconductors. It has been found that the magnetic flux in certain magnesium diboride films is intrinsically motionless, or “frozen,” in applied magnetic fields up to 14 Tesla. Such a complete apathy to an applied magnetic field has never been seen before in any other superconductor. While the theoretical explanation for this behavior has eluded scientists, the experimental finding has drawn a lot of attention. This behavior may make it possible to fabricate superconducting wire that can carry very large electric currents.
- Using Electron Spin, not Electron Charge, to Carry Information. Today’s computers are based on resistive circuitry using the movement of charged electrons. The resistance generates heat, and the removal of this heat is a fundamental limiting factor in creating the next generation of ultra small and ultra fast circuit elements. In a remarkable discovery, theorists have determined that in certain materials a spin current can be created with the application of a suitably oriented electric field, with no dissipation of energy. The spin current could potentially be used to carry out the same logic operations with no energy loss. This has been verified recently with experiments on gallium arsenide. This discovery may lead to computers with much greater capabilities including speed and capacity due to smaller circuit elements and with a significant reduction in energy loss.
- Plutonium Helps Understand Superconductivity’s Mysteries. Magnetic resonance studies of the fundamental mechanism responsible for superconductivity in $PuCoGa_5$ reveal strong similarities to the high-$T_c$ copper oxide materials. These results confirm earlier theories that this unique family of plutonium superconductors is nearly magnetic. This is a new class of superconducting materials and forms a conceptual bridge between two families of magnetically mediated superconductors, the heavy fermion metals and the copper oxides. The discovery of additional classes of superconducting materials enhances our ability to understand the mechanisms responsible for high temperature superconductivity.
- Ultrafast Studies of Nanocrystals. The fastest phase transition between nanocrystal structures ever recorded has been observed by ultrafast laser techniques. The reversible structural change in nanocrystals of vanadium dioxide switches the material from a semiconductor to a metallic phase,

increasing the electrical conductivity by a factor of 100-10,000 depending on nanoparticle size. Correspondingly large changes from optical transparency to high reflectivity occur at the same time. Lasers with pulses as short as one ten-trillionth of a second were used to track the phase change in vanadium dioxide nanoparticles. This discovery may be key to possible applications requiring extremely rapid switching from transparent to reflective states. These include protective overlayers for sensitive infrared detectors, nonlinear optical switches, fiber-optic pressure sensors, and electrically or optically triggered transistors that could switch hundreds of times faster than conventional silicon devices.

- First Direct Observations of Quasiparticles. Quasiparticles provide a convenient simplification to describe the behavior of electrons in a superconductor. A quasiparticle can be thought of as a single particle moving through a system, surrounded by a cloud of other particles either pushed away or dragged along by its motion. Prior investigations of their dynamics have been indirect. Through the use of a new optical technique it was possible to perform the first direct study of the dynamics of quasiparticles in a superconductor. It was discovered that the quasiparticles can propagate remarkably far, several hundreds of nanometers. Knowledge of the dynamics of quasiparticles, specifically their rates of diffusion, scattering, trapping, and recombination, is critical for the both the applications and fundamental understanding of superconductivity.
- Confining Electrons in New Two-dimensional Materials. Transition metal oxides, like semiconductors, are materials that confine electrons to a plane. It may now be possible to construct near-perfect layered materials of two perovskite structured materials. It has been shown through computational models that a single layer of $LaTiO_3$ in $SrTiO_3$ will serve as an electron donor and positive charge layer to retain those electrons in a thin layer as a two-dimensional electron gas (2DEG). Electrons behaving like a 2DEG appear to be an exotic phenomenon, but they are not. Many semiconductor electronic devices operate by creating just such a gas by an applied electric field inducing a thin conducting region at an interface—the field effect transistor being the prime example. Such thin electron layers have become a valuable tool for scientists studying the ways in which electrons organize their collective behavior. By expanding the materials available to create 2DEGs, new, more diverse opportunities have been created to expand our knowledge of electronic behavior that in turn can produce new applications.
- Inexpensive Route to Solar Cells Using Nanomaterials. New and novel semiconductor nanocrystal-polymer solar cells with surprisingly high efficiencies have been fabricated. In a solar cell, the conversion of light energy to electrical current occurs at the nanometer scale. Thus the development of methods for controlling materials on this scale creates new opportunities for more advanced solar cells. These advances are required because, although solar cells based on silicon and gallium arsenide have achieved high efficiencies and have found a variety of markets, more widespread applications remain limited by their high cost of production. These new cells are formed in an inherently inexpensive process from a colloidal solution of semiconductor nanocrystals in a semiconducting polymer. The unique features of nanosized objects are exploited to optimize the cell performance by controlling the shape of the nanocrystals. The performance of the new cells already rivals that of the best polymer-based devices. While the power conversion efficiency is still below that of current amorphous silicon and single crystal devices, there are opportunities to increase performance further by adding additional nanocrystal components to capture more of the solar spectrum. Furthermore, the same methods can be extended to address other optoelectronic applications, such as photodetectors and light emitting diodes.

- Predicting Magnetism in Nanomaterials. As recording media and sensors become smaller and ever-denser, it is increasingly important to control magnetism in nanostructures. But the physical properties of magnetic nanostructures are linked in complex ways and are difficult to predict, much less control. In this work, the magnetic properties of a cobalt nano-wire next to a platinum surface step were predicted from first-principles. The results are in perfect agreement with experiment and show the importance of a proper quantum mechanical description of the interplay of different magnetic phenomena. This work, based on newly developed quantum mechanical models implemented on high-performance computers, shows that accurate predictions can be made for a nanostructure comprised of a few hundred atoms. With continued theoretical development and more powerful computers, this paves the way toward prediction and control of more complex and useful magnetic structures.
- Explaining Materials Deformation Mechanisms from Atomic-scale Measurements. Using the world's most advanced electron microscope, the first direct observations of atomic details in complex crystalline dislocation cores revealed the atomic mechanisms underlying the deformation of intermetallic compounds with complex crystal structures. It was discovered that the diffusion of chromium atoms into and out of the crystal dislocation cores hinders dislocation motion in Laves-phase $Cr_2Hf$, a model intermetallic compound, thus providing a clue as to the origin of the brittleness and poor low temperature ductility of these intermetallic alloys. The poor low-temperature ductility of these intermetallic alloys has prevented their fabrication and use for decades. Some of the most attractive high-strength alloys for advanced high-temperature fission and fossil energy conversion applications possess similar complicated atomic configurations and lack the low-temperature ductility required for their fabricated by conventional cold deformation processes without crack formation. This discovery provides new atomistic insight into the behavior of crystal dislocations in complex intermetallic compounds necessary to design new fabricable alloys with the required strength at high service temperatures.
- Discovery of Mechanism of Surface Mass Transport. Researchers have discovered that trace concentrations of sulfur can enhance the rate of mass transport on copper surfaces by many orders of magnitude and have established the atomic scale mechanism by which this enhancement occurs. This discovery was enabled by low-energy electron microscopy measurements of the motion of singe-atom-high steps on copper exposed to calibrated doses of sulfur. By comparing observations of the motion of these steps with theoretical predictions based on calculations of the electronic structure of the surface, this research established that surface mass transport is catalyzed by the formation of a large number of mobile copper sulfide clusters. Such highly mobile clusters are believed to be a common feature of impure surfaces. The enhanced mass transport allows the formation of much flatter and more defect free surfaces. This discovery provides insight to many previous puzzling observations of anomalous surface mass transport. It is an important advance towards the capability to control the nanoscale morphology of surfaces, a critical necessity for nanoscale applications.
- Superior Iron-based Alloys and Steels. Fundamental laws of alloying coupled with advanced microanalytical characterization led to the discovery that yttrium containing iron-based alloys substantially enhance the stability of the amorphous (non-crystalline) state. Two technical implications are: (1) large bulk physical dimensions of this class of amorphous alloys can be made and (2) this understanding provides a new direction for designing bulk amorphous metals for structural and functional applications. Bulk tool steel was fabricated that was twice as hard as conventional tool steel. These achievements are milestones in the science of amorphous metals and

the design of functional complex metallic alloys. Even more important, this research has demonstrated that microalloying is a new approach for designing bulk amorphous alloys. Their unique atomic configurations and the absence of a crystalline lattice allow bulk amorphous metals to outperform their crystalline counterparts by exhibiting superior magnetic and mechanical properties and corrosion resistance coupled with high thermal stability.

- Fracture Resistance Mechanism in Ceramics. Structural ceramics are complex structures of micron-sized matrix grains separated by a nanoscale intergranular film. For many years it has been observed that certain additives, specifically rare-earth atoms, influence the ceramic's fracture resistance. But detailed information about how this effect is achieved and how it can be controlled had been inaccessible with current diagnostic capabilities. Now, new scanning transmission electron microscopy (STEM) and associated chemical analysis techniques have revealed the local atomic structure and bonding characteristics of the grain boundaries with close to atomic resolution. Applied to silicon nitride ceramics containing a range of rare-earth additives, these methods together have revealed how each atom bonds at a specific location depending on atom radius, electronic configuration and the presence of oxygen; this variation in bonding sites can be directly related to the fracture resistance or toughness of the ceramic.

- Better Protective Coatings. Previously unattainable insight into stress development and failure mechanisms in thermally grown surface oxides on metal alloys has been obtained by a new in-situ synchrotron x-ray technique. This technique enabled, for the first time, the uncoupling and isolation of mechanical stress contributions from oxide growth, phase transformations, and creep deformation processes. For pure thermally-grown alumina, steady state oxidation creates compressive stresses. However, when certain "reactive elements" are added to the alloy, it is found that tensile stresses develop instead. Maximizing the tensile offset can lead to dramatic improvement in performance of a protective oxide. A 10 percent shift in the tensile direction can translate to a 40 percent improvement in operating lifetime. Better control of early stage oxidation leads to thinner, and thus longer lifetime protective oxides by speeding the transformation to a stable oxide structure. These results underpin future alloy development for high-temperature nuclear and fossil energy generation technologies and more fuel efficient jet engine applications where operating lifetime has great economic value.

- New Composite Materials that Respond to Magnetic Fields. Magnetic-field-structured composites are a novel class of material in which magnetic particles, dispersed in a polymerizable medium, are organized into chains and other structures by magnetic fields while the polymer solidifies. These chains of particles can be electrically conductive, and this electrical conductivity can be extremely sensitive to temperature, pressure, and chemical vapors that penetrate and swell the polymer. In the present work it was demonstrated that even modest magnetic fields produced by simple copper coils cause these materials to contract significantly, like artificial muscles. This contraction was found to be accompanied by an enormous, 50,000-fold increase in electrical conductivity. This is by far the largest "magnetoresistance" effect ever observed in such modest magnetic fields and paves the way to using magnetic fields to control heat and current transport in micro and nano machines, and to tailoring the sensing response of these materials.

- The "Giant Proximity Effect." The reproducible confirmation of the existence of a Giant Proximity Effect (GPE) has challenged experimentalists for over a decade. In the traditional Proximity Effect (PE), a very thin layer of normal metal, when placed between two thicker superconductor slices, behaves like a superconductor. That is, superconducting or paired electrons retain phase coherence even while separated by the normal metal gap. In the newly discovered GPE, the normal-metal barrier layer is as much as 100 times thicker than in the PE case, a result that stands outside of any present theories. In addition to challenging the theoretical community and providing new clues to the causes of high-temperature superconductivity, this result may lead to new advances in superconducting circuitry as it is relatively easy to prepare reproducible thick barriers which will improve device uniformity and yield.

- World's Smallest Nanomotor. The smallest synthetic motor—a 300 nanometer gold rotor on a carbon nanotube shaft—has been demonstrated. This "nanomotor" continues the dramatic advances in the miniaturization of electromechanical devices and is a key step in the realization of practical synthetic nanometer-scale electromechanical systems (NEMS). In initial testing, the rotor rotated on its nanotube shaft for thousands of cycles with no apparent wear or degradation in performance. This is attributed to the unique low-friction characteristics of the carbon nanotube shaft. The new motor design has significant potential for NEMS applications. It should be possible to fabricate arrays of orientationally-ordered nanotube-based actuators on substrates by using alignment techniques.
- Magnetohydrodynamic Turbulence in Liquid Metals. Application of a strong magnetic field can completely change flow characteristics of an electrically conducting fluid. The transformation may occur in processes ranging from the generation of sunspots to crystal growth. One particular aspect of this phenomenon, the damping of flow variations along the magnetic field lines and the corresponding development of elongated or even two-dimensional flow structures, affect nearly all aspects of turbulent flow behavior, including heat transfer and mixing. In a series of high resolution numerical experiments it has been shown that the anisotropy of flow (or directionality of flow) patterns is a robust universal feature determined primarily by the strength of the magnetic field, conductivity, and kinetic energy. Furthermore, the elongation of flow patterns is approximately the same for flow structures of different size. This property can be effectively employed for accurate modeling of magnetohydrodynamic turbulence. The results of the work are relevant to technological applications, such as continuous casting of steel, crystal growth, and development of lithium breeding blankets for fusion reactors.
- Nanoparticle Catalysts. Methods were developed for depositing and stabilizing nanometer-sized platinum group metals, including palladium and rhodium, on surfaces of carbon nanotubes in supercritical fluid carbon dioxide. Uniformly distributed monometallic and bimetallic nanoparticles with narrow size distributions are formed on the surfaces of the carbon nanotubes. The carbon nanotube-supported palladium and rhodium nanoparticles demonstrated improved performance over commercial carbon-based palladium and rhodium catalysts for hydrogenation of olefins and aromatic compounds. These new nanoscale catalysts are currently being tested as electrocatalysts for low temperature polymer electrode fuel cells applications.

**Selected FY 2005 Facility Accomplishments**

- The Advanced Light Source (ALS)
  - Beam-Size Stability Improved. Over the last five years, elliptically polarizing undulators (EPUs) have been used very successfully at the ALS to generate high-intensity photon beams with variable photon polarization (from linear to circular). However, users were not completely satisfied with the EPUs performance because they degraded the beam quality by increasing the photon beam size. Based on detailed magnet measurements, a system was developed that maintains a constant beam size. It is now being employed in routine user operation solving a problem that has affected many other light sources.

- New Undulator Beamline for High-Resolution Photoemission Electron Microscopy. Beamline 11.0.1 is a new elliptically polarizing undulator (EPU) beamline dedicated to photoemission electron microscopy (PEEM) at the ALS. An EPU, the third installed at the ALS, delivers light into the new beamline, which began commissioning March 2005. With full polarization control and continuous coverage optimized over key energy regions, this beamline will be an attractive user facility for organic and magnetic polarization-contrast microscopy. This beamline will have an aberration-corrected photoemission electron microscope (PEEM-3) with a spatial resolution of approximately 5 nanometers.

- New In-Vacuum Undulator Beamline for Femtosecond X-ray Studies. Beamline 6.0.1 for soft x-ray science with ultrashort photon pulses of 200 femtoseconds was ready for commissioning in July 2005. The beamline is unique in the U.S. and will be made available to users in FY 2006. The primary components are a vacuum undulator to produce x-rays over a wide photon-energy range, optical components, including a spectrograph for recording an entire x-ray absorption spectrum from one photon pulse, and a high-repetition-rate femtosecond laser system.

▪ The Advanced Photon Source (APS)

- More Stable Beams. Using a technique pioneered at the APS, 175 girders supporting accelerator components in the APS storage ring have been displaced by as much as 6 mm during scheduled tri-annual maintenance periods over the last seven years, eliminating the stray radiation background signals. As a result, photon beam position monitors (BPMs) for insertion devices over the entire storage ring circumference are now operating on line. The APS leads the world in the use of photon BPMs for insertion device beamlines. Use of these monitors has improved long-term x-ray beam angular stability by more than a factor of five. Users are able to scan the x-ray photon energy by changing the insertion device gap on demand, while still maintaining superior photon beam stability on their samples. The payoff is improved ability to resolve micron and nanometer-sized features in samples

- Improved Timing Experiments. The x-ray pulse structure at the APS is on the order of 100 picoseconds. This pulse width enables special classes of timing experiments where the physical phenomena require fast time resolution. Recent experiments at the APS using this technique have involved the study of porphyrins that may one day form the building blocks of novel catalysts, photonic devices, and efficient solar-power units. The APS has a special operating mode to facilitate these types of measurements. In this mode, a single x-ray timing pulse is isolated from the other x-ray pulses. The intensity in the pulse is determined by the amount of charge stored in the isolated electron bunch that generates the photon pulse. Recent changes to the storage ring top-up injection method, which allows the APS linear accelerator to vary the injection charge along with increasing the injection frequency from two minutes to one minute, have resulted in doubling the single pulse-intensity without adversely affecting the non-timing experiments.

- Improved Mirrors for X-ray Focusing. Elliptically-shaped mirrors based on new technology developed at the Advanced Photon Source are being used to achieve unprecedented focusing of high-brightness x-ray beams. These mirrors are especially useful for producing the microbeams that are used to probe the composition and structure of materials. They are being applied to studies such as microstructural analyses of structural changes arising from welding operations and detailed investigations of the three-dimensional structure of complex crystalline samples.

- Nanoprobe Beamline Commissioned for First Experiments. The world's first hard x-ray nanoprobe was activated in March 2005, at the APS. The Nanoprobe beamline is a central component of the new Center for Nanoscale Materials at Argonne National Laboratory. The x-ray nanoprobe will have a spatial resolution of 30 nanometers or better, the highest of any hard x-ray microscopy beamline in the world. It will offer fluorescence, diffraction, and transmission imaging in the x-ray spectral range of 3-30 keV, making it a valuable tool for studying nanomaterials.

- The National Synchrotron Light Source (NSLS)
  - New X-ray Micro-Diffraction Instrument. This instrument to be used for nanoscale research was developed at the X13B beamline to take advantage of the small source size of the in-vacuum mini-gap undulator in the X13 straight section of the NSLS x-ray ring. It consists of five main subsystems: monochromator, focusing optics, sample manipulator, charge-coupled detector (CCD) area detector, and a point detector with two degrees of freedom. The sample stages are equipped with integrated submicron position encoders for excellent positional precision and repeatability. The point detector assembly allows the use of analyzer crystals to obtain better resolution. A key design feature is the close attention paid to mechanical coupling of the focusing optics to the sample positioner to reduce vibrations and improve the microscope stability for the users.
  - Elliptically-Polarized Wiggler Beamline Upgrade. The Elliptically-Polarized Wiggler (EPW) located in the X13 straight section of the NSLS x-ray is a unique radiation source that produces time-varying elliptically-polarized x-rays for magnetism studies. A major upgrade was performed on beamline X13A to enhance its performance. It included replacement of the existing horizontal focusing mirror, which had been plagued by poor reflectivity as well as mechanical and thermal stability problems, with a new water-cooled spherical mirror. The new mirror system increases the horizontal photon collecting angle by a factor of two and is fully motorized to allow precise manipulation and optimization of the mirror's position. In addition, the beamline interlock and control systems were upgraded. The beamline upgrade has resulted in an order of magnitude increase in the photon intensity delivered to the sample, and the elimination of mechanical and thermal instabilities. These improvements have led to more efficient use of the beamline and increased magnetic sensitivity in the measurements.
  - Development of a Photon-Counting Silicon Microstrip Array Detector. The NSLS detector group has developed an extremely versatile 1-dimensional position sensitive detector. It is based on custom microelectronics developed at Brookhaven National Laboratory, and consists of a linear array of silicon photodiodes, each 0.125 x 4 mm, which is connected to a set of 32-channel custom integrated circuits and a microprocessor system. The detector system's performance is several orders of magnitude better than one can achieve with charge-coupled type detectors. It is easily adaptable to as large an array as is needed by the application. For example, arrays of 320 and 640 strips, 40 and 80mm long have been fabricated for real-time x-ray scattering.
  - X-ray Ring Lattice Symmetry Restored. The most direct benefit for the NSLS user community was the restoration of the x-ray ring magnetic field lattice symmetry, which for many beamlines resulted in a 25 percent reduction of the horizontal beam size and an increase in photon intensity delivered to a sample. The desired eight fold symmetry of the x-ray ring magnet lattice can be lost from errors in the x-ray ring quadrupole field strengths. The quadrupole errors can be partially compensated by trim coils available in the x-ray ring for one of the quadrupole magnet families. These errors were determined from an elaborate analysis of the electron orbit measurements taken as quadrupole magnet field strengths were systematically varied. This

improvement allowed the NSLS to restore the eight fold symmetric x-ray ring magnet settings for routine operations.

- The Stanford Synchrotron Radiation Laboratory (SSRL)
  - First SPEAR3 Run Completed. In the commissioning run for the new SPEAR3 accelerator, the facility proved to be exceptionally reliable, providing very stable beam for a very high percent (97) of the scheduled time. This is higher than ever recorded with SPEAR2, and an exceptional achievement for a new storage ring. The user run commenced in March and the SPEAR3 storage ring operated at 3 GeV/100 mA and provided 30+ hour life times. (The average uptime over the past five years was 96%.) During the run, users on 239 different proposals received beam time in a total of 466 experimental starts involving 1,516 researchers.
  - First High-Current SPEAR3 Tests Performed. SSRL conducted three special 8-hour shifts of SPEAR3 operation with currents above the official safety envelope value of 100 mA. These high-current test shifts took place on swing shifts with the experimental floor cleared of non-radiation workers. The main purpose of these tests was to determine if multi-bunch electron beam instabilities will be encountered at higher current operation, in which case a program to implement a costly multi-bunch feedback system would have to be launched. Other potential problems, primarily excessive component heating, are also of concern. The current reached in these tests was limited to 225 mA by the power rating of some absorbers in a legacy insertion device chamber. This current was reached and a comprehensive search revealed no apparent beam instabilities.
  - New Methods Developed for Studying Structures of Nanomaterials. The reactivity and properties of nanomaterials are highly influenced by particle size and atomic-scale structure. Researchers at SSRL have recently demonstrated that the combined use of several x-ray scattering and absorption measurement techniques leads to quantum leaps in understanding the structures of nanomaterials. X-ray scattering measurements allow experimenters to combine size and shape information with structural information to remove the small-particle size contribution to x-ray diffraction peak broadening, whereas x-ray absorption measurements provide complementary, metal-specific information on local atomic structure in disordered materials. Measurements on zinc sulfide have conclusively demonstrated that structural relaxation of surface atoms causes inhomogeneous internal strain, markedly altering its material properties. This multi-technique nano-characterization approach has further been advanced by developing methods for the routine characterization of bacterial nano-minerals under fully-hydrated *in-situ* conditions. Bacterial nanominerals are an important class of naturally occurring nanomaterials that help to control the composition of the atmosphere, the potability of natural waters, and the arability of soils. This multiple-technique method provides unique information of wide interest to the nanoscience community.

- The Intense Pulsed Neutron Source (IPNS)
  - Simultaneous Measurement of Mixed-conductor Lattice Relaxation, Diffusion, and Gas Conversion. The General Purpose Powder Diffractometer (GPPD) at the IPNS is equipped with a specially designed controlled-atmosphere furnace, where samples in pellet or hollow-tube form are exposed to mixtures of gases to control oxygen and hydrogen content from highly oxidizing to highly reducing environments. Using two separate gas delivery "circuits," simulated membrane operation conditions can be achieved whereby the responses of oxygen-permeable membranes to strong oxygen partial pressure gradients can be studied. Exhaust gases are

analyzed with a Residual Gas Analyzer to probe for leakage and to quantify gas conversion reactions. Dense ceramic components with mixed-conduction properties and high oxygen permeability are important as membranes for oxygen separation and solid oxide fuel cell applications. Membranes are typically operated at elevated temperatures (800-1000°C) and exposed to large oxygen partial pressure gradients. This experiment reproduces the conditions under which these membranes will be used commercially and provides insights into the unusual differential oxygen partial pressure stability of these materials.

- Accelerator Systems Improvements. Efforts include: completion of the beamline-magnet power supply upgrades, replacing the originals with higher-efficiency and better regulated units; completion of a full year of operation of the first of two new kicker-magnet power supplies; and completion of full-power tests of the new third-rf system that will be installed in the synchrotron ring to provide new proton beam capture and handling capabilities.
- National Neutron and X-ray Scattering School. During August 2005, Argonne National Laboratory again hosted the National School on Neutron and X-Ray Scattering. The school continues to attract outstanding graduate students and post-doctoral appointees with 150 applications for the 60 positions available in 2005. The intensive training introduces students to the theory of, and provides hands-on experimentation in, x-ray and neutron scattering.

▪ The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE)

- Neutron Scattering Winter Schools. The First and Second Annual LANSCE Neutron Scattering Winter Schools were held, with 30 students from a wide geographical distribution attending each School. The 2004 topic was magnetism and the 2005 topic was mechanical properties of materials. During nine intensive days in Los Alamos, students had lectures from world experts on the key materials issues for the School theme, modeling and theory, and neutron scattering techniques addressing these issues. In addition, the students had the opportunity to gain hands-on experience in neutron-scattering techniques and data analysis.
- New Sample Environments. A major emphasis on sample environments in FY 2005 has greatly enhanced the low temperature, high field, and high pressure possibilities for user experiments. Investments in new low temperature sample environments, high pressure instrumentation, sample goniometers, and support staff have made users more productive. Along with the 11-Tesla superconducting magnet commissioned in 2004, the Lujan Center's suite of sample environments for condensed matter physics has dramatically improved in FY 2005. A rheometer designed to synchronize with the 20 Hz Lujan Center pulsed neutron beam is expected to be tested in FY 2005. It will provide a unique capability to impose accurate hydrodynamic shear on polymer solutions and colloidal suspensions while performing structural measurements by small-angle neutron scattering.
- Instruments Enhancement. The High Intensity Powder Diffractometer (HIPD) and the Single Crystal Diffractometer (SCD) have received upgrades to software, shielding, alignments, and hardware that have increased their neutron intensity, user throughput, and efficiency. New hardware and software controls on the Low-Q Diffractometer (LQD) and a new detector have made small angle neutron scattering (SANS) more effective.

- The High Flux Isotope Reactor (HFIR)
  - Common Guide Casings for Seven New Instruments Installed. Neutron guides transport cold neutrons (energies ~0.1–20 meV) with little loss in flux. This permits one to transport neutron beams from the source to instruments several tens of meters away. This lowers the instrumental background noise from gamma rays and unwanted neutrons since one can place the instruments far from the source. Also, the guides have a slight curvature which removes the "line-of-sight" view of the neutron source and further reduces this background. The guides are made by coating glass with layered coatings called supermirrors which are highly reflective for neutrons. These flat, coated glass plates are then assembled to form hollow rectangular cross-sectioned pipes with the coated sides forming the interior walls of the pipes. These guides will be illuminated with neutrons produced by the new HFIR cold source to be installed early in 2006.
  - HB-4 Shield Tunnel and Velocity Selector Shielding Installed. A great deal of neutron shielding is required to shield the exit of the new HFIR cold source and components of the cold neutron beamlines. The first and largest general section of shielding for the new instruments was constructed. Also, the lead shielding for the velocity selectors for the two small angle neutron scattering (SANS) instruments was assembled. These components are essential for the new Center for Neutron Scattering cold neutron spectrometers.
  - SANS 1 Detector Tank and Internal Components Installed. The largest component for the first Small Angle Neutron Scattering (SANS) instruments has been installed. This giant tank will contain the detector for this instrument. The 1 meter square detector will ride on rails inside the evacuated volume of the tank.
  - The Neutron Reflectometer Commissioned. A new instrument, the neutron reflectometer, was commissioned for use in the general user program at the HFIR Center for Neutron Scattering. This machine is optimized for the studies of surfaces and interfaces. It is the fifth Cold Neutron Source instrument fully commissioned and will be used for the studies of polymers, biomaterials, thin solid films, and surfactants.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Materials Sciences and Engineering Research** .............................. | **290,400** | **274,220** | **335,009** |
| ▪ **Structure and Composition of Materials** ................................ | **24,907** | **16,943** | **22,245** |

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

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

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 2007, 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 are increases to support the development of advanced electron microscopy and scanning probe techniques ($+763,000), ultrafast electron scattering probes as companion tools to ultrafast photon probes ($+1,000,000), for mid-scale instrumentation to develop new experimental tools and techniques for atomic scale structural characterization ($+2,000,000), for research related to the hydrogen economy ($+100,000), and for solar energy conversion ($+1,439,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Mechanical Behavior and Radiation Effects** .......................... | **14,008** | **13,037** | **18,195** |

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials. Concerns include the behavior of materials under repeated or cyclic stress, high rates of stress application as in impact loading, and over a range of temperatures corresponding to the stress and temperature conditions in present and anticipated future 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 in order to develop predictive models for the design of materials having superior mechanical behavior, with some emphasis on very high temperatures. The focus of basic research in radiation effects is to achieve an atomic-level fundamental understanding of mechanisms of radiation damage and how to design radiation-tolerant materials. Concerns include radiation induced embrittlement and radiation assisted stress-corrosion cracking. Other issues 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

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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 2007, 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 for ongoing materials research in support of materials related to advanced nuclear reactor fuel cycles ($+5,158,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Physical Behavior of Materials** ................................................ | **25,551** | **24,677** | **29,756** |

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 critical.

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 2007, 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 are increases to support solar conversion research ($+4,379,000) and research activities related to the hydrogen economy ($+700,000).

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Synthesis and Processing Science** ............................................ | **15,149** | **17,083** | **21,022** |

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 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 2007, 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 in ways 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 initiate new emergent behavior research ($+1,000,000), research activities related to hydrogen economy ($+1,500,000), and solar energy conversion ($+1,439,000).

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|---|---|---|---|
| ▪ **Engineering Research** ............................................................... | **5,306** | **2,444** | **1,000** |

This activity supports fundamental atomic or nanoscale 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.

The performance, safety, and economics of fission, fusion, fossil, and transportation energy conversion systems depend on a thorough understanding of heat transfer in regimes of complex, multi-phase fluid flow and the ability to provide reliable early warning of impending catastrophic fracture or other failure.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

In FY 2007, in order to emphasize other research activities described herein, selected activities in engineering research will be terminated, including nanoindentation, fluid behavior during solidification, heat transfer, and multiphase fluid flow.

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| ▪ **Neutron and X-ray Scattering** ................................................ | **46,061** | **45,141** | **62,055** |

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 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, together with the electron scattering probes 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 2007, activities will be initiated in ultrafast materials science research with an emphasis on understanding the physics of strongly correlated systems and systems at the nanoscale; properties and behavior of materials at high pressure magnetic fields; real-time, in-situ characterization of materials synthesis; exploratory research on next generation instrument concepts for synchrotron light sources and neutron sources; and studies of structure and dynamics in hydrogen storage materials ($+9,614,000). Additional funding is provided for the development of new research activities in photon-based ultrafast materials science ($+4,000,000), the development of mid-scale instrumentation including end stations at the synchrotron light sources and neutron scattering facilities ($+1,000,000), and research related to the hydrogen economy ($+2,300,000).

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| ▪ **Experimental Condensed Matter Physics**............................... | **41,024** | **36,691** | **47,480** |

This activity supports condensed matter physics with emphases in electronic structure, surfaces, and 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

| | (dollars in thousands) | |
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| FY 2005 | FY 2006 | FY 2007 |

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 which underpin various technology programs in Energy Efficiency and Renewable Energy (EERE). Research in superconductivity and photovaltaics especially 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. The petroleum recovery efforts of Fossil Energy (FE) and the clean-up efforts of Environmental Management (EM) programs are supported through research on granular materials and on fluids.

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

In FY 2007, 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 initiate mid-scale instrumentation for the synthesis of new materials and the growth of high quality single crystals ($+2,500,000) and for solar energy conversion ($+4,939,000). Additional funding is provided for research related to the hydrogen economy ($+3,350,000).

- **Condensed Matter Theory** ........................................................ **19,798** **22,888** **27,408**

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. Examples include fracture mechanics—

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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 2007, major activities will include both 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 lay the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties. Within this funding, there are increases to support new emergent behavior research ($+1,500,000), research related to hydrogen production, storage, and use ($+1,100,000), and for solar energy conversion ($+1,920,000).

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| ▪ **Materials Chemistry** ........................................................ | **46,860** | **40,694** | **49,748** |

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 (NMR), 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 2007, major activities will include the 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

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

inorganic/organic components in engineered assemblies with unprecedented efficiencies for the conversion of solar photons to fuels and chemicals. Within this activity, there are increases for direct solar conversion to fuels research ($+5,129,000) and for the development of new tools, techniques and mid-scale instrumentation to measure forces, atomic configuration, and physical and chemical properties with ultrahigh sensitivity to further advance nanoscale science ($+1,500,000). Additional funding is provided for research related to the hydrogen economy ($+2,425,000).

| | FY 2005 | FY 2006 | FY 2007 |
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| ▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)** | **7,643** | **7,280** | **8,000** |

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, 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, and nuclear physics, fusion energy sciences, fossil energy sciences, and energy efficiency and renewable energy sciences. In FY 2007, funding is increased for EPSCoR research activities ($+720,000). The following table shows EPSCoR distribution of funds by state.

**EPSCoR Distribution of Funds by State**

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| Alabama | 695 | 685 | 258 |
| Alaska | — | — | — |
| Arkansas | 145 | 135 | 139 |
| Delaware | — | — | — |
| Hawaii | — | — | — |
| Idaho | 476 | 375 | 375 |
| Kansas | 626 | 135 | — |
| Kentucky | 224 | — | — |
| Louisiana | 660 | 462 | 375 |
| Maine | — | — | — |
| Mississippi | 667 | 132 | — |
| Montana | 375 | 455 | 133 |
| Nebraska | 120 | 265 | 269 |
| New Hampshire[a] | — | — | — |
| Nevada | — | 90 | 105 |
| New Mexico | 135 | 135 | — |
| North Dakota | 406 | 273 | — |
| Oklahoma | 485 | 350 | 350 |
| Rhode Island[a] | — | — | — |

[a] Becomes eligible in FY 2006.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Puerto Rico | 375 | 375 | — |
| South Carolina | 716 | 660 | 525 |
| South Dakota | 125 | 125 | — |
| Tennessee | — | 140 | 140 |
| Vermont | 705 | — | — |
| U.S. Virgin Islands | — | — | — |
| West Virgina | 315 | 225 | 135 |
| Wyoming | 270 | 140 | 140 |
| Technical Support | 123 | 60 | 110 |
| Other[a] | — | 2,063 | 4,946 |

- **Electron-beam Microcharacterization** **7,614** **7,945** **7,945**

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 on 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 2007, user operations, scientific research of the staff, and development of new instruments or techniques will continue to be supported at the electron beam microcharacterization user facilities.

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[a] Uncommitted funds in FY 2006 and FY 2007 will be competed among all EPSCoR states.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Accelerator and Detector Research** .......................................... | **4,000** | **2,119** | **3,000** |

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 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 in order to achieve high power spallation sources. There is also joint interest in collaboration with NSF on Energy Recovery Linac (ERL) research. There is a coordinated effort between the DOE and NSF to facilitate the development of x-ray detectors. There are ongoing industrial interactions through the SBIR/STTR awards for the development of x-ray detectors.

In the area of neutron science, there is research to develop improved high intensity, low emittance proton sources for accelerator-driven neutron sources. More efficient proton sources can increase the reliability and lifetime due to lower RF power requirements.

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 2007, activities in novel accelerator and source concepts as well as detector research will continue.

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| ▪ **General Plant Projects** ............................................................... | **3,250** | **—** | **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.

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

Capital Equipment funding for new and upgraded instrumentation prior to the installation and commissioning of the cold source has been competed.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Linac Coherent Light Source (LCLS)** | **4,000** | **—** | **—** |

Research and development (R&D) funds were provided to support the physics design of several key LCLS components: the photocathode gun, the linac, the undulator, and the beam optics. These R&D activities were carried out at SLAC and other collaborating institutions in order to reduce the technical risk and provide more confidence in the project's cost and schedule estimates prior to establishing a project performance baseline. No funding is requested in FY 2006 or FY 2007.

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| ▪ **Nanoscale Science Research Centers** | **600** | **993** | **500** |

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

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| ▪ **The Center for Nanoscale Materials** | **12,000** | **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, including clean rooms, 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 which 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 be the highest spatial resolution instrument of its kind in the world, which will permit nondestructive examination of magnetic, electronic, and photonic materials important both for basic science and as foundations for future nanotechnologies.

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| ▪ **Spallation Neutron Source Instrumentation I** | **3,143** | **12,579** | **10,500** |

Funds are provided to continue a Major Item of Equipment with a total estimated cost of $68,500,000 for five instruments for the Spallation Neutron Source that will be installed after the SNS line item project is completed in FY 2006. These instruments will complement the initial suite of five instruments that are being built as part of the SNS construction project, which has capacity for 24 instruments. The instrument concepts for the Major Item of Equipment project were competitively selected using a peer review process. The project will be managed by Oak Ridge National Laboratory with participation by both Argonne and Brookhaven National Laboratories as well as by the State University of New York at Stony Brook. The instruments will be installed at the SNS on a phased schedule between FY 2007 – 2011. A new Major Item of Equipment, described below, will fund approximately four to five additional instruments.

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| ▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)** | **1,900** | **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.

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| ▪ **Transmission Electron Aberration Corrected Microscope (TEAM)** | **5,586** | **6,206** | **5,508** |

Funds are provided for a Major Item of Equipment with a Total Estimated Cost in the range of $11,200,000 to $13,500,000 and a Total Project Cost in the Range of $25,000,000 to $30,000,000. The TEAM project will construct and operate a new aberration-corrected electron microscope and

| | (dollars in thousands) | |
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| FY 2005 | FY 2006 | FY 2007 |

make this capability widely 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.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)** | — | — | **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 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 close 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 Complex. The TEC 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 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.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Spallation Neutron Source Instrumentation II** | — | — | **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 approximately five instruments for the Spallation Neutron Source that will be installed after the SNS line item project is completed in FY 2006. These instruments will effectively complete the suite of instruments 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.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **Facilities Operations** | **330,826** | **444,676** | **644,885** |
| ▪ **Operation of National User Facilities** | **330,826** | **444,676** | **644,885** |

The operations of the scientific user facilities are funded at a level that will permit service to users at optimal capacity, an increase from FY 2006. 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 second year of a transition of programmatic ownership for SLAC linac operations from HEP to BES as the LCLS project proceeds. FY 2007 funding is requested for National

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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 2005 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 (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.

## Facilities

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| Advanced Light Source | 44,800 | 42,783 | 49,802 |
| Advanced Photon Source | 100,500 | 95,890 | 108,604 |
| National Synchrotron Light Source | 36,750 | 36,196 | 40,763 |
| National Synchrotron Light Source-II | 1,000 | — | 25,000 |
| Stanford Synchrotron Radiation Laboratory | 32,388 | 25,475 | 35,836 |
| High Flux Isotope Reactor | 46,900 | 43,330 | 51,598 |
| Radiochemical Engineering Development Center | 4,500 | — | — |
| Intense Pulsed Neutron Source | 16,800 | 15,500 | 18,531 |
| Manuel Lujan, Jr. Neutron Scattering Center | 9,588 | 10,000 | 10,582 |
| Spallation Neutron Source | 37,600 | 101,001 | 171,409 |
| Center for Nanophase Materials Sciences | — | 17,800 | 19,190 |
| Center for Integrated Nanotechnologies | — | 11,900 | 19,190 |
| Molecular Foundry | — | 8,100 | 19,190 |
| Center for Nanoscale Materials | — | 3,500 | 19,190 |
| Linac Coherent Light Source (LCLS) | — | 3,500 | 16,000 |
| Linac for LCLS | — | 29,700 | 40,000 |
| Total, Facilities | 330,826 | 444,675 | 644,885 |

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **—** | **18,820** | **24,228** |

In FY 2005, $13,551,000 and $1,626,000 were transferred to the SBIR and STTR programs, respectively. The FY 2006 and FY 2007 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

| | | | |
|---|---|---|---|
| **Total, Materials Sciences and Engineering** | **621,226** | **737,715** | **1,004,212** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Materials Sciences and Engineering Research** | |
| ▪ **Structure and Composition of Materials** | |
| Increases are provided for developing advanced electron microscopy and scanning probe techniques ($+763,000), research to advance the hydrogen economy ($+100,000), ultrafast science ($+1,000,000), mid-scale instrumentation ($+2,000,000), and solar energy conversion ($+1,439,000) | +5,302 |
| ▪ **Mechanical Behavior and Radiation Effects** | |
| Increase is provided for ongoing research in support of materials related to advanced nuclear reactor fuel cycles | +5,158 |
| ▪ **Physical Behavior of Materials** | |
| Increases are provided for research to advance the hydrogen economy ($+700,000) and solar energy conversion ($+4,379,000). | +5,079 |
| ▪ **Synthesis and Processing Science** | |
| Increase is provided for emergent behavior ($+1,000,000), research to advance the hydrogen economy ($+1,500,000), and solar energy conversion ($+1,439,000) | +3,939 |
| ▪ **Engineering Research** | |
| Termination of selected activities in engineering research including fluid behavior during solidification and heat transfer | -1,444 |
| ▪ **Neutron and X-ray Scattering** | |
| Increases are provided for research and instrumentation for studies of strongly correlated materials, systems at the nanoscale, materials in high fields, and other studies relevant to energy needs ($+9,614,000). Increases are also provided for research to advance the hydrogen economy ($+2,300,000), ultrafast science ($+4,000,000), and mid-scale instrumentation ($+1,000,000) | +16,914 |
| ▪ **Experimental Condensed Matter Physics** | |
| Increases are provided for research to advance the hydrogen economy ($+3,350,000), mid-scale instrumentation ($+2,500,000), and solar energy conversion ($+4,939,000) | +10,789 |
| ▪ **Condensed Matter Theory** | |
| Increases are provided for research to advance the hydrogen economy ($+1,100,000), emergent behavior ($+1,500,000), and solar energy conversion ($+1,920,000) | +4,520 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Materials Chemistry** | |
| Increases are provided for research to advance the hydrogen economy ($+2,425,000), mid-scale instrumentation ($+1,500,000), and solar energy conversion ($+5,129,000) | +9,054 |
| ▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)** | |
| Increases is provided for additional EPSCoR research activities | +720 |
| ▪ **Accelerator and Detector Research** | |
| Increase is provided for additional research in new accelerator and detector concepts, including accelerator concepts for light sources not necessarily based on storage-ring technologies | +881 |
| ▪ **General Plant Projects** | |
| Increase is provided for general plant projects as part of the BES stewardship responsibilities | +737 |
| ▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor** | |
| Funding for new and upgraded instrumentation prior to installation and commissioning of the cold source is complete.. | -2,000 |
| ▪ **Nanoscale Science Research Centers** | |
| Scheduled decrease for Other Project Costs for the Nanoscale Science Research Centers. Funding is provided for Other Project Costs for the BNL Center for Functional Nanomaterials. No Other Project Costs are required for the remaining Nanoscale Science Research Centers | -493 |
| ▪ **The Center for Nanoscale Materials** | |
| Scheduled decrease for the Major Item of Equipment for the ANL Center for Nanoscale Materials due to its completion | -14,000 |
| ▪ **Spallation Neutron Source Instrumentation I** | |
| Scheduled decrease for Instrumentation for the Spallation Neutron Source. | -2,079 |
| ▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)** | |
| Scheduled decrease for R&D on instrumentation for the LCLS | -1,500 |
| ▪ **Transmission Electron Aberration Corrected Microscope (TEAM)** | |
| Scheduled decrease for the Major Item of Equipment for the Transmission Electron Aberration Corrected Microscope | -698 |
| ▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)** | |
| Initiate Major Item of Equipment for approximately four instruments at the Linac Coherent Light Source. | +10,000 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Spallation Neutron Source Instrumentation II** | |
| Initiate a new Major Item of Equipment for approximately four to five additional instruments for the Spallation Neutron Source | +10,000 |
| **Total, Materials Sciences and Engineering Research** | **+60,879** |
| **Facilities Operations** | |
| ▪ **Operation of National User Facilities** | |
| Increase for the Advanced Light Source to support accelerator operations and for increased support for users | +7,019 |
| Increase for Advanced Photon Source to support accelerator operations and for increased support for users | +12,714 |
| Increase for National Synchrotron Light Source to support accelerator operations and for increased support for users | +4,567 |
| Increase for National Synchrotron Light Source-II – Other Project Costs per FY 2007 project data sheet | +25,000 |
| Increase for the Stanford Synchrotron Radiation Laboratory to support accelerator operations and for increased support for users | +10,361 |
| Increase for High Flux Isotope Reactor to support reactor operations | +8,268 |
| Increase for Intense Pulsed Neutron Source to support accelerator operations and for increased support of users. | +3,031 |
| Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and for increased support for users | +582 |
| Increase for Spallation Neutron Source to support operations in the first full year of operation. | +70,408 |
| Increase for the Center for Nanophase Materials Sciences for continued operations. | +1,390 |
| Increase for Center for Integrated Nanotechnologies for continued operations | +7,290 |
| Increase for Molecular Foundry for continued operations. | +11,090 |
| Increase for Center for Nanoscale Materials for continued operations. | +15,690 |
| Increase for Linac Coherent Light Source Other Project Costs per FY 2007 project datasheet. | +12,500 |
| Increase for Stanford Linear Accelerator Center in support of the linac operations | +10,300 |
| **Total, Facilities Operations** | **+200,210** |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **SBIR/STTR** | |
| Increase in SBIR/STTR funding because of an increase in total operating expense........... | +5,408 |
| **Total Funding Change, Materials Sciences and Engineering** ........................................ | **+266,497** |

# Chemical Sciences, Geosciences, and Energy Biosciences

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Chemical Sciences, Geosciences, and Energy Biosciences | | | |
| Chemical Sciences, Geosciences, and Energy Biosciences Research | 225,928 | 208,831 | 255,113 |
| Facilities Operations | 6,437 | 6,251 | 6,805 |
| SBIR/STTR | — | 5,468 | 6,581 |
| Total, Chemical Sciences, Geosciences, and Energy Biosciences | 232,365 | 220,550 | 268,499 |

### 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 $255,113,000 research component of this subprogram is support for General Plant Projects and General Purpose Equipment totaling $17,466,000.

### 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 provides support for chemistry comparable to that of the National Science Foundation. It 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 2005 Research Accomplishments**

- Timing the World's Shortest X-Ray Pulses. Light sources based on particle accelerators, such as the Linac Coherent Light Source (LCLS), will revolutionize x-ray science due to their unprecedented brightness and extremely short pulse duration. To take full advantage of x-ray pulses that last only a few femtoseconds ($10^{-15}$ seconds), they must be timed relative to equally short pulses from an optical laser. Such measurements are vital to a wide range of LCLS experiments in which a sample is excited by an optical pulse and probed by an x-ray pulse. At the Stanford Linear Accelerator Center, ultrashort x-ray pulses were generated when 80-femtosecond electron pulses from an accelerator were sent through an undulator magnet; the x-ray and electron pulses were perfectly coincident in time. A crystal placed near the path of the electron beam experienced intense electric fields that altered the optical properties of the crystal, the electro-optic (EO) effect. An optical laser beam passing through the crystal sensed the EO effect, turning the time delay between the optical pulse and the electron/x-ray pulse into a spatial displacement on a detector. The current timing resolution of 60 femtoseconds could be improved to 5 femtoseconds, matching the projected performance of accelerator-based light sources into the foreseeable future.
- Molecular Fragmentation Observed in Unprecedented Detail. Researchers working at the Advanced Light Source have advanced our ability to observe the total destruction of a molecule to new levels of sophistication, challenging theoretical understanding and paving the way for research to be performed at next-generation light sources. When a hydrogen molecule is exposed to x-ray photons of the appropriate energy, the two electrons it possesses can be ejected at once, leaving behind two positively charged nuclei that rapidly explode. Thus, absorption of one x-ray photon causes the complete destruction of the molecule. Using modern techniques of three-dimensional imaging and ultrafast timing, the motions of all four particles from a single event can be related to one another. The results are surprising and challenge our current theoretical understanding of how x-rays interact with matter.
- Complete Ionization of Clusters in Intense VUV Laser Fields. BES-supported researchers have developed a theory that explains recently-observed ionization behavior of xenon clusters that were exposed to intense, coherent vacuum ultraviolet (VUV) pulses from a free-electron laser (FEL). Surprisingly, at intensities that produce only single ionization of an isolated xenon atom, the clusters irradiated by the FEL showed massive ionization in which every atom in the cluster was highly ionized, producing ions with charge states up to +8. This implies that each xenon atom in the cluster absorbed about 30 VUV photons. The key difference between clusters and isolated atoms is that energetic electron-ion collisions occur within the clusters and modify the single-photon absorption cross section, thus allowing a large number of photons to be absorbed. This process is called "inverse bremsstrahlung" and, when incorporated into a simple linear absorption model, clearly reproduces the experimental observations. Theories such as this will be needed to understand the behavior of matter when it is exposed to intense, coherent X-ray pulses from next-generation light sources such as the LCLS.
- The Roaming Atom: Straying from the Lowest-energy Reaction Pathway. A fundamental tenet of modern chemical reaction theory is the concept of the transition state, a transient molecular entity

that lies on the most direct pathway from reactants to products and whose properties govern the rate of reaction. Recently, it was shown that in a simple chemical reaction, the decomposition of formaldehyde, a substantial fraction of the dissociating molecules avoid the region of the transition state entirely. These studies combine ion imaging experiments with theoretical trajectory calculations to reveal that the dissociation takes place via a mechanism in which one hydrogen atom begins to roam away from the molecule and nearly dissociates, then returns to react with the remaining hydrogen atom. Along with other recent findings on reactions such as $O + CH_3$, these results challenge conventional notions of chemical reactions and raise the question of how common such processes might be. A key question is whether such a mechanism applies only to reactions forming hydrogen, during which a light hydrogen atom may rapidly explore regions far from the conventional transition state.

- New Combustion Intermediates Discovered. A complete mechanism for the combustion of simple hydrocarbon fuels includes dozens of distinct molecular species and hundreds of chemical reactions. The identification of which molecules to include in a combustion chemistry mechanism still requires experimental detection, particularly for reactive intermediates. A class of unstable molecules known as enols, which have OH groups adjacent to carbon-carbon double bonds, are not currently included in standard combustion models. In work performed at the Advanced Light Source, significant quantities of 2, 3, and 4-carbon enols were observed using photoionization mass spectrometry of flames burning representative compounds from modern fuels. Concentration profiles of the enols taken in the model flames demonstrate that their presence cannot be accounted for by isomerization reactions that convert more stable molecules into enols. This leads to the conclusion that an entire class of important reaction intermediates is absent from current combustion models, and the models will need substantial revision.
- Unified Molecular Picture of the Surfaces of Aqueous Solutions. A long-term controversy exists regarding the detailed, molecular nature of the surface of an aqueous solution containing molecular ions (or electrolytes). Joint theoretical and experimental studies have led to a new, unified view of the structure of the interface between air and aqueous electrolytes. Molecular dynamics simulations have shown that in basic salt solutions positively charged ions (cations) are repelled from the interface, while negatively charged ions (anions) exhibit a propensity to migrate toward the surface that correlates with the anion's polarizability and physical size. In acidic solution, however, there is a high propensity for cations to be located at the air/solution interface. In this case, both cations and anions are concentrated at the surface and reduce the surface tension of water. These conclusions have been verified by surface-selective nonlinear vibrational spectroscopy experiments. Understanding the behavior of ions at aqueous surfaces is important to the heterogeneous chemistry of seawater aerosols and to the tropospheric ozone destruction in the Arctic and Antarctic due to reactions on ice pack covered with sea spray.
- Self-Assembled Artificial Photosynthesis. In natural photosynthesis, self-assembly of light-absorbing molecules, or chromophores, at specific distances and orientations is especially important in two parts of the overall photosynthetic system: the antenna component, where light is collected; and the reaction center, where charge is separated. Recently, a green organic chromophore was discovered that exhibits photophysical and photoredox properties similar to those of natural chlorophyll a. When conjoined with four similar chromophores, the molecules self-assemble in solution to form an antenna-reaction center complex. Self-organization of the large structure is believed due to the propensity of these similar chromophores to align in a cofacial stacking arrangement. The self-

assembled organic has attributes that closely mimic the primary events in photosynthesis: efficient light energy capture over a wide spectral range, energy funneling toward a core electron-transferring unit, and excited-state symmetry breaking of a molecular pair resulting in charge separation. The structure of the new array was determined at the Advanced Photon Source.

- Two-Dimensional Spectroscopy Reveals Energy Transport Pathways In Photosynthesis. Photosynthetic antennas capture solar photons and transport the absorbed energy to the photosynthetic reaction center where charge separation occurs. Energy transfer by the antenna is nearly 100 percent efficient, although the mechanism for the process has been elusive. A novel spectroscopic technique known as a two-dimensional photon echo, commonly used in the infrared, has been extended to the visible spectral region and has revealed important details about energy transfer in photosynthetic light harvesting. In antenna pigments from green sulfur bacteria, distinct energy transport pathways have been identified that depend on the spatial properties of the pigment-protein complex. Contrary to the accepted model of a sequential cascade in energy from high- to low-lying excited states, these results reveal excited states that are distributed over two or more chlorophyll molecules and a pathway in which energy levels are skipped on the way to the lowest level. The new two-dimensional electronic spectroscopic method, which measures electronic couplings and maps the flow of excitation energy, opens the door to investigation of other photoactive systems and can be applied to improving the efficiency of molecular solar cells.
- How Water Networks Accommodate an Excess Electron. In bulk water an excess electron can become trapped within a cavity formed by a network of hydrogen-bonded water molecules. This “solvated electron” is a critical chemical intermediate in the radiolysis of aqueous solutions. One approach to understanding the solvated electron is to study the structure and dynamics of clusters of water containing an excess electron in the gas phase. This approach has not yet been successful because these anionic water clusters are hard to make and because an accurate theoretical description for them is lacking. Recent work has shown that anionic clusters containing four to six water molecules can be created within gas-phase matrices of inert argon clusters, where their infrared spectra can be obtained. Analysis of these spectra using density functional theory shows that the diffuse electron interacts most strongly with a single water molecule that is hydrogen bonded to two other waters in a rearranged network. The spectra also exhibit evidence for the rapid exchange of energy between the vibrations of the hydrogen atoms on the unique molecule and the excess electron. This new technique can now be extended to larger water clusters that better mimic the solvated electron in bulk water.
- Gold, a Magnificent Nanoscale Catalyst. When gold atoms are assembled as tiny clusters smaller than 8 nanometers and attached to the surface of titanium oxide, they acquire the remarkable ability to dissociate oxygen at room temperature and insert that oxygen into very specific locations in molecules. The origin of such unusual reactivity—discovered some 10 years ago—has until recently evaded a widely accepted explanation. Numerous parameters in the material are important and usually cross-correlated: gold particle dimension and shape, metal oxidation state, oxide support reducibility, and interaction of the gold with the support. Separating those parameters in these materials, which are macroscopically amorphous, would demand special analytical techniques that are able to focus on the detailed properties of individual chemical bonds in the solid. Therefore, researchers pursued a different route using existing and well-known surface science techniques: they accurately synthesized and stacked one-atom-thick layers of gold extended in two dimensions, and supported them on top of perfect oxide crystals of known structure. They demonstrated that the

nanoscale properties of gold metal are achievable by controlling the layer thickness to between 2 and 3 atoms. Such knowledge can now be extended to the manipulation of selective oxidation chemistry or the discovery and assembly of new catalysts.

- Theory Guides Scientists on How to Extract Hydrogen from Natural Sources and Store it Efficiently. Two of the keys to a hydrogen economy are having an abundant supply of hydrogen and having materials that can store such hydrogen in a readily accessible form. Both of those challenges can be addressed by designing materials—chemical catalysts—that bind atomic hydrogen with medium strength and release molecular or gaseous hydrogen with very little heating. A random or systematic search for such catalysts, even with high-throughput techniques, would be very expensive and take many years. Scientists resorted to so-called density-functional theory, which is an electronic structure theory of matter, and other theories that describe chemical reactivity to design the ideal bimetallic catalysts, combinations of two metals, in special atomic arrangements that would result in solids with the desired properties. They arrived at a new theoretical construct called near-surface alloys of metals, such as a crystal of platinum containing a single layer of nickel atoms in its second row, that possesses the unique catalytic behavior sought. Having by now mapped entire families of such new theoretical materials—a feat unachievable by direct experimental means—these scientists have embarked on the challenge of fabricating these new structures and have already demonstrated their concept with a few successful examples.

- Devising the Next-Generation Wonder Molecules—Fine Chemistry inside Nano Cages. In the future drugs, fibers, fuel additives, molecular electronics devices, solar energy conversion dyes, and flavors may be synthesized in a similar manner using sets of discrete cavities to contain and isolate single molecules or just reacting pairs of molecules and catalysts. The "single-molecule catalysis" concept would allow maximum control of the environment surrounding a molecule, the spatial arrangement adopted by its atoms, the type of bonds made available for reaction, and even how the energy is coupled to and transferred to the molecule. Such level of control would result in the ability to break bonds or insert or remove atoms or change the spatial arrangement of atoms in very specific ways and not others. The resulting products would possess properties—chemical, biological, optical, electronic, or mechanical—superior to those achievable through less controllable chemistry. Researchers are beginning to show that this goal may be achievable. So-called supramolecular or larger-than-molecules cages made with organometallic compounds were used to host other organometallic complexes that have catalytic properties, such as the ability to specifically break carbon-hydrogen bonds. They have shown that certain carbon-hydrogen bonds are selectively broken and that only certain members of a chemical family undergo reaction, and not others. They have even shown that the constrained environment also leads to enhanced rate of production of the most desired product, which is in itself a revolutionary discovery.

- Controlling the Crash-landing of Biomolecules on Surfaces. Researchers have, for the first time, demonstrated that peptide ions retain at least one proton after soft landing on chemically modified, "fluffy" surfaces. Controlled deposition on surfaces holds great potential for applications such as selective chemical separations and analysis. Soft landing refers to the intact capture of large size-selected, charged molecules on surfaces of liquids or solids. Previous research suggests that soft landing provides a means for highly specific deposition of molecules of any size and complexity on surfaces using only a tiny fraction of material normally used in standard synthetic approaches. In the present studies, peptide ions are attractive as model systems that can provide important insights on the behavior of soft-landed macromolecules. The researchers used a specially designed mass spectrometer configured for studying interactions of large ions with surfaces. The special characteristics of the instrument enabled quantitative investigation of the effect of the speed and mass of ions on the soft landing process. For example, it was determined that even collisions with high energies can result in deposition of intact ions on surfaces.

- Removal of Radium Ions from Water using Special "Grabber" Molecules. Researchers demonstrated a process that is highly selective for binding radium cations. It is a significant challenge to remove radioactive radium cations from wastewater since the large excess of other non-radioactive ions in solution can interfere with the selective extraction of radium. In the new work, a specially designed molecule was used to selectively bind radium. This supramolecular assembly made from isoguanosine is just the right size to extract radium in the presence of other cations such as magnesium and sodium.
- How Molecules Move through Small Holes. Measurements of transport through 15-nanometer pores have been compared to theoretical results to yield new understanding of differential transport at small scales. This knowledge is important for an understanding of separation processes at the molecular level, and could lead to a new generation of analytical devices based on microfluidic platforms. By adjusting physical parameters such as the channel diameter, and applying the appropriate external electrical potential, arrays of nanochannels—formed by nanocapillary array membranes—can be made to behave like digital fluidic switches, and the movement of molecules from one side of the array to the other side can be controlled. Combining model calculations with experimental characterization provides important insights into the mechanism of molecular transport and, additionally, provides quantitative measures of the surface characteristics of the interior of the pores.
- Using Thorium and Uranium to Activate the Carbon-Hydrogen and Carbon-Nitrogen Bonds in Molecules. The extent of electron-sharing in bonds with metals is an important property in catalysis. The correlation of bond covalency with reactivity can be elucidated by determining the reactivity of actinide (thorium, uranium, and other elements in the same row of the periodic table) ions with multiply bonded functional groups. Pyridine N-oxide ($C_5H_5N$-O), which has a relatively stable benzene-like ring, can transfer oxygen atoms to certain transition metals. Chemists have discovered that some uranium and thorium compounds can make C-H bonds in pyridine N-oxide more reactive by forming metal-carbon bonds. The structures of the products produced in these new reactions have been confirmed by x-ray crystallography. These reactions provide examples of C-H and C=N bond activation that is mediated by actinide metals. These studies may offer insights into catalytic removal of nitrogen-containing compounds from petroleum feedstocks, which is necessary to reduce nitrogen oxide emission in fuels.
- Elusive Carbon Dioxide Binding Mode Discovered in New Uranium Complex. Carbon dioxide ($CO_2$) is a stable molecule with two strong carbon-oxygen bonds. Inorganic chemists seek to mimic the catalytic chemical processes by which carbon dioxide is modified by plants to form sugars. This process can remove $CO_2$ from the atmosphere and minimize atmospheric release of $CO_2$ in industrial processes such as refinement of hydrocarbons. A new exquisitely-designed uranium complex has been found to react with $CO_2$ such that one electron is transferred from the $U^{3+}$ center to $CO_2$, producing a species with an unusual linear $CO_2$ that binds to uranium and has one weaker oxygen-carbon bond. Uranium is an essential component of this species because the $U^{3+}$ ion is large, electron-rich, and has the right structure to participate in bonding. This species is unique in that the $CO_2$ remains linear, with one C-O bond longer and weaker than the other. The molecular structure,

bond lengths and oxidation state were established experimentally. The linear M-O-C-O coordination had previously been seen only in an iron enzyme. The new uranium-$CO_2$ complex represents a chemical image of a catalytic process and may make it possible to design new catalysts to reduce the concentration of $CO_2$ in the atmosphere.

- Plutonium is Caged and Illuminated by Synchrotron Light. A new complexant, which was synthesized to extract plutonium and other actinide elements selectively, has shown promise to remove plutonium from mammals. Microscopic crystals (about the thickness of a human hair) of a plutonium complex have been produced to provide a structural model in order to design new actinide-selective binders. Using the Advanced Light Source, researchers determined the detailed structure of these crystals and showed that individual plutonium ions are trapped in cavities produced by eight oxygen atoms from the binder molecules. This structural determination will serve as a model of such complexes on which to base the design of novel molecules that are cages for toxic metals.
- Sheer Energy: Thinner, Cheaper Fuel Cell Catalysts. Fuel cells are a major source of clean energy in the hydrogen economy. Their economic development critically depends on cheaper electrocatalysts for oxygen reduction. The slow nature of this reaction causes a major limit in fuel cell efficiency. High precious metal content is another drawback of existing technology. Researchers coated five cheaper metals with a layer of platinum one atom thick and tested them. For most of the platinum "monolayers," the reaction occurred more slowly than it does on the thicker platinum layer currently used in fuel cells. But adding a monolayer of platinum to the cheaper metal palladium sped up the reaction. Theoretical computations predicted how the platinum monolayers are affected by atoms from the underlying layer of metal. The theory agreed well with the experiments and showed that a platinum monolayer on palladium balances two competing needs: it is reactive enough to break the bonds between oxygen atoms yet does not cling to the oxygen atoms so tightly that it prevents them from reacting with hydrogen. This method can dramatically decrease the expensive metal loading in fuel cells and improve cost and performance.
- Advances in Computational Chemistry Research. Basic research in computational chemistry has resulted in a superior method for the prediction of chemical behavior from computational quantum mechanics and statistical mechanics. The method is based on treating the solvent in which a molecule is placed as a continuum, and determining the cavity-formation energy from statistical mechanics, and the electric contributions from quantum mechanics. This work has now been published and a leading chemical process simulation company has incorporated this method into the most recent release of their industry dominating process simulator. This work will impact modern industrial plant and process design and lead to higher energy efficiencies through effective modeling of manufacturing processes.
- Is $CO_2$ Gone When You Put It In The Ground? There are only two options for dealing with increasing $CO_2$ concentrations in the atmosphere—get rid of new $CO_2$ actively or discontinue producing it and wait for natural processes to remove the excess over a very long time. Both approaches will likely be needed in the future. Researchers have been developing capabilities for realistic modeling of $CO_2$ injection into deep geological formations and for understanding dynamic processes associated with the injection in order to provide a scientific basis for evaluating the injections feasibility. Computational models were developed for coupling fluid properties, chemical and thermodynamic data, and rock-fluid interaction measurements. Reservoir dynamics were investigated on different levels of complexity and scale for natural and engineered systems. These

types of calculations also form the basis for understanding possible leaks which may be major regulatory and insurance concerns for large scale geological $CO_2$ sequestration. The improved computational codes from this project were also used as the basis for design calculations for $CO_2$ injection at the Frio Test Site as part of the Office of Fossil Energy funded Climate Change Technology Program.

- Improving Our Vision of the Subsurface. Large scale subsurface seismic measurements, although adequate for simple oil and gas exploration or waste site characterization, are inadequate for high hydrocarbon recovery rates or more effective environmental remediation or monitoring. Research is providing a better understanding of geophysical measurements of compressional and shear wave velocities, elastic moduli, and seismic anisotropy as they vary as functions of porosity, permeability, fluid contents, and stresses. A fiber-optic "optical" strainmeter has been developed that provides spatially averaged properties over a centimeter or "core" length scale intermediate between point measurements and a meter-scale bulk-measurements. The increased accuracy and sensitivity in measuring elastic deformation during applied sinusoidal stress will enable better discrimination between strain (elastic wave transmission efficiency) and phase lags (attenuation indicative of fluid content and type). In addition, the highly precise optical strain gage measurements will allow higher resolution testing of the significance of different types of heterogeneity at the core scale, in order to enable prediction of these properties at larger scales. The fiber optic sensor has been demonstrated to have a significantly higher sensitivity than other strain gages.
- The Auxin Receptor: A Holy Grail in Plant Science. The plant growth hormone called auxin is a small molecule, indole acetic acid (IAA)—too small to have the expected breadth of "informational" content to achieve its myriad effects of controlling the growth of leaves, stems, roots, flowers, fruits, and growth changes in response to light and gravity. Recent research demonstrated that IAA interacts directly with a much larger molecule, a protein, which was earlier shown to affect plant growth by stimulating the expression (activation) of certain growth-related genes. Now the solution to the mystery of auxin action is becoming clear. It turns out to be similar to an electric switch, but a bit more complex. We are beginning to unravel the molecular details of auxin's biological activity.

## Detailed Program Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Chemical Sciences, Geosciences, and Energy Biosciences Research** | **225,928** | **208,831** | **255,113** |
| ▪ **Atomic, Molecular, and Optical (AMO) Science** | **16,627** | **15,397** | **19,248** |

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; the 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

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

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 micro-characterization centers, and neutron scattering facilities. Furthermore, by studying energy transfer within isolated molecules, AMO science provides the very 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 2007, 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; 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 coherent control of quantum systems ($+851,000), ultrafast science ($+2,000,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Chemical Physics Research** ........................................................ | **32,946** | **31,866** | **37,813** |

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.

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 significantly 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

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

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 is 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.

The SciDAC computational chemistry program addresses two fundamental research efforts: (1) chemically reacting flows and (2) the chemistry of unstable species and large molecules. Each of these research efforts is carried out by a team of related scientists working with the appropriate Integrated Software Infrastructure Centers supported under SciDAC by the SC Advanced Scientific Computing Research program.

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

In FY 2007, 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 condensed phase and interfacial molecular science ($+1,000,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,697,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Photochemistry and Radiation Research**................................ | **30,446** | **25,489** | **32,007** |

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 Laboratory, 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

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|

(dollars in thousands)

charge separation in molecule-based biomimetic assemblies should also be applicable in the future development of molecular optoelectronic devices. A strong interface with the Office of Energy Efficiency and Renewable Energy (EE) solar conversion programs exists at National Renewable Energy Laboratory (NREL), involving shared research, analytical and fabrication facilities, and involving a jointly shared project on dye-sensitized solar cells.

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, nuclear energy production, and medical diagnosis and radiation therapy.

This activity is the dominant supporter (85%) of solar photochemistry in the U.S., and the sole supporter of radiation chemistry.

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 2007, 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 ultrafast science ($+1,000,000), solar energy conversion ($+3,909,000), and research related to the hydrogen economy ($+1,609,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Molecular Mechanisms of Natural Solar Energy Conversion** ........................................ | **13,640** | **12,411** | **18,188** |

This activity supports fundamental research at the interface between the biological and physical sciences to characterize the molecular and chemical mechanisms involved in the conversion of solar energy to stored chemical energy. Research supported includes the characterization of the chemical processes occurring during photosynthesis, the kinetic and catalytic mechanisms of enzymes involved in the synthesis chemical fuels, and the biochemical mechanisms involved in the fixation of carbon dioxide. The approaches used include biophysical, biochemical, and molecular structure/function analyses. The goal is to enable the future biotechnological exploitation of both natural and synthetic systems and to provide insights and strategies into the design of non-biological and hybrid processes. This activity encourages fundamental research that employs novel approaches that integrate biological sciences with physical sciences in order to understand the molecular details of energy conversion by natural systems.

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

In FY 2007, 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.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

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 for biophysical characterization of biomolecular complexes ($+500,000), chemical imaging ($+750,000), emergent behavior ($+500,000) solar energy conversion ($+3,909,000), and research related to the hydrogen economy ($+118,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Metabolic Regulation of Energy Production** ........................ | **19,427** | **17,554** | **17,601** |

This activity supports fundamental research in the molecular processes that constitute and regulate metabolic pathways that are involved in cellular chemical conversions of importance to energy. Understanding the molecular mechanisms of chemical transformations and the control of chemical transformation pathways in living systems, such as plants, provides the basis for modifying biological processes and designing bioinspired, synthetic systems for applications in energy technologies. The research goal is to develop a predictive and experimental context for the manipulation of metabolism to accumulate a desired product and to design and synthesize robust bioinspired and biomimetic systems, including hybrid systems that achieve desired chemical transformations with high efficiency and specificity. Research supported includes the molecular characterization of metabolic pathways and the signaling pathways that enhance or limit their activity in living systems, and structure/function studies of key biomolecular components, signal transducers, molecular machines, 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 chemical catalysis in living systems and provides the basis for manipulation of biological chemistry and the development of bioinspired and biomimetic systems for specific chemical transformations.

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

In FY 2007, increased emphasis will be placed upon understanding interactions that occur within the nanoscale range; this includes signal reception at biological surfaces and membranes, enzyme-substrate recognition, and the structure/function of molecular complexes and molecular machines that enable and control chemical transformations. An emerging area will be the development of new imaging tools and methods to examine metabolic and signaling pathways at both the physical-spatial and temporal scale. Within this funding, there is an increase for research related to the hydrogen economy ($+47,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Catalysis and Chemical Transformation** ................................ | **37,871** | **38,107** | **47,459** |

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

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

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 which 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.

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 2007, 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 ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), solar energy conversion ($+3,659,000), and research related to the hydrogen economy ($+3,443,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Separations and Analyses** | **15,490** | **17,287** | **24,041** |

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 2007, 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) will allow multiple analytical measurements to be 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 molecular science for advanced chemical separations ($+1,000,000), chemical imaging ($+1,750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), research related to the hydrogen economy ($+808,000), and solar energy conversion ($+1,696,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Heavy Element Chemistry** ........................................................ | **10,506** | **9,354** | **17,128** |

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

| | (dollars in thousands) | | |
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| | FY 2005 | FY 2006 | FY 2007 |

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 products 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 in order 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 2007, 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 advanced fuel cycles for future nuclear energy needs. 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 mid-scale instrumentation ($+500,000) and research related to advanced fuel cycles ($+7,274,000).

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| ▪ **Geosciences Research** ................................................................ | **22,212** | **20,494** | **22,345** |

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.

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.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

In FY 2007, funding will continue to provide the majority of individual investigator basic research funding 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 quality portfolios. Within this funding, there are increases for nanoscale geochemistry ($+851,000), chemical imaging ($+500,000) and mid-scale instrumentation ($+500,000).

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| ▪ **Chemical Energy and Chemical Engineering** ........................ | **11,938** | **3,731** | **1,817** |

This activity supports research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes. Also included is fundamental research in areas critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems including anode, cathode, and electrolyte systems and their interactions with emphasis on improvements in performance and lifetime. The program covers a broad spectrum of research including fundamental studies of composite electrode structures; failure and degradation of active electrode materials; thin film electrodes, electrolytes, and interfaces; and experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena.

Capital equipment is provided for such items as computer work stations and electrochemical apparatus.

In FY 2007, in order to emphasize other priorities, there will be reductions in research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research.

| | | | |
|---|---|---|---|
| ▪ **General Plant Projects (GPP)** .................................................. | **9,832** | **13,124** | **13,408** |

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 Biosciences subprogram. The total estimated cost of each GPP project will not exceed $5,000,000.

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|---|---|---|---|
| ▪ **General Purpose Equipment (GPE)**........................................ | **4,993** | **4,017** | **4,058** |

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.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Facility Operations** | **6,437** | **6,251** | **6,805** |

The facility operations budget request, which includes operating funds, capital equipment, and GPP, 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 | 6,437 | 6,251 | 6,805 |

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **—** | **5,468** | **6,581** |

In FY 2005 $5,213,000 and $626,000 were transferred to the SBIR and STTR programs, respectively. The FY 2006 and FY 2007 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

| | | | |
|---|---|---|---|
| **Total, Chemical Sciences, Geosciences, and Energy Biosciences** | **232,365** | **220,550** | **268,499** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Chemical Sciences, Geosciences, and Energy Biosciences Research** | |
| ▪ **Atomic, Molecular, and Optical (AMO) Science** | |
| Increases are provided for coherent control of quantum systems ($+851,000), ultrafast science ($+2,000,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000) | +3,851 |
| ▪ **Chemical Physics Research** | |
| Increases are provided for condensed phase and interfacial molecular science ($+1,000,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,697,000). | +5,947 |
| ▪ **Photochemistry and Radiation Research** | |
| Increases are provided for research related to the hydrogen economy ($+1,609,000), ultrafast science ($+1,000,000), and solar energy conversion ($+3,909,000) | +6,518 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Molecular Mechanisms of Natural Solar Energy Conversion** | |
| Increases are provided for biophysical characterization of biomolecular complexes ($+500,000), research related to the hydrogen economy ($+118,000), chemical imaging ($+750,000), emergent behavior ($+500,000), and solar energy conversion ($+3,909,000). | +5,777 |
| ▪ **Metabolic Regulation of Energy Production** | |
| Increase is provided for research related to the hydrogen economy | +47 |
| ▪ **Catalysis and Chemical Transformation** | |
| Increases are provided for research related to the hydrogen economy ($+3,443,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), and solar energy conversion ($+3,659,000) | +9,352 |
| ▪ **Separations and Analyses** | |
| Increases are provided for molecular science for advanced chemical separation ($+1,000,000), research related to the hydrogen economy ($+808,000), chemical imaging ($+1,750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,696,000). | +6,754 |
| ▪ **Heavy Element Chemistry** | |
| Increases are provided for mid-scale instrumentation ($+500,000) and research relevant to advanced fuel cycles ($+7,274,000) | +7,774 |
| ▪ **Geosciences Research** | |
| Increases are provided for nanoscale geochemistry ($+851,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000) | +1,851 |
| ▪ **Chemical Energy and Chemical Engineering** | |
| Reductions in research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research | -1,914 |
| ▪ **General Plant Projects (GPP)** | |
| Increase in general plant projects intended to help alleviate recurring maintenance costs by improving infrastructure. | +284 |
| ▪ **General Purpose Equipment (GPE)** | |
| Small increase for GPE maintenance of equipment | +41 |
| **Total, Chemical Sciences, Geosciences and Energy Biosciences Research** | **+46,282** |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Facility Operations** | |
| Increase for the Combustion Research Facility to support operations | +554 |
| **SBIR/STTR** | |
| Increase in SBIR/STTR funding because of an increase in operating expenses. | +1,113 |
| **Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences** | **+47,949** |

## Construction

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Construction | | | |
| Spallation Neutron Source (ORNL) | 79,891 | 41,327 | — |
| Project Engineering Design, Nanoscale Science Research Centers | 1,996 | — | — |
| Project Engineering Design, Linac Coherent Light Source (SLAC) | 19,914 | 2,518 | 161 |
| Linac Coherent Light Source (SLAC) | 29,760 | 82,170 | 105,740 |
| Center for Functional Nanomaterials (BNL) | 18,317 | 36,187 | 18,864 |
| The Molecular Foundry (LBNL) | 31,828 | 9,510 | 257 |
| Center for Nanophase Materials Science (ORNL) | 17,669 | — | — |
| Center for Integrated Nanotechnologies (SNL/LANL) | 30,650 | 4,580 | 247 |
| Project Engineering Design, National Synchrotron Light Source-II (BNL) | — | — | 20,000 |
| Project Engineering Design, Advanced Light Source User Support Building (LBNL) | — | — | 3,000 |
| Total, Construction | 230,025 | 176,292 | 148,269 |

### Description

Construction is needed to support the research in each of the subprograms in the BES program. Experiments necessary in support of basic research require that state-of-the-art facilities be built or existing facilities modified to meet unique research requirements. Reactors, x-ray light sources, and 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 under construction—the Linac Coherent Light Source, the Center for Functional Nanomaterials, design of 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 in order 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 2005 | FY 2006 | FY 2007 |
| ▪ **Spallation Neutron Source (SNS), ORNL** | **79,891** | **41,327** | **—** |

The purpose of the SNS Project is to provide a next-generation short-pulse spallation neutron source for neutron scattering. The SNS will be used by researchers from academia, national and federal labs, and industry for basic and applied research and for technology development in the fields of condensed matter physics, materials sciences, magnetic materials, polymers and complex fluids, chemistry, biology, earth sciences, and engineering. When commissioning is complete, the SNS will be significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence. The facility will be used by 1,000–2,000 scientists and engineers annually. Interest in the scientific community in the SNS is increasing.

The SNS consists of a linac-ring accelerator system that delivers short (microsecond) proton pulses to a target/moderator system where neutrons are produced by a process called spallation. The neutrons so produced are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations. There will initially be one partially instrumented target station with the potential for adding more instruments and a second target station later.

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.

In FY 2001, two grants were awarded to universities for research requiring the design, fabrication, and installation of instruments for neutron scattering. These instruments will be sited at the SNS, with commissioning beginning late in FY 2006, shortly after the SNS facility itself is commissioned. Both awards were made based on competitive peer review conducted under 10 CFR Part 605, Financial Assistance Program.

Funds appropriated in FY 2002 continued R&D, design, procurement, construction activities, and component installation. Essentially all R&D supporting construction of the SNS was completed, with instrument R&D continuing. Title II design was completed on the linac and was continued on the ring, target, and instrument systems. The completed ion source and portions of the drift tube linac were delivered to the site and their installation was begun. Other system components for the accelerator, ring, target, and instruments continued to be manufactured. Work on conventional facilities continued, with some reaching completion and being turned over for equipment installation, such as the ion source building and portions of the klystron building and linac tunnel. Construction work began on the ring tunnel.

Funds appropriated in FY 2003 continued instrument R&D and design, procurement, construction, installation, and commissioning. The ion source was commissioned; the drift tube linac was installed and commissioning was begun; installation of other linac components progressed; and installation of ring components began. Target building construction and equipment installation continued.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

Numerous conventional facilities, including the klystron, central utilities, and ring service buildings and the linac and ring tunnels, were advanced. Site utilities became available to support linac commissioning. In FY 2003, a Major Item of Equipment (MIE) was initiated for five SNS instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Beam Spectrometer. The MIE is funded at $3,143,000 in FY 2005, $12,579,000 in FY 2006, and $10,500,000 in FY 2007. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories in collaboration with the SNS based on scientific merit and importance to users from universities, industries, and government laboratories. A second Major Item of Equipment is initiated in FY 2007 for an additional four to five instruments.

Funds appropriated in 2004 continued instrument R&D, design, and procurement. The drift-tube linac and cavity-coupled linac portions of the warm linac commissioning were completed. Other commissioning activities continued in the linac. Cryogenic refrigerator installation and system cool down were advanced. High-energy beam transport installation and testing were completed. Ring fabrication and assembly activities continued. Target fabrication and assembly activities continued. Most SNS buildings are completed with the exception of ongoing construction work in the target and instrument facilities and the central laboratory and office building.

Funds appropriated in FY 2005 continued R&D, procurement, and installation of equipment for instrument systems. Commissioning of Linac Systems was completed. Commissioning of the high-energy beam transport and accumulator ring was begun; installation and testing for the ring-target beam transport system was performed. Installation and testing was performed and preparation for the readiness review was started for target systems. The remaining major construction contracts were completed. Procurement, installation, and testing continued for integrated control systems.

Funds appropriated in FY 2006 will complete the SNS Project. Procurement and installation of equipment for instrument systems will be performed. An accelerator readiness review will be completed and target systems will be commissioned. All requirements to begin operations will be met and all SNS facilities will be turned over to operations. The estimated Total Project Cost is $1,411,282,560, and the construction schedule continues to call for project completion by mid-2006.

| | | | |
|---|---|---|---|
| ▪ **Project Engineering and Design, Nanoscale Science Research Centers** ........ | **1,996** | **—** | **—** |

Project Engineering and Design funds provide Title I and Title II design-only funding for Nanoscale Science Research Centers (NSRCs) at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Sandia National Laboratories (Albuquerque), and Brookhaven National Laboratory. These funds were used to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. NSRCs provide state-of-the-art facilities for materials nanofabrication and advanced tools for nanocharacterization to the scientific community.

| | | | |
|---|---|---|---|
| ▪ **Project Engineering and Design, Linac Coherent Light Source, SLAC** ........ | **19,914** | **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 nanosctructured materials, at atomic or near-atomic resolution. These are only a few examples of breakthrough science that will be enabled by LCLS, planned to be the world's first "fourth generation" x-ray light source.

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.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

Funds were appropriated in FY 2006 and are requested in FY 2007 for Project Engineering Design (PED) Title I and Title II design work. Additional information on the LCLS Project is provided in the LCLS PED data sheet, project number 03-SC-002.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Linac Coherent Light Source, SLAC** ...................................... | **29,760** | **82,170** | **105,740** |

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 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 will support physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Central Laboratory and Office Building. In addition, the injector will be completed and construction of the downstream linac and electron beam transport to the undulator hall will begin. Undulator module assembly will be started along with construction of x-ray transport/optics/diagnostics systems.

FY 2007 budget authority is requested to continue physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Central Laboratory and Office (CLO) building.

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

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, BNL**............................................... | **18,317** | **36,187** | **18,864** |

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 funding is requested to 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 data sheet. Additional information is provided in the construction project data sheet 05-R-321.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL** | **31,828** | **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 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 data sheet. Additional information is provided in the construction project data sheet 04-R-313.

| | | | |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL** | **17,669** | **—** | **—** |

The Center for Nanophase Materials Sciences (CNMS), a BES Nanoscale Science Research Center, will include a research center and user facility that will integrate nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation. A new building will provide state-of-the-art clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be equipment to synthesize, manipulate, and characterize nanoscale materials and structures. The Center, collocated at the Spallation Neutron Source complex, will have as its major scientific thrusts nano-dimensioned soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. A major focus of the CNMS will be to exploit ORNL's unique facilities and capabilities in neutron scattering.

FY 2004 and FY 2005 funding was requested for the construction of the Center for Nanophase Materials Science located at Oak Ridge National Laboratory. Performance was measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet.

| | | | |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, SNL/LANL** | **30,650** | **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

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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 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 data sheet. Additional information is provided in the construction project data sheet 03-R-313.

| | | | |
|---|---|---|---|
| ▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS-II), BNL** | **—** | **—** | **20,000** |

The NSLS-II would be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of 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 will be the best storage-ring-based synchrotron light source in the world, but, more importantly, NSLS-II will be transformational in that it will open new regimes of scientific discovery and investigation.

FY 2007 funding is requested to begin Project Engineering and Design (PED) Title I and Title II design. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 07-SC-06.

| | | | |
|---|---|---|---|
| ▪ **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 is requested to begin Project Engineering and Design. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 07-SC-12.

| | | | |
|---|---|---|---|
| **Total, Construction** | **230,025** | **176,292** | **148,269** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Spallation Neutron Source, ORNL** | |
| Decrease in funding for construction of the Spallation Neutron Source at ORNL, representing the scheduled completion of the project. | -41,327 |
| ▪ **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 the scheduled decrease in activities. | -2,357 |
| ▪ **Linac Coherent Light Source, SLAC** | |
| Increase in funding to continue construction for the LCLS project. | +23,570 |
| ▪ **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. | -17,323 |
| ▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL** | |
| Decrease in funding for construction of the Molecular Foundry at LBNL, representing the scheduled ramp down of activities. | -9,253 |
| ▪ **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 scheduled ramp down of activities. | -4,333 |
| ▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS II), BNL** | |
| Increase in funding to initiate Project Engineering and Design | +20,000 |
| ▪ **Project Engineering and Design, Advanced Light Source (ALS) User Support Building, LBNL** | |
| Increase in funding to initiate Project Engineering and Design | +3,000 |
| **Total Funding Change, Construction** | **-28,023** |

# 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 2005 | FY 2006 | FY 2007 |
| Major User Facilities | | | |
| Advanced Light Source at Lawrence Berkeley National Laboratory. | 44,800 | 42,783 | 49,802 |
| Advanced Photon Source at Argonne National Laboratory | 100,500 | 95,890 | 108,604 |
| National Synchrotron Light Source at Brookhaven National Laboratory | 36,750 | 36,196 | 40,763 |
| Center for Nanophase Materials Sciences at Oak Ridge National Laboratory | — | 17,800 | 19,190 |
| Center for Integrated Nanotechnologies at Sandia National Laboratories/Albuquerque and Los Alamos National Laboratory | — | 11,900 | 19,190 |
| Molecular Foundry at Lawrence Berkeley National Laboratory | — | 8,100 | 19,190 |
| Center for Nanoscale Materials at Argonne National Laboratory | — | 3,500 | 19,190 |
| Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center. | 32,388 | 25,475 | 35,836 |
| High Flux Isotope Reactor at Oak Ridge National Laboratory. | 46,900 | 43,330 | 51,598 |
| Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory. | 4,500 | — | — |
| Intense Pulsed Neutron Source at Argonne National Laboratory. | 16,800 | 15,500 | 18,531 |
| Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory. | 9,588 | 10,000 | 10,582 |
| Spallation Neutron Source at Oak Ridge National Laboratory. | 37,600 | 101,001 | 171,409 |
| Combustion Research Facility at Sandia National Laboratories/California. | 6,437 | 6,251 | 6,805 |
| National Synchrotron Light Source-II at Brookhaven National Laboratory | 1,000 | — | 25,000 |
| Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center | — | 3,500 | 16,000 |
| Linac for LCLS | — | 29,700 | 40,000 |
| Total, Major User Facilities | 337,263 | 450,926 | 651,690 |

### 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 2005 | FY 2006 | FY 2007 |
| General Plant Projects | 16,532 | 13,695 | 15,624 |
| Accelerator Improvement Projects | 10,245 | 8,032 | 25,112 |
| Capital Equipment | 86,639 | 69,123 | 131,657 |
| Total, Capital Operating Expenses | 113,416 | 90,850 | 172,393 |

## Construction Projects

(dollars in thousands)

| | Total Estimated Cost (TEC) | Prior Year Appro-priations | FY 2005 | FY 2006 | FY 2007 | Unappro-priated Balances |
|---|---|---|---|---|---|---|
| 07-SC-06, PED, BNL, National Synchrotron Light Source-II | 75,000 | — | — | — | 20,000 | 55,000 |
| 07-SC-12, PED, LBNL, Advanced Light Source User Support Building | 3,000 | — | — | — | 3,000 | — |
| 05-R-320, SLAC, Linac Coherent Light Source | 315,000[a] | — | 29,760 | 82,170 | 105,740 | 61,356 |
| 05-R-321, BNL, Center for Functional Nanomaterials | 79,700[b] | — | 18,317 | 36,187 | 18,864 | 366 |
| 04-R-313, LBNL, The Molecular Foundry | 83,604[c] | 34,794 | 31,828 | 9,510 | 257 | — |
| 03-SC-002, PED, SLAC, Linac Coherent Light Source | 35,974 | 13,381 | 19,914 | 2,518 | 161 | — |
| 03-R-312, ORNL, Center for Nanophase Materials Sciences | 63,740[d] | 43,583 | 17,669 | — | — | — |
| 03-R-313, SNL, Center for Integrated Nanotechnologies | 73,754[e] | 34,118 | 30,650 | 4,580 | 247 | — |
| 02-SC-002 PED, Nanoscale Science Research Centers | 19,828 | 17,832 | 1,996 | — | — | — |
| 99-E-334, ORNL, Spallation Neutron Source | 1,192,283 | 1,071,065 | 79,891 | 41,327 | — | — |
| Total, Construction | | | 230,025 | 176,292 | 148,269 | |

[a] Includes $35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source datasheet.
[b] Includes $5,966,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[c] Includes $7,215,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[d] Includes $2,488,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[e] Includes $4,159,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

## **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 2005 | FY 2006 | FY 2007 | Completion Date |
|---|---|---|---|---|---|---|---|
| ANL, Center for Nanoscale Materials....... | 72,500[a] | 36,000 | 10,000 | 12,000 | 14,000 | — | FY 2006 |
| ORNL, Spallation Neutron Source Instrumentation I[b] .......... | 68,500 | 68,500 | 13,022 | 3,143 | 12,579 | 10,500 | FY 2007–FY 2011 est. |
| LBNL, Transmission Electron Aberration Corrected Microscope.... | 25,000–30,000 | 11,200–13,500 | — | — | 2,000 | 3,500 | TBD |
| ORNL, Spallation Neutron Source Instrumentation II .......... | 40,000–60,000 | 40,000–60,000 | — | — | — | 10,000 | TBD |
| SLAC, Linac Coherent Light Source Instumentation ............... | 50,000–60,000 | 50,000–60,000 | — | — | — | 10,000 | TBD |
| Total, Major Items of Equipment ................. | | | 23,022 | 15,143 | 28,579 | 34,000 | |

[a] This includes $36,000,000 provided by the State of Illinois for construction of the building.
[b] This FY 2003 MIE includes five instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Beam Spectrometer.