Basic Energy Sciences

Funding Profile by Subprogram

(dollars in thousands)

	FY 2004 Comparable Appropriation	FY 2005 Original Appropriation	FY 2005 Adjustments	FY 2005 Comparable Appropriation	FY 2006 Request
Basic Energy Sciences					
Research					
Materials Sciences and Engineering	558,831	628,228	+6,904[ab]	635,132	746,143
Chemical Sciences, Geosciences, and Energy Biosciences	213,778	253,422	-13,947[ab]	239,475	221,801
Total, Research	772,609	881,650	-7,043	874,607	967,944
Construction	218,653	231,880	-1,855[a]	230,025	178,073
Total, Basic Energy Sciences	991,262[c]	1,113,530	-8,898	1,104,632	1,146,017

Public Law Authorizations:
Public Law 95-91, "Department of Energy Organization Act, 1977"
Public Law 103-62, "Government Performance and Results Act of 1993"

Mission

The mission of the Basic Energy Sciences (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, and safety of energy generation, conversion, transmission, and use. For example, research on toughened

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[a] Includes a reduction of $8,898,000 for a rescission in accordance with P.L. 108-447, the Consolidated Appropriations Act, 2005, as follows: Materials Sciences and Engineering ($-5,019,000); Chemical Science, Geosciences and Energy Biosciences ($-2,024,000); and Construction ($-1,855,000).
[b] Includes a reallocation of funding within BES in accordance with H. Rpt. 108-792, accompanying P.L. 108-447, as follows: Materials Sciences and Engineering ($+11,923,000) and Chemical Science, Geosciences and Energy Biosciences ($-11,923,000) to optimize funding for research and facility operations within the BES program.
[c] Includes reductions of $5,984,000 rescinded in accordance with P.L. 108-137, the Consolidated Appropriations Act, 2004, $17,258,000, which was transferred to the SBIR program, and $2,071,000, which was transferred to the STTR program.

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 plant growth aids the development of renewable biomass resources and solar photoenergy 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.

Key scientific emphases of these subprograms will lead the coming revolutions in: science of the ultrasmall (the nanometer length scale); science of the ultrafast (the femtosecond time scale); and science of complex systems (systems whose properties cannot be described by the properties of their individual components, e.g., high-temperature superconductivity and coupled chemical reactions). Advances in these three areas will deliver the foundations and discoveries for a future built around controlled chemical processes and materials designed one atom at a time. Focus areas necessary to achieve this goal involve research programs of individual investigators and groups of investigators; the development of advanced tools and instruments for x-ray, neutron, and electron diffraction, scattering, and imaging; the development of other advanced probes of matter, e.g. using high electric or magnetic fields; and theory, modeling, and simulation using high-end computing. 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 instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with 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 microcharacterization centers reveal the atomic details of metals and alloys; glasses and ceramics; semiconductors and superconductors; polymers and biomaterials; proteins and enzymes; catalysts, 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 five 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.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Results	FY 2003 Results	FY 2004 Results	FY 2005 Targets	FY 2006 Targets
Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence					
Materials Sciences and Engineering					
N/A	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: Demonstrate first 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.	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 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: Demonstrate first 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).	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	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]	Improve Simulation: As a part of the SciDAC program, perform a three-dimensional combustion reacting flow simulation involving more than 10 reacting species and 0.2 billion grid points.	Improve Simulation: Perform a three-dimensional combustion reacting flow simulation involving more than 30 reacting species and 20 million grid points.
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. [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]*	*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 improvement is expected in FY 2006 as compared to the level of achievement for FY 2005. That is due to the performance levels for resolution (temporal and spatial) has 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 become available.

FY 2001 Results	FY 2002 Results	FY 2003 Results	FY 2004 Results	FY 2005 Targets	FY 2006 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. [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]*	*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 (NAS); (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, 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 into the FY 2005 and FY 2006 Budget Request 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 2006. 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 (www.sc.doe.gov/measures.htm) 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.

Funding by General and Program Goal

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
General Goal 5, World-Class Scientific Research Capacity			
Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence			
Materials Sciences and Engineering	558,831	635,132	746,143
Chemical Sciences, Geosciences and Energy Biosciences	213,778	239,475	221,801
Construction	218,653	230,025	178,073
Total, General Goal 5, World-Class Scientific Research Capacity	991,262	1,104,632	1,146,017

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 2004, the program funded research in more than 175 academic institutions located in 49 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 microbatteries;
- thermoacoustic refrigeration devices that cool without moving parts and without the use of freons;
- compound semiconductors, leading to the world's highest efficiency photovoltaic solar cells;
- catalysts for the production of new polymers (annually, a multibillion dollar industry) and for a host of other products and energy-efficient processes;
- high-strength, lightweight magnets for sensors and for small motors used in power steering and other vehicle functions;
- strong, ductile alloys for use in high-temperature applications;
- nonbrittle ceramics for use in hammers, high-speed cutting tools, engine turbines, and other applications requiring lightweight and/or high-temperature materials;
- new steels, improved aluminum alloys, magnet materials, and other alloys;
- polymer materials for rechargeable batteries, car bumpers, food wrappings, flat-panel displays, wear-resistant plastic parts, and polymer-coated particles in lubricating oils;
- processes for extraction of radioactive and hazardous metal ions from solutions for nuclear fuel purification/reprocessing and for cleanup of radioactive wastes; and
- a host of new instruments, e.g., instruments based on high-temperature superconductors that can sense the minute magnetic fields that emanate from the human brain and heart.

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.

The new millennium will take us deep into this world of complex nanostructures. Here, simple structures interact to create new phenomena, and large complicated structures can be designed atom by atom for desired characteristics. We will design new tiny objects "from scratch" that have unprecedented optical, mechanical, electrical, or chemical properties that address the needs of human society.

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), 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. During the past eight years, BESAC subcommittees have reviewed the synchrotron radiation light sources, the neutron scattering facilities, and the electron-beam microcharacterization 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/SC-80/sc-81/docs.html#DOE). 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 (2004). This COV review cycle will begin 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.

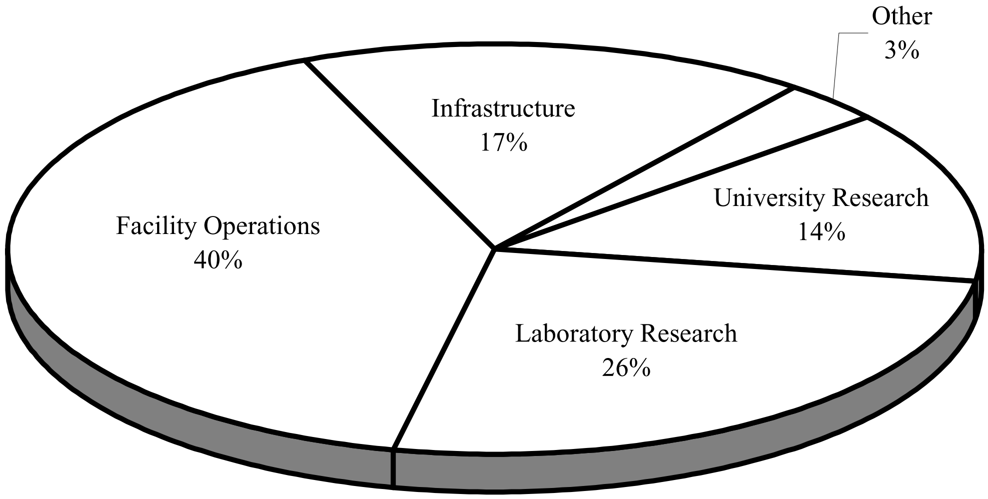
Inputs to our prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, these considerations have led to: increased investments in science at the nanoscale to take advantage of 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., catalysis) 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 to existing facilities such as the High Flux Isotope Reactor or the Stanford Synchrotron Radiation Laboratory 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 2006 budget request continues priorities established in the past few years. Construction of the Spallation Neutron Source will be completed in accord with the established baseline. A significant investment in the area of nanoscale science includes construction and operations funding for four new Nanoscale Science Research Centers at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, the combination of Sandia National Laboratories and Los Alamos National Laboratory, and Brookhaven National Laboratory. Finally, continued support for a Major Item of Equipment (MIE) is requested for the fifth and final Nanoscale Science Research Center at Argonne National Laboratory. That Center is being built in partnership with the State of Illinois, which provided $36,000,000 in FY 2003 and FY 2004 for the construction of the building. BES funding will provide clean rooms, instrumentation, and ultimately operations support for the Center. Project Engineering Design and Construction funding also are provided for the Linac Coherent Light Source (LCLS), a 4th generation light source that will provide orders of magnitude higher intensities of 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.

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 remain significant budget components in FY 2006, including the Spallation Neutron Source, the Nanoscale Science Research Centers, and the Linac Coherent Light Source.

Basic Energy Sciences Budget Allocation
FY 2006



Research

The BES program is one of the Nation's largest supporters of fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences. 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, that 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 2006, there are a number of significant program milestones and increases, including the following:

- Construction of the Spallation Neutron Source will be completed, and the facility will begin operation at the planned funding level.
- All five Nanoscale Science Research Centers are nearing completion; four of them will begin operation in FY 2006. The Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Molecular Foundry at Lawrence Berkeley National Laboratory, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory all will begin operation at the planned funding levels. In addition, the Center for Nanoscale Materials at Argonne National Laboratory will begin limited operation following the completion of its building (funded by the State of Illinois) and prior to the completion of the BES-funded Major Item of Equipment, which provides the instrumentation for that Center.
- The Linac Coherent Light Source will continue Project Engineering Design (PED) and will begin construction at the planned levels. Funding is provided separately for preconceptual design of instruments for the facility. Funding is also provided to partially support operation of the SLAC linac. This marks the beginning of the transition to LCLS operations at SLAC.
- The Transmission Electron Aberration Corrected Microscope project is initiated as a Major Item of Equipment.
- Research to realize the potential of a hydrogen economy will be increased from $29,183,000 to $32,500,000. The research program is based on the BES workshop report "Basic Research Needs for the Hydrogen Economy."

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

In order to accomplish these very high-priority, forefront activities, some difficult choices had to be made. In particular, the BES support for the Radiochemical Engineering and Development Center at Oak Ridge National Laboratory is terminated. The operations budgets of the remaining facilities are funded at about the same level as in FY 2005, which will decrease the available beam time and service to users. Finally, research activities are funded at a level approximately 3% less than in FY 2005; while no research activities are terminated, there are reductions throughout.

Nanoscience and Nanoscale Science Research Centers (NSRCs) are user facilities for the synthesis, processing, fabrication, and analysis of materials at the nanoscale. They are designed to enable the nanoscale revolution by collocating multiple research disciplines, multiple techniques, and a wide variety of state-of-the-art instrumentation in a single building. The NSRCs are designed to promote rapid advances in the various areas of nanoscale science and technology.

NSRCs are sited adjacent to or near an existing BES synchrotron or neutron scattering facility to enable rapid characterization of newly fabricated materials. Contained within NSRCs will be clean rooms; chemistry, physics, and biology laboratories for nanofabrication; and one-of-a-kind signature instruments and other instruments, e.g., nanowriters and various research-grade probe microscopies, not generally available outside of major user facilities. NSRCs will serve the Nation's researchers broadly and, as with the existing BES facilities, access to NSRCs will be through submission of proposals that will be reviewed by mechanisms established by the facilities themselves.

NSRCs were conceived in FY 1999 within the context of the NSTC Interagency Working Group on Nanoscale Science, Engineering, and Technology as part of the DOE contribution to the National Nanotechnology Initiative. Planning for the NSRCs has included substantial participation by the research community through a series of widely advertised and heavily attended workshops attracting a total of about 2,000 researchers.

As was described in the recent National Research Council report “Small Wonders, Endless Frontiers – A Review of the National Nanotechnology Initiative,” new processes that couple top-down and bottom-up assembly techniques “will allow the fabrication of highly integrated two- and three-dimensional devices and structures to form diverse molecular and nanoscale components. They would allow many of the new and promising nanostructures, such as carbon nanotubes, organic molecular electronic components, and quantum dots, to be rapidly assembled into more complex circuitry to form useful logic and memory devices. Such new devices would have computational performance characteristics and data storage capacities many orders of magnitude higher than present devices and would come in even smaller packages. Nanomaterials and their performance properties will also continue to improve. Thus, even better and cheaper nanopowders, nanoparticles, and nanocomposites should be available for more widespread applications. Another important application for future nanomaterials will be as highly selective and efficient catalysts for chemical and energy conversion processes. This will be important economically not only for energy and chemical production but also for conservation and environmental applications. Thus, nanomaterial-based catalysis may play an important role in photoconversion devices, fuel cell devices, bioconversion (energy) and bioprocessing (food and agriculture) systems, and waste and pollution control systems.”

The following table summarizes the BES investments in research at the nanoscale.

Nanoscale Science Research Funding

	(dollars in thousands)				
	TEC	TPC	FY 2004	FY 2005	FY 2006
Research					
Materials Sciences and Engineering			73,501	66,995	112,632
Chemical Sciences, Geosciences, and Biosciences			27,833	28,360	26,914
Capital Equipment					
Major Item of Equipment — ANL, Center for Nanoscale Materials			10,000	12,000	14,000
Nanoscale Science Research Centers					
PED – All sites			2,982	1,996	0
Construction					
BNL, Center for Functional Nanomaterials	79,700	81,000	0	18,317	36,553
LBNL, Molecular Foundry	83,700	85,000	34,794	31,828	9,606
ORNL, Center for Nanophase Materials Sciences	63,740	64,740	19,882	17,669	0
SNL/A and LANL, Center for Integrated Nanotechnologies	73,800	75,800	29,674	30,650	4,626
Total, BES Nanoscale Science Funding			198,666	207,815	204,331

Basic Research in Support of the Hydrogen Economy. In FY 2006, $32,500,000 is requested for 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 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. A total of $21,473,000 in new funding will be awarded as a result of this solicitation. 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, which will be peer reviewed according to the guidelines in 10 CFR 605. Awards will be 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.

President's Hydrogen Initiative

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
Materials Sciences and Engineering Research	3,055	14,761	16,600
Chemical Sciences, Geosciences, and Biosciences	4,655	14,422	15,900
Total Hydrogen Initiative	7,710	29,183	32,500

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. The funding level for operation of the light sources, the Intense Pulse Neutron Source, and the High-Flux Isotope Reactor will be approximately equal to that in FY 2005; without cost of living increases, the level of operations will be about ten percent less than that in FY 2005. The reduction in funding from FY 2005 to FY 2006 for some of these facilities is a result of one-time increases in FY 2005 for capital equipment or other special needs such as fuel and maintenance at the High Flux Isotope Reactor. 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 2004 Actual[a]	FY 2005 Estimate	FY 2006 Estimate
All Facilities			
Optimal Hours[b]	36,800	29,800	32,200
Scheduled Hours	28,004	29,800	28,800
Unscheduled Downtime	8%	<10%	<10%
Number of Users	8,545	8,680	7,850
Advanced Light Source			
Optimal Hours[b]	5,700	5,600	5,600
Scheduled Hours	5,162	5,600	5,100
Unscheduled Downtime	4%	<10%	<10%
Number of Users	1,898	1,900	1,700
Advanced Photon Source			
Optimal Hours[b]	5,700	5,000	5,000
Scheduled Hours	5,113	5,000	4,500
Unscheduled Downtime	2%	<10%	<10%
Number of Users	2,773	2,800	2,500
National Synchrotron Light Source			
Optimal Hours[b]	5,700	5,500	5,500
Scheduled Hours	5,287	5,500	5,000
Unscheduled Downtime	4%	<10%	<10%
Number of Users	2,299	2,300	2,100
Stanford Synchrotron Radiation Laboratory			
Optimal Hours[b]	5,300	3,700	5,000
Scheduled Hours	2,651	3,700	4,200
Unscheduled Downtime	3%	<10%	<10%
Number of Users	741	800	800
High Flux Isotope Reactor			
Optimal Hours[b]	6,100	3,300	4,400
Scheduled Hours	3,096	3,300	4,000
Unscheduled Downtime	29%	<10%	<10%
Number of Users	48	100	100

[a] Scheduled hours for FY 2004 show actual number of hours delivered to users.
[b] Optimal hours for FY 2005 and FY 2006 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. This constitutes a definitional change from previous years. The figures for FY 2004 reflect the theoretical maximum number of hours the facilities could operate annually under ideal circumstances and maximum funding.

	FY 2004 Actual[a]	FY 2005 Estimate	FY 2006 Estimate
Intense Pulsed Neutron Source			
Optimal Hours[b]	4,700	3,600	3,600
Scheduled Hours	4,052	3,600	3,200
Unscheduled Downtime	0%	<10%	<10%
Number of Users	279	280	250
Manuel Lujan, Jr. Neutron Scattering Center			
Optimal Hours[b]	3,600	3,100	3,100
Scheduled Hours	2,643	3,100	2,800
Unscheduled Downtime	19%	<10%	<10%
Number of Users	507	500	400

Cost and Schedule Variance

	FY 2004 Actual	FY 2005 Estimate	FY 2006 Estimate
Spallation Neutron Source			
Cost Variance	+0.3%		
Schedule Variance	-1.25		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	Instrument Systems Design Complete	Ring Beam Available to Target
		Linac Beam Available to Ring	Approve Critical Decision 4 – Start of Operations
Linac Coherent Light Source (SLAC)			
Cost Variance	0%		
Schedule Variance	0%		
Major (Levels 0 and 1) Milestones Completed or Committed to		Approve Critical Decision 2b – Performance Baseline	Approve Critical Decision 3b – Start Construction
		Approve Critical Decision 3a – Start Long-Lead Procurement	

[a] Scheduled hours for FY 2004 show actual number of hours delivered to users.
[b] Optimal hours for FY 2005 and FY 2006 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. This constitutes a definitional change from previous years. The figures for FY 2004 reflect the theoretical maximum number of hours the facilities could operate annually under ideal circumstances and maximum funding.

	FY 2004 Actual	FY 2005 Estimate	FY 2006 Estimate
Center for Nanophase Materials Sciences (ORNL)			
Cost Variance	+.03%		
Schedule Variance	-.03%		
Major (Levels 0 and 1) Milestones Completed or Committed to		Approve Critical Decision 4a – Start Initial Operations	Approve Critical Decision 4b – Start Full Operations
Center for Integrated Nanotechnologies (SNL/LANL)			
Cost Variance	+0.4%		
Schedule Variance	-0.1%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 3a – Start Utility Construction Approved Critical Decision 3b – Start of Full Construction	None	Approve Critical Decision 4a – Start Initial Operations
The Molecular Foundry (LBNL)			
Cost Variance	-0.1%		
Schedule Variance	-0.1%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 3 – Start Construction	None	Approve Critical Decision 4a – Start of Initial Operations
Center for Nanoscale Materials (ANL)			
Cost Variance	+4.3%		
Schedule Variance	-10.1%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 2 – Performance Baseline Approve Critical Decision 3 – Start Construction	None	Approve Critical Decision 4a – Start of Initial Operations
Center for Functional Nanomaterials (BNL)			
Cost Variance	+0.8%		
Schedule Variance	-0.5%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approve Critical Decision 2 – Performance Baseline	Approve Critical Decision 3 – Start Construction	

	FY 2004 Actual	FY 2005 Estimate	FY 2006 Estimate
SSRL SPEAR3 Upgrade			
Cost Variance	0%	N/A	N/A
Schedule Variance	0%	N/A	N/A
Major (Levels 0 and 1) Milestones Completed or Committed to	Complete Accelerator Readiness Review Start Commissioning Approve Critical Decision 4 – Start Operations	None	None

Construction and Infrastructure

Spallation Neutron Source (SNS) Project

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 completed in 2006, the SNS will be significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence – ISIS at the Rutherford Laboratory in England. The facility will be used by 1,000-2,000 scientists and engineers annually. Interest in the scientific community in the SNS is increasing.

Neutron scattering will play a role in all forms of materials research and design, including the development of smaller and faster electronic devices; lightweight alloys, plastics, and polymers for transportation and other applications; magnetic materials for more efficient motors and for improved magnetic storage capacity; and new drugs for medical care. The high neutron flux (i.e., high neutron intensity) from the SNS will enable broad classes of experiments that cannot be done with today's low-flux sources. For example, high flux enables studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions.

FY 2006 budget authority is requested to 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 remains constant at $1,411,700,000. Additional information on the SNS Project is provided in the SNS construction project data sheet, project number 99-E-334.

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 electrons and 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 range. The characteristics of the light from the LCLS will open new realms of scientific inquiry and applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. Optical devices beyond the undulator manipulate the direction, size, energy, and duration of the x-ray beam and carry it to whatever experiment is under way. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation. Most other free-electron lasers store the light from many passes of the electron beam through the undulator in an optical cavity before putting it to use. The LCLS will require just a single pass by the electron beam through the undulator, thanks largely to the low emittance of the electron beam at the front end of the system.

FY 2006 budget authority is requested to initiate 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 Lab Office (CLO) Complex.

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.

Nanoscale Science Research Centers (NSRCs)

Funds are requested for construction of NSRCs located at Lawrence Berkeley National Laboratory, at Sandia National Laboratories/Los Alamos National Laboratory, and at Brookhaven National Laboratory. Funds are also requested to continue the Major Item of Equipment for an NSRC at Argonne National Laboratory. Additional information on the NSRCs is provided in the Construction Project data sheets, project numbers, 03-R-313, 04-R-313, and 05-R-321 and in the Materials Sciences and Engineering subprogram.

General Plant Project (GPP) and General Plant 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. 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 8,500 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. 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.

	FY 2004	FY 2005 est.	FY 2006 est.
# University Grants	1,100	1,350	1,200
Average Size	$145,000	$150,000	$150,000
# Permanent Ph.D.s (FTEs)	3,650	4,240	3,940
# Postdoctoral Associates (FTEs)	1,050	1,220	1,140
# Graduate Students (FTEs)	1,690	1,960	1,820

Materials Sciences and Engineering

Funding Schedule by Activity

(dollars in thousands)

	FY 2004	FY 2005	FY 2006	$ Change	% Change
Materials Sciences and Engineering					
Materials Sciences and Engineering Research	260,693	294,367	270,742	-23,625	-8.0%
Facilities Operations	298,138	325,242	457,069	+131,827	+40.5%
SBIR/STTR	0	15,523	18,332	+2,809	+18.1%
Total, Materials Sciences and Engineering	558,831	635,132	746,143	+111,011	+17.5%

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.

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 microcharacterization, 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, and is responsible for the construction of the Spallation Neutron Source, the five Nanoscale Science Research Centers, and the Linac Coherent Light Source.

Selected FY 2004 Research Accomplishments

- The Ultimate Analysis: Single-Atom Spectroscopy in Bulk Solids. A longstanding dream in materials sciences and engineering has been to see and study those specific individual atoms that are critical to bulk properties and to determine their location and active configuration. Now, through an enhanced scanning transmission electron microscope with improved optics, researchers are able to observe an individual atom within its bulk environment and characterize its chemical state via spectroscopic means, determining its valence and bonding with nearest neighbors. The advance was made possible by correction of lens aberrations in the electron microscope to give a smaller yet brighter beam with a diameter of approximately 1 Ångstrom. Single-atom sensitivity, the ultimate analysis, opens up all areas of materials science and engineering to fundamental investigations in a revolutionary way.
- New Thin-film Texture Discovered with Potential for Nanotech Applications. One of the most fundamental structural properties of a thin film is its "texture," which is the orientation of individual grains with respect to the deposition substrate. Three types of texture are commonly observed: random, where no single orientation is dominant; fiber-texture, where the film grains are parallel to the growth direction, but random about that direction; and epitaxial, where the film orientation is fixed in three dimensions with respect to the substrate. The new, fourth type of texture, named axiotaxy, was observed in a number of thin film systems in which the film and substrate share a common plane orientation as a consequence of crystal lattice matching. This new texture provides a potential method for assembling large numbers of nanocrystals in regular patterns for nanotech applications.
- Negative Refraction - New Frontier for Superlenses. The first demonstration of negative and positive refraction of visible light at the same crystal interface was recognized as one of the "Top 15 Physics News Stories of 2003" by the American Institute of Physics. Nature provides us with optical refraction which is always positive: that is, the incident and transmitted light through an interface of two different media are on opposite sides of the interface normal. For negative refraction, they are on the same side of the interface normal. The beauty of negative refraction is total transmission and zero reflection, regardless of the angle of light incidence. These properties lend themselves to the creation of "super lenses." Laser beams can be steered in nano-photonic devices without loss, and optical telescopes can be built with higher resolution. The new interface uses a ferroelastic twin domain boundary such as a yttrium vanadate (YVO_4) bi-crystal and is applicable to any frequency of the electromagnetic spectrum. As a vision for the future, electron beams could be focused more efficiently in highly sensitive electron microscopes.
- Multi-band Semiconductors for High Efficiency Solar Cells. A new semiconductor material has been discovered that has multiple energy gaps, instead of the usual one, allowing for ultra-efficient energy capture of sunlight. Multi-band semiconductors were theoretically predicted over 20 years ago, but only now through the properties of so-called "highly mismatched alloys" (HMAs) have they been achieved. HMAs are compound semiconductors in which a small fraction of the anions are replaced with more electronegative atoms, producing a material with a new band having a strong quantum mechanical interaction with either the occupied valence band or the empty conduction band of the host semiconductor. Using this approach it was predicted, and subsequently demonstrated experimentally, that a II-VI semiconductor compound (ZnMnTe) with a small fraction (~1%) of the group VI constituent, i.e., tellurium, replaced by oxygen operates as a multiband semiconductor. Theoretical evaluation indicates that a single junction solar cell fabricated from this material could achieve a power conversion efficiency of 56%.

- Individual Carbon Nanotubes as Nanoscale Light Sources. A single carbon nanotube with a diameter of only 1.4 nanometer was used to fabricate the smallest source of light that can be controlled by electric current. The emission spectrum (color) of the light varied as a function of nanotube length and diameter. The center of the spectrum is determined by the nanotube diameter while the width of the spectrum depends on the length of the nanotube. Long nanotubes (50,000 nanometers) had narrow, symmetric emission spectra (characteristic of cold electrons) centered at the bandgap of the nanotube, which is inversely proportional to the nanotube diameter. Short nanotubes (500 nanometers) were also peaked at the bandgap of the nanotube, but showed broad, asymmetric spectra with a tail on the high-energy side, characteristic of hot electrons. These spectra show the cooling of hot electrons in nanotubes as a function of length through excitation of vibrations of the nanotube. The demonstrated understanding and control of optical properties using nanotubes could be important for optoelectronic nanotechnology.
- Magnetic Resonance Imaging at the Nanoscale. An innovative magnetic resonance approach to characterizing nano-porosity in a variety of materials has been developed. Magnetic resonance imaging (MRI) has been tremendously successful in visualizing resident deformities and the presence of disease in soft, porous biological tissues of the liver or kidney, yet the limited resolution precludes characterization at the nanometer scale. By using a technique of percolating inert gas through a nanoporous structure and then determining both the "sticking coefficient" of the gas and the time it takes for the gas to move away from the pore structure, MRI can now evaluate both the pore size distribution and the nature of the pore connectivity. This allows the analysis of highly porous structures that are present in many living systems and those created artificially in the laboratory such as filters to sequester pollutants, catalysts for chemical reactions, highly efficient insulators, and high strength to weight ratio materials for structural applications. By understanding the relationship between processing parameters and porosity of the resultant materials, advances in porous materials can be made.
- Nano-Trains: Nanoparticle Transport Using Motor Proteins. An active transport system that can be used to pick up, transport, and deposit nanoparticles within a microfluidic system has been developed. The active transport system is powered by the motor protein kinesin, a naturally occurring molecular machine. In the presence of a fuel source (adenosine triphosphate, or ATP), the head groups in the motor proteins “walk” rapidly along protein fibers called microtubules. With the tails of kinesin fixed to a surface the proteins can be used to propel the microtubules across the surface. The microtubules can now be modified to carry various size particles, ranging from 10 micrometers to 10 nanometers, and in large quantities, by functionalizing segments of the microtubules to carry cargo, like train “cars,” while leaving other segments unfunctionalized to act as “engines” by allowing free interaction with the motor proteins. This discovery suggests that highly non-equilibrium structures could be developed using the same active transport strategies that organisms employ for tissue assembly and muscle actuation.
- How Do Complex Fluids Jam? Is the mechanism for flow jamming the same for solid particulate matter (such as powders, coal, grain, pills, etc.) as for foam (bubbles in a fluid)? Two processes that rely on flowing foam are oil extraction and mineral separation. A major feature of both is that the flow can spontaneously stop, or jam, as the bubbles block each other. A better understanding of the causes of jamming will improve processes relying on flow. Recent studies using model foam systems have measured the coexistence between a flowing phase and a jammed phase. A surprising result was that this behavior was different from jamming observed in solid particulate systems. It

provided evidence for at least two different mechanisms of jamming, a critical step in furthering the understanding of the jamming process.

- Electron Transport in Semiconductor Quantum Wires. Spintronics (electronic phenomena that depend on electron spins) may provide a route to future generations of high-speed, low-power, nanoelectronics and may open up new areas of technology such as solid-state-based quantum computing. Significant challenges exist to realize these goals, including how to detect – or read – the electron spin in an electrical measurement. It has recently been demonstrated how such detection can be achieved in practice by exploiting the unique features of electron transport in semiconductor nanostructures known as quantum wires. Experiments show that the spin state of one quantum wire can be detected by studying the conductance of another wire located in close proximity. Theoretical work supports the idea that these experiments provide non-local detection of the electron spin opening pursuit of applications of this work to solid-state approaches to quantum computing.
- Superfluid Excitons at High Magnetic Field. A grand challenge for condensed matter physics is the observation of a new phase of matter created by the "condensation" of excitons, which are electron-hole pairs. Because excitons are bosons, any number can occupy a single quantum state. Thus, at low temperature, they should condense into the lowest energy level. Unfortunately, observation of this has been hindered by the rapid recombination of the electron and hole. Using magnetic fields to create stable exciton gases in doped double-layer semiconductor structures, the first evidence for condensation of an exciton gas was found in quantum tunneling measurements. The signature of the condensation was that both the conventional and Hall resistances of the sample become extremely small at low temperature. This nascent superfluidity is the strongest evidence yet for excitonic Bose condensation.
- Going from Good to Great: Doubling the Superconducting Upper Critical Field of Magnesium Diboride. In January 2001, a simple compound, magnesium diboride (MgB_2) was discovered to superconduct at a remarkably high temperature of 40 K, double the 20 K value for the niobium-based industrial standard. However, in its pure form, the material stops superconducting in a low magnetic field. During the past year, it was determined that the material continues to be superconducting in high fields if a small amount of carbon, about 5%, is substituted for boron. This has led to a better understanding of the superconductivity in this unique compound. The results indicate that, if the current carrying capability and mechanical properties can be further enhanced, carbon-doped MgB_2 could become the next industrial standard superconductor --better, cheaper, and lighter than niobium alloys.
- Wiring for Nanocircuits: Stabilized Silicon Nanotubes. Recent theoretical predictions have indicated that silicon nanotubes can be stabilized by attaching a string of 3d transition elements along the outside of the tube. These same calculations predict that the resulting nanotubes will be strongly conducting -- an important property needed by a candidate material for wiring together nanoelectronic components. The often considered carbon nanotubes, however, can be weakly metallic, semiconducting, or insulating depending on a property that is quite difficult to control-the winding ratio of the tube. The stabilization and metallization of the silicon nanotube can be accomplished with a small amount of nickel, about one nickel atom for every five silicon atoms. The compound tube structure studied is also smaller than most carbon nanotubes.
- Lashing Together Nanoparticles to Make Real Things. Theorists have shown that one can cause nanoparticles to self-assemble into ordered arrays by attaching short polymer strings to the particles to act as tethers. This is important because it is necessary to assemble large numbers of nanometer-

sized particles to create something of size appropriate to our world. It must be done as a loose assembly of the nanoparticles to retain their special properties but often also be arranged in special geometric patterns to realize the desired property. The technique demonstrated by detailed simulations is to attach short polymer strands to the particles at specified points and then let nature take its course. While currently only a theoretical prediction, the scheme is quite feasible and is expected to be in use within two to five years. In the meantime, the theorists are busy developing a "handbook" of how to position the tethers, how long they should be, and what they should be made of to accomplish a particular desired structure.

- A New Class of White Light Phosphors: Advancing the Solid State Lighting Initiative. A new class of tunable, white light emitting phosphors based on single size semiconductor nanoparticles or quantum dots (QDs) has been discovered. This breakthrough meets one of the most critical needs in the Department's Solid-State Lighting Initiative, whose aim is to replace present day highly inefficient light bulbs by solid state lighting devices and thereby have revolutionary effects on conserving electric energy. This accomplishment was made possible by the finding that, for sufficiently small cadmium sulfide and cadmium selenide QDs of diameters two nanometers or less, the onset of light absorption (determined by dot size) and the emission energy, or color (determined by interfacial chemistry), can be independently controlled. The decoupling of these two features allows wide separation of the absorption and emission to eliminate self-absorption of the emitted light, and allows one to tune the emission throughout the visible range from a population of single-size dots. Key to this discovery is the ability to tailor the energies and lifetimes of interface states by the addition of suitable surfactants that bind to selected sites on the QD surface (which determine the emission), or the addition of suitable electron or hole traps (e.g., zinc or sulfide ions, respectively).
- Catalyst Active Sites Imaged in Real Time. The atomic-scale formation and dynamics of active sites on a catalytic surface have been imaged for the first time. Using movies made from a series of state-of-the-art atomic-level scanning tunneling microscope images, the time-dependent behavior of sites on the surface of palladium metal was observed while diatomic hydrogen gas was adsorbed and then dissociated into two hydrogen atoms. The catalytic dissociation of hydrogen on a metal surface is pervasive in catalytic chemistry. Contrary to the prevailing view of the past three decades, it was found that three adjacent and empty surface sites are required for this process to occur - two empty sites are not sufficient. This surprising result calls into question the conventional thinking on the structure of active sites on catalyst surfaces. Further real-time measurements will help establish the molecular-level understanding of the formation of the active sites that determine the catalytic activity of a surface.
- Basic Research Leads to Terabit Memory Devices. A decade-long basic research project has led to the first successful application by industry of a novel approach in nanotechnology, 'molecular self-assembly,' to enable continued miniaturization of semiconductor circuitry such as FLASH memories. The essential element in this new approach lies in directing the orientation of highly-dense arrays of nanoscopic cylindrical domains in thin films of diblock copolymers (BC). Using routine lithographic processes, the BC films are transformed into large area arrays of cylindrical nanopores with very high aspect ratios. Establishing the ability to produce such high density arrays in a simple, robust, and inexpensive manner using conventional processing (new tooling is not required and will not be required with further advances in the self-assembly technique) has broken new ground in fundamental studies of nanoscience and the rapid transfer of this technology to the industrial sector.
- Fundamentals of How Liquid Metals Solidify Answered with Synchrotron Radiation Experiments. Materials properties are determined, in large measure, by the nature of the solidification process.

During the cooling process, the metal atoms in the liquid phase are thought to pack together with almost the same order as the resultant solid. In fact, early experiments demonstrated that liquids cooled far below their melting point still maintain a large degree of disorder. As the temperature is further lowered, a well ordered crystalline solid is eventually reached, but the nucleation pathway to the crystalline form remained a mystery. By combining levitated molten metal drops with a newly developed, in-situ synchrotron x-ray diffraction technique for measuring structure during solidification, investigators have verified for the first time that atoms in a liquid metal arrange themselves with the local symmetry of an icosahedron, a Platonic solid consisting of 20 tetrahedra (4-sided pyramid shaped polyhedra). As cooling proceeds, the icosahedral arrangement transitions to the final crystalline form. This discovery proves that atomic scale structure in the liquid actually plays a role in crystallization, something that is not treated in current nucleation theory.

- X-Ray Microscopy in 3D on a Micron Scale. Metal deformation, ranging from the centuries old heating and beating of sword edges to the rolling of metal sheets in modern industrial mills, is one of the oldest and most important materials processing techniques, yet it remains one of the least understood. Although elaborate recipes have been developed to produce alloys with desired properties, they are all based on expensive and inefficient search and discovery methods. To address this, a new, nondestructive, submicron-resolution 3D x-ray microscopy technique with high-precision nanoscale indentations to study the fundamental aspects of deformation in ductile materials has been developed. X-ray microscopy measurements made using penetrating synchrotron x-ray microbeams are providing detailed, quantitative information on the deformation microstructure for sizes below that of a human hair, but too large for electron microscopy. These results provide previously missing information that is critical for testing advanced theories and computer modeling and for making new materials, with predictable properties, in a more efficient manner.
- Understanding Fundamental Magnetic Properties Could Lead to Sensor Development. Magnetic excitations provide insight into the spin structure and spin dynamics of materials. One material studied exhibits colossal magnetoresistance, a property that makes it interesting for sensor applications. The magnetic structure of this material ($Pr_{0.5}Sr_{0.5}MnO_3$) was determined to be ferromagnetically aligned layers that are coupled antiferromagnetically. The magnetic excitations (also called spin waves) were measured using inelastic neutron scattering at the High Flux Isotope Reactor at Oak Ridge National Laboratory. The spin wave dispersion follows the behavior expected from linear spin wave theory. With refinements in analyzer efficiency and film preparation techniques, the measurement technique will then be applied to thin films. This should allow a search for spin wave excitations in antiferromagnetic films of Fe-Pt.

Selected FY 2004 Facility Accomplishments

- The Advanced Light Source (ALS)
  - New Insertion Device Installed for Ultrafast X-Ray Pulses. Light from a high-power, ultrafast laser will travel with the electron beam through the new permanent-magnet wiggler at the ALS, thereby modulating the energy of a portion of the electron beam. The energy modulation results in a spatial separation of the modulated slice of the beam, which is only 200 femtoseconds long, so that it can be used to generate ultrafast x-ray pulses for experiments at photon energies from 100 eV to10 keV.
  - High-pressure Facility Enables State-of-the-art Geophysics and Materials Research. At the newly commissioned ALS research facility, x-rays from a superconducting bend-magnet source, a high-efficiency micro-focused beamline, and a high-power laser-heated high-pressure cell (diamond

anvil cell) will be used for a wide range of experiments, such as determining the high-pressure/high-temperature phase diagrams and equations of state of materials at pressures up to the Mbar range and at temperatures up to several thousand Kelvin.

- New Research on Solvated or Buried Systems Possible. Real-world materials that inhabit wet environments or are buried in the interior of more complex structures pose challenges to researchers. *In situ* electronic and structural properties of such materials are now accessible due to the high brightness of third-generation synchrotron radiation sources and the development of liquid-cell sample chambers. The technology developed at the ALS has already been demonstrated for the characterization of nanoparticles and opens the way for studies of advanced battery and hydrogen storage material.
- Fast Orbit Feedback Stabilizes Electron Beam Position. Today's synchrotron radiation instrumentation requires that the position of the illuminating x-ray beam be rock solid, which in turn imposes the same condition on the position of the electron beam. ALS scientists and engineers have commissioned a new feedback system (fast orbit feedback) that senses the beam position and sends signals to the control system to correct any vertical and horizontal position errors to within 2 μm and 3 μm, respectively.

▪ The Advanced Photon Source (APS)

- A New Technique for Understanding Materials under Extreme Conditions. Nuclear resonant inelastic x-ray scattering and extreme-brilliance x-ray beams are being used to measure, for the first time, the velocity of sound in tiny samples of materials under extreme conditions. The ability to obtain detailed information from minuscule amounts of materials under extreme conditions is critical to many experiments, from geophysics to national security.
- Taking the Heat from Higher-Brightness X-rays. Two new beamlines require two or three in-line undulators to achieve the required high photon intensity. To accommodate the expected higher APS storage ring beam current and concurrent heat loads that will be more than three times hotter than the surface of the sun, a novel insertion device front end has been developed.
- Powering Up to Higher X-ray Beam Brilliance. Radio frequency (rf) technology at the APS is one of several innovations laying the foundation for an eventual increase in storage ring current to 300 mA. This power exceeds the rf output power of all the TV and radio stations in a major U.S. city such as Washington, D.C., and will provide researchers with more brilliant x-ray beams.
- Glowing Results from a Unique Application of X-ray Fluorescence. The intense photon flux from an APS insertion device beamline has been used for the first application of x-ray-induced fluorescence techniques to perform in-situ measurements in high-pressure metal-halide arcs. These data, not obtainable in any other way, are essential to developing a clearer understanding of high-pressure arc systems, among the most energy-efficient sources of white light.

▪ The National Synchrotron Light Source (NSLS)

- Superconducting Undulator Test Facility Constructed. A state-of-the-art cryogenic Vertical Test Facility was designed and constructed for use in developing superconducting undulators (SCU). This device allows precise magnetic field mapping of superconducting undulator prototypes at cryogenic temperatures and measures thermal performance and quench behavior under realistic operating conditions, including simulated beam heating. A SCU design has been developed which incorporates a novel cryogenic thermal management system to intercept the high beam heat loads expected in future ultra-high brightness synchrotron light sources.

- Hard X-ray Microprobe Completed for Environmental Sciences. A new hard x-ray microprobe beamline, X27A, will provide additional and enhanced x-ray micro-spectroscopy capabilities to the NSLS environmental science user community. The beamline can be operated in three different modes and can focus x-rays to a spot the size of a few microns. The detector array will enable both elemental mapping as well as fluorescence yield x-ray absorption spectroscopy studies of complex environmental samples.
- Infrared Spectrometer Installed on Surface Science Beamline. Corrosion and catalysis involves the interaction between gas molecules and another material such as a metal surface. Infrared spectroscopy from metal surfaces is an important tool for studying the interactions with adsorbed molecules. A portion of the U4IR surface science beamline was re-built to incorporate a new infrared spectrometer. This new spectrometer provides improved spectral resolution, spectral range, and increased collection rates over the previous instrument.
- X-ray Beamline Renovated for Materials Sciences. The X21 hybrid wiggler x-ray beamline and two experimental stations have been substantially rebuilt to accommodate new experimental programs that address elastic x-ray scattering studies of materials under high magnetic fields, thin films grown in-situ, and materials studied with small angle x-ray scattering, with appropriate setups permanently installed in the stations.

▪ The Stanford Synchrotron Radiation Laboratory (SSRL)

- SPEAR3 Project Completed. The four-year SPEAR3 Upgrade Project, jointly funded by the Department of Energy and the National Institutes of Health, was completed on time and within budget (SPEAR stands for the Stanford Positron Electron Accelerating Ring). The 3-GeV SPEAR3 light source produces x-ray beams having 1 to 2 orders of magnitude higher photon brightness than the SPEAR2 accelerator it replaced, enabling enhanced scientific capabilities comparable to those of other third generation light sources.
- SPEAR3 Commissioned and Operation for Users Commenced. The SPEAR3 storage ring was commissioned within a remarkably short time, beginning with equipment turn-on in mid-November 2003, and ending with the first 100-mA beam delivery to users in early March 2004. The speedy commissioning enabled the SSRL user program to begin again only 11 months after the SPEAR2 shutdown.
- First Diffraction Patterns are demonstrated with the SPPS. The first measurements of diffraction patterns from several prototypical samples were achieved at the sub-picosecond pulse source (SPPS). The first signals from the electro-optic pulse length and jitter experiment have been recorded yielding resolution limited pulse lengths of 1 picosecond. The preliminary jitter results indicate root-mean-square timing of the order of 250-300 femtoseconds.
- Source of Excessive Beam Emittance Found. Important progress in understanding the sources of excessive electron beam emittance from a photo-cathode gun has been made at the SSRL Gun Test Facility, setting the path for achieving the design goal for the Linac Coherent Light Source (LCLS) electron gun. The discovery indicates that a time dependent kick significantly increases the projected beam emittance. Eliminating the beam kick will enable operation of the high-charge gun with a sufficiently low emittance for x-ray Free Electron Laser operation at the LCLS.

- The Intense Pulsed Neutron Source (IPNS)

  - IPNS Instruments Upgraded. The IPNS continues to make major instrument upgrades to maintain world class science capabilities for its users: 1) more than one half of the user instruments have migrated to a new data acquisition system that enables faster and more flexible data binning; 2) installation of neutron guides and frame definition choppers has boosted flux on sample for some instruments by 2-20 times; and 3) improved detectors and collimation and larger detector coverage have significantly reduced the time required to collect neutron data. Successful commissioning of a new IPNS target from recycled disks recovered from end-of-life targets has provided a cost effective alternative to the construction of entirely new IPNS targets and enables IPNS operations for an additional six years.

  - IPNS Hosts the National Neutron and X-Ray Scattering School. During the two-week period of August 15-29, 2004, 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 134 applications for the 60 positions available in 2004.

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

  - Goniometer Installed on Small-Angle Neutron Scattering Instrument. The goniometer is able to position the sample in the neutron beam with any orientation. Thus, it provides for a complete measurement of diffraction space, giving information on the crystal three-dimensional structure over large length scales from 1 to about 100 nm. Research problems that will benefit from this new capability include flux-lattice studies in superconductors, super lattice structures, and self-assembling colloidal structures.

  - Spin Echo Spectrometry Demonstrated. This technique, achieved for the first time at a pulsed neutron source, has application to diffraction problems in nanoscale materials systems and was demonstrated on a dilute solution of 58 nm diameter polystyrene spheres in deuterium oxide.

  - High-Intensity Powder Diffractometer (HIPD) Refurbished. The instrument is now fully operational for studies of atomic and magnetic structure of crystalline and noncrystalline powders, liquids, phase transitions, small samples, and absorbing materials. Due to its very high counting rates, time-resolved measurements are also possible as recently demonstrated in a diffraction study of the curing process of cement.

- The High Flux Isotope Reactor (HFIR)

  - Operational Milestone Celebrated. On April 21, 2004, HFIR began its 400th operating cycle in its 38 year history. The length of an operating cycle depends on the time it takes for the reactor's uranium fuel to become depleted. A celebration marking this anniversary was held on May 15.

  - Neutron Scattering Instruments Upgraded. The upgraded HFIR has state-of-the-art neutron scattering instruments that are among the world's best. In FY 2004, the HB-2B Residual Stress Diffractometer was brought into operation in the HFIR Beam Room. The HB-2D triple-axis monochromator shield was installed at the end of the HB-2 tunnel, and the Reflectometer and SNS Detector Station on this beam tube are operational. The WAND diffractometer, one of the instruments in the US-Japan International Collaboration, will also be operational, completing an important milestone in the HFIR Upgrade project.

- Cold Source Comprehensive Hazards Analysis Completed. One of the premier features of the HFIR upgrade will be the addition of an environment of super-cold liquid hydrogen. This environment literally chills the neutrons so they have less thermal energy with longer wavelengths, which make them valuable tools for the study of larger, more complex atomic and molecular structures. The HFIR Cold Source Comprehensive Hazards Analysis was completed and submitted to DOE in support of the October 4, 2004 milestone.
- Reactor Equipment Upgraded. New Instrument Air System compressors, dryers and receivers were installed in FY 2004. These components replace obsolete equipment and will simplify the system by reducing the number of valves in the system significantly.

Detailed Justification

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
Materials Sciences and Engineering Research......	**260,693**	**294,367**	**270,742**
▪ **Structure and Composition of Materials**...........	**22,833**	**31,185**	**26,403**

This activity supports basic research on atomic-scale structure, composition, and bonding and on their relationship to the behavior and performance of materials, predictive theory and modeling, and new materials systems. This activity also supports four electron beam microcharacterization user centers: the Center for Microanalysis of Materials at the University of Illinois, 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 characterize localized atomic positions and configurations, chemical gradients, bonding forces, etc.

The properties of materials used in all areas of energy technology depend upon their structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the structural characteristics of advanced materials. This dependence occurs because the spatial and chemical inhomogeneities in materials (e.g., dislocations, grain boundaries, magnetic domain walls, and precipitates) determine and control critical behaviors such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, 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 2006, 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.

The overall decrease in structure and composition of materials is attributable to an increase for research related to the hydrogen economy ($+135,000) and a decrease due to reduced research activities in metal and ceramic grain boundary characterization and FY 2005 one-time increments in areas of transmission electron microscopes ($-4,917,000).

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
▪ **Mechanical Behavior and Radiation Effects**.....	**13,444**	**13,469**	**12,221**

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 of 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 2006, there will be a decrease in mechanical behavior and radiation effects research attributable to a reduction in activities related to understanding and inhibiting the degradation of structural materials and a decrease due to the FY 2005 one-time funding enhancement for nanomechanics research ($-1,248,000).

▪ **Physical Behavior of Materials**...........................	**22,148**	**26,657**	**24,512**

This activity supports basic research at the atomic and molecular level to understand, predict, and control physical behavior 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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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 mission 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 2006 the overall decrease in physical behavior of materials is attributable to an increase in research related to the hydrogen economy ($+355,000) and a decrease due to FY 2005 one-time enhancements in areas of organic electronic materials, and electronic and magnetic materials research ($-2,500,000).

▪ **Synthesis and Processing Science**	**12,710**	**14,271**	**14,771**

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.

These activities underpin 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.

In FY 2006, funding will include continued support for research on nanoscale synthesis and processing. This activity will address the significant experimental and theoretical challenges in understanding what is occurring so that the benefits of nanoscale phenomena can be realized in larger scale components. The properties of materials change dramatically as the grain size in materials approaches the nanometer scale. At conventional grain sizes, a gain in strength of a material typically results in a loss in both ductility and fracture toughness resulting in a brittle material. However, by using nanocomposites and understanding deformation physics, it should be possible to make materials that are strong, tough (resistant to impact fracture), and ductile. There is also great need for nanoparticles of uniform size, composition, and surface stability because experiments have shown that fracture toughness may undergo a profound increase as the grain size falls below 10 to 50 nm in high-temperature structural ceramics. These materials might be used in advanced fuel efficient engines, turbines, and machine cutting tools.

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 2006 the overall increase in synthesis and processing science is attributable to a decrease due to the reduced research in the area of welding and joining of materials and FY 2005 one-time increments in areas of guided self-assembly ($-1,258,000), and an increase for research related to the hydrogen economy ($+125,000) and nanoscale science focusing on theory, modeling an computation ($+1,633,000).

	FY 2004	FY 2005	FY 2006
▪ **Engineering Research**	**10,975**	**7,902**	**5,000**

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. 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.

On-going activities in FY 2006 will include research in the mechanics of nanoscale systems including nanotube driven motors and nano-systems containing both physical and biological components, nanoindentation, and fluid behavior during solidification including the competition between amorphous and crystalline phase development. Research in heat transfer, multiphase fluid flow, and granular materials will be decreased or terminated. ($-2,902,000).

	FY 2004	FY 2005	FY 2006
▪ **Neutron and X-ray Scattering**	**44,928**	**49,970**	**44,058**

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 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, are the primary tools for characterizing the atomic, electronic, and magnetic structures of materials.

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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. An additional $303,000 will be applied to this research.

In FY 2006 the overall decrease in neutron and x-ray scattering is attributable to an increase in research related to the hydrogen economy ($+303,000), and a decrease in neutron powder diffraction and due to FY 2005 one-time increments in areas of instrumentation physics and neutron scattering research ($-6,215,000).

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

▪ **Experimental Condensed Matter Physics**	**42,631**	**45,647**	**42,004**

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 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 (EE/RE). Research in superconductivity and photovaltaics especially is coordinated with the technology programs in EE/RE. 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.

In FY 2006, funding provides support for investigation of fundamental questions in condensed matter physics at the nanoscale. As the size of a nanoscale structure becomes less than the average length for scattering of electrons or phonons, new modes of transport for electrical current and/or heat may become possible. Also thermodynamic properties, including collective phenomena and phase transitions such as ferromagnetism, ferroelectricity, and superconductivity can change when structures contain a smaller number of atoms, with a much greater proportion of surface atoms. The potential impacts of understanding the physics are very significant. For example, nanoscale structures provide a path toward the next generation of magnets for memory, more efficient electric motors, better thermoelectric materials, and materials for more efficient solar energy conversion. Research efforts for the development of nanomaterials for both energy conversion and hydrogen energy

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

storage, which exhibit size-dependent properties that are not seen in macroscopic solid state materials will be continued. 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.

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

The overall decrease for experimental condensed matter physics is attributable to an increase for research related to the hydrogen economy ($+296,000) and a decrease due to FY 2005 one-time increments in crystal growth, scanning tunneling microscopy, transmission electron microscopy, and correleated electron materials research and reduced research activities in thermal physics ($-3,939,000).

	FY 2004	FY 2005	FY 2006
▪ **Condensed Matter Theory**	**18,126**	**18,872**	**19,975**

This activity supports basic research in theory, modeling, and simulations, and it complements the experimental work. 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, for more complex materials and hybrid structures, even the outlines of a theory remain to be made. 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 – 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.

This activity also supports the Center for X-ray Optics at LBNL, and the Center for Synthesis and Processing of Advanced Materials, which consists of collaborating projects at national laboratories, universities, and industry.

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

In FY 2006, the overall increase for theoretical condensed matter physics is attributable to an increase for research related to theory, modeling, and computation in nanoscience ($+3,000,000) and to hydrogen production, storage, and use ($+125,000) and a decrease due to FY 2005 one-time enhancements in areas of materials theory, and improvements to existing instruments, including computer clusters ($-2,022,000).

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
▪ **Materials Chemistry**...	**40,338**	**45,422**	**41,740**

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, 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 2006, funding will continue to explore multi-disciplinary approaches (with biology, chemistry, physics and computational science playing major roles) to model, design and synthesize new and novel materials. Also of interest is the development of new organic electronic materials with novel magnetic, conducting, and optical properties; single crystal growth of advanced materials that will lead to better characterization, and consequently, better understanding of their properties; and polymer interfaces. The overall decrease for materials chemistry is attributable to an increase for research related to basic research for hydrogen production, storage, and use ($+500,000) and a decrease due to FY 2005 one-time increments in areas of nanoscale polymer materials research, and improvements to existing instruments, including nuclear magnetic resonance and novel atomic force microscopes, and a reduction for smaller group activities ($-4,182,000), including single investigator projects at DOE national laboratories.

▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**......................	**7,673**	**7,643**	**7,280**

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, 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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

and nuclear physics, fusion energy sciences, fossil energy sciences, and energy efficiency and renewable energy sciences. The following table shows EPSCoR distribution of funds by state. The decrease in EPSCoR is attributable to a reduction in new competitions in FY 2006 ($-363,000).

EPSCoR Distribution of Funds by State

	(dollars in thousands)		
	FY 2004 Estimate	FY 2005 Estimate	FY 2006 Estimate
Alabama	987	510	600
Alaska	0	0	0
Arkansas	140	0	135
Delaware[a]	0	0	0
Hawaii[b]	0	0	0
Idaho	328	102	375
Kansas	527	560	135
Kentucky	247	224	0
Louisiana	647	198	462
Maine	0	0	0
Mississippi	578	535	132
Montana	515	375	375
Nebraska	0	0	125
Nevada	0	0	0
New Mexico[b]	135	0	135
North Dakota	410	139	273
Oklahoma	525	135	350
Puerto Rico	375	375	375
South Carolina	854	266	535
South Dakota	125	0	125
Tennessee[a]	0	0	0
Vermont	877	709	0
US Virgin Islands[a]	0	0	0
West Virginia	248	201	90
Wyoming	130	130	140
Technical Support	25	110	110
Other[c]	0	3,074	2,808
Total	7,673	7,643	7,280

[a] Delaware, Tennessee, and U.S. Virgin Islands became eligible for funding in FY 2004.
[b] Hawaii and New Mexcio became eligible for funding in FY 2002.
[c] Uncommitted funds in FY2005 and FY2006 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**	**2,000**	**2,000**	**2,000**

Capital equipment funds are provided for new and upgraded instrumentation, such as spectrometers, diffractometers, and detectors.

▪ **Linac Coherent Light Source (LCLS)**	**2,000**	**4,000**	**0**

Research and development (R&D) funds are 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 will be 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. The completion of funding is in accordance with the approved project schedule.

▪ **Nanoscale Science Research Centers**	**400**	**600**	**993**

Funds are provided for three Nanoscience Research Centers to support pre-operational activities leading up to the start of research operations. These Centers are the Center for Nanophase Materials Sciences (CNMS) located at ORNL, the Molecular Foundry located at LBNL, and the Center for Integrated Nanotechnologies (CINT) located at Sandia National Laboratories and Los Alamos National Laboratory.

▪ **The Center for Nanoscale Materials**	**10,000**	**12,000**	**14,000**

Funds are provided for a Major Item of Equipment (MIE) 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 is being constructed by the State of Illinois for the Center at a cost of $36,000,000 and which will be dedicated to the Center operations. The building will be 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. The Center will build on ANL's recognized strengths in magnetism, superconductivity, and novel materials with "spintronic" functionality.

▪ **Instrumentation for the Spallation Neutron Source**	**7,387**	**7,643**	**8,079**

Funds are provided for a MIE with a total estimated cost in the range of $50,000,000 to $75,000,000 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 MIE 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 TEC range will be narrowed to a cost and schedule performance baseline

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

following completion of Title I design and External Independent Reviews. It is anticipated that these five instruments will be installed at the SNS on a phased schedule between FY 2007 – 2011.

▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)**	**0**	**1,500**	**1,500**

Funds are provided to continue R&D on instrumentation for the LCLS. These instruments will complement the instrument that is being built as part of the LCLS construction project. This R&D activity will evolve after determination of the scope of the project, i.e., the number and type of instruments to be fabricated. The instrument concepts that are being supported with these funds will be competitively selected using a peer review process. The activity is patterned after that described above for the SNS. The project will be managed by the Stanford Linear Accelerator Center with participation by partners as determined by the peer review process.

▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	**3,100**	**5,586**	**6,206**

Funds are provided for a MIE 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 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.

Facilities Operations	**298,138**	**325,242**	**457,069**
▪ **Operation of National User Facilities**	**298,138**	**325,242**	**457,069**

As noted earlier, in order to accomplish the highest-priority goals, some difficult choices had to be made. In particular, the BES support for the Radiochemical Engineering and Development Center at Oak Ridge National Laboratory is terminated. The operations of the remaining facilities are funded at about the same level as in FY 2005, which will decrease the available beam time and service to users by about ten percent. In general, the decrease in funding from FY 2005 to FY 2006 represent one-time increments in capital equipment and other specialized increments in FY 2005. These include: Advanced Light Source, Advanced Photon Source, National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory, and High Flux Isotope Reactor. The Spallation Neutron Source and the Nanoscale Science Research Centers operate at their planned FY 2006 levels. 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 beginning of a 3-4 year transition of programmatic ownership for SLAC linac operations from HEP to BES as the LCLS project proceeds. The Combustion Research Facility is funded in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. The facility operations budget request, presented in a consolidated manner

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

later in this budget, includes operating funds, capital equipment, and accelerator and reactor improvements (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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
Advanced Light Source	43,937	45,600	42,367
Advanced Photon Source	95,740	99,950	98,000
National Synchrotron Light Source	37,398	37,400	37,400
Stanford Synchrotron Radiation Laboratory	29,670	30,654	28,300
High Flux Isotope Reactor	40,284	46,930	40,032
Radiochemical Engineering Development Center	6,100	4,500	0
Intense Pulsed Neutron Source	16,768	17,055	17,055
Manuel Lujan, Jr. Neutron Scattering Center	9,844	10,053	10,300
Spallation Neutron Source	18,397	33,100	106,872
Center for Nanophase Materials Sciences	0	0	18,086
Center for Integrated Nanotechnologies	0	0	12,709
Molecular Foundry	0	0	8,554
Center for Nanoscale Materials	0	0	3,894
Linac Coherent Light Source (LCLS)	0	0	3,500
Linac for LCLS	0	0	30,000
Total, Facilities	298,138	325,242	457,069

SBIR/STTR	**0**	**15,523**	**18,332**

In FY 2004, $12,433,000 and $1,492,000 were transferred to the SBIR and STTR programs, respectively. The FY 2005 and FY 2006 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

Total, Materials Sciences and Engineering	**558,831**	**635,132**	**746,143**

Explanation of Funding Changes

	FY 2006 vs. FY 2005 ($000)
Materials Sciences and Engineering Research	
▪ **Structure and Composition of Materials**	
Overall decrease in structure and composition of materials research because of increase for research related to the hydrogen economy ($+135,000) and decrease in metal and ceramic grain boundary characterization research and FY 2005 one-time increments in areas of electron microcopy and improvements to existing instruments ($-4,917,000).	-4,782
▪ **Mechanical Behavior and Radiation Effects**	
Decrease in mechanical behavior and radiation effects research because of reduction in degradation of structural materials research and FY 2005 one-time increment for nanomechanics research	-1,248
▪ **Physical Behavior of Materials**	
Overall decrease in physical behavior of materials research because of increase for research related to the hydrogen economy ($+355,000) and reduction due to FY 2005 one-time research increments ($-2,500,000)	-2,145
▪ **Synthesis and Processing Science**	
Overall increase because of decrease in research in the area of welding and joining of materials ($-1,258,000) and increase for research related to the hydrogen economy ($+125,000) and nanoscale science focusing on theory, modeling and computation ($+1,633,000)	+500
▪ **Engineering Research**	
Decrease in engineering research because of decrease for research activities in heat transfer, multiphase fluid flow, and granular materials	-2,902
▪ **Neutron and X-ray Scattering**	
Overall decrease in neutron and x-ray scattering research because of increase for research related to the hydrogen economy ($+303,000) and decrease in neutron powder diffranction and due to FY 2005 one-time research increments ($-6,215,000)	-5,912
▪ **Experimental Condensed Matter Physics**	
Overall decrease in experimental condensed matter physics research because of increase for research related to the hydrogen economy ($+296,000) and decrease in thermal physics research due to FY 2005 one-time research increments ($-3,939,000)	-3,643

	FY 2006 vs. FY 2005 ($000)
▪ **Condensed Matter Theory**	
Increase in condensed matter theory research because of increase for research related to theory, modeling, and computation in nanoscience ($+3,000,000) and hydrogen production, storage, and use ($+125,000) and reduction due to FY 2005 one-time research increments ($-2,022,000)	+1,103
▪ **Materials Chemistry**	
Overall decrease in materials chemistry research because of increase for research related to the hydrogen economy ($+500,000) and reduction for smaller group activities and FY 2005 one-time research increments ($-4,182,000).	-3,682
▪ **Experimental Program to Stimulate Competitive Research (EPSCOR)**	
Decrease in EPSCoR because of reduction in new competitions in FY 2006.	-363
▪ **Linac Coherent Light Source**	
Decrease for research and development per schedule for the Linac Coherent Light Source.	-4,000
▪ **Nanoscale Science Research Centers**	
Increase for other project costs per schedule associated with the Nanoscale Science Research Centers.	+393
▪ **The Center for Nanoscale Materials**	
Increase for MIE for the ANL Center for Nanoscale Materials.	+2,000
▪ **Instrumentation for the Spallation Neutron Source**	
Increase for Instrumentation for the Spallation Neutron Source.	+436
▪ **Transmission Electron Aberration Corrected Microscope (TEAM)**	
Increase for MIE for the Transmission Electron Aberration Corrected Microscope.	+620
Total, Materials Sciences and Engineering Research	**-23,625**
Facilities Operations	
▪ **Operation of National User Facilities**	
Decrease for the ALS as a result of a one time FY 2005 increment for modifications to permit eventual top-up mode injection, which will permit stable x-ray beam intensities rather than the current gradual decline in x-ray beam intensity over the period of several hours.	-3,233
Decrease for the Advanced Photon Source as a result of one-time FY 2005 increment for beamline modifications	-1,950

	FY 2006 vs. FY 2005 ($000)
Decrease for Stanford Synchrotron Radiation Laboratory as a result of one-time FY 2005 increment for optics and beamline modifications to take advantage of the increased brightness following the SPEAR 3 upgrade	-2,354
Decrease for High Flux Isotope Reactor as a result of one-time FY 2005 increment for fuel purchases, maintenance, and instrument modifications	-6,898
Decrease due to termination of BES support for the Radiochemical Engineering Development Center. This marks the beginning of a consolidation of hot-cell activities at ORNL, which will subsequently be funded by other customers.	-4,500
Increase for the Manuel Lujan Jr., Neutron Scattering Center for operations	+247
Increase for the Spallation Neutron Source to begin operations	+73,772
Increase for the Center for Nanophase Materials Sciences to begin operations	+18,086
Increase for the Center for Integrated Nanotechnologies to begin operations	+12,709
Increase for the Molecular Foundry to begin operations	+8,554
Increase for the Center for Nanoscale Materials to begin operations	+3,894
Increase for the Linac Coherent Light Source Other Project Costs per FY 2006 project datasheet. These funds will be used to start commissioning of the injector linac subsystems, primarily the laser dedicated to the photocathode gun. These commissioning activities will also involve preparing the applications software and other activities that will ultimately be needed to commission the LCLS linac	+3,500
Increase for SLAC Linac in support of the Linac Coherent Light Source. This marks the beginning of the transition to BES the LCLS operations at SLAC	+30,000
Total, Facilities Operations	**+131,827**
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expense funding	+2,809
Total Funding Change, Materials Sciences and Engineering	**+111,011**

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

	(dollars in thousands)				
	FY 2004	FY 2005	FY 2006	$ Change	% Change
Chemical Sciences, Geosciences, and Energy Biosciences					
Chemical Sciences, Geosciences, and Energy Biosciences Research	207,886	227,465	210,290	-17,175	-7.6%
Facilities Operations	5,892	6,169	6,169	0	0.0%
SBIR/STTR	0	5,841	5,342	-499	-8.5%
Total, Chemical Sciences, Geosciences, and Energy Biosciences	213,778	239,475	221,801	-17,674	-7.4%

Description

Support is provided in the broad chemical sciences 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.

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 equal 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 2004 Research Accomplishments

- Potential for Greatly Enhanced Efficiency in Nanocrystalline Solar Cells. An incident solar photon striking a semiconductor solar cell normally produces a single electron-hole pair (exciton) and some excess heat. Experimentalists have recently demonstrated that two or more excitons can be created by absorption of a single photon in an array of lead-selenide nanocrystals. This process is called "impact ionization" and is observed when the photon energy is greater than three times the band gap of the nanocrystal. Multiple excitons from a single photon are formed on the picosecond time scale, and the process occurs with up to 100% efficiency depending on the excess energy of the absorbed photon. If this process could be translated into an operational solar cell, the gain in efficiency for converting light to electrical current would be greater than 35%.
- High Order Harmonic Generation Using Ions. High harmonic generation (HHG) is a process in which highly nonlinear optical effects, driven by ultrafast, intense laser pulses in an atomic gas, are used to turn visible bursts of photons into bursts in the extreme ultraviolet and soft x-ray spectral regions. There is a cutoff at high frequencies for HHG that is determined by the ionization potential of the atom and by defocusing and phase mismatch of the pump-laser beam due to ionization. Recent experiments have significantly extended the range of HHG to photon energies up to 250 eV through the use of atomic ions, which have higher ionization potentials and are thus capable of producing more energetic harmonic orders. In this work an ultrashort, intense optical laser pulse was focused into a hollow fiber filled with low-pressure argon gas. The fiber serves as a waveguide to phase-match the fundamental excitation pulse with the HHG soft x-ray pulse. This work demonstrates that HHG from ions can extend laser-based, coherent up-conversion into the soft x-ray region of the spectrum.
- Manipulation of Carbon Monoxide Oxidation to Carbon Dioxid. The formation of a chemical bond involves the approach of two reactants to short distances so that a new bond can form. How close do the two reactants need to be for them to interact with each other? In this novel experiment, a single carbon monoxide (CO) molecule on a surface was pushed toward two oxygen (O) atoms that were formed in the dissociation of O_2 by tunneling electrons. Using inelastic electron tunneling spectroscopy in a cryogenically cooled microscope, the hindered rotational mode of the CO molecule was measured as its distance from the two O atoms decreased. The change in this vibrational energy signaled the onset of a significant CO-O interaction prior to the formation of carbon dioxide (CO_2). A shift of 20% in the hindered rotation energy was observed when the CO molecule was within 2.50 Å from each of the two O atoms. Spatially resolved mapping of the hindered rotational mode led to a tilted CO in the O-CO-O complex. The controlled positioning of the two reactants allowed direct visualization of the chemistry. This research probed individual reactive encounters of the type that constitute a surface-mediated catalytic process. Exacting control of catalysis will require such molecular-level characterization.
- Direct Numerical Simulations of Homogeneous Charge Compression Ignition. Homogeneous charge compression ignition (HCCI) has the potential to reduce nitrogen oxide and particulate emissions from internal combustion engines while improving overall efficiencies. A major challenge posed by

this method of combustion is control of the heat release rate, and in particular, a means to spread the heat rate out in time to suppress the occurrence of damaging engine knock. Direct numerical simulations (DNS) of lean hydrogen-air ignition at high pressure and constant volume in the presence of temperature inhomogeneities are helping researchers understand the HCCI combustion process. Starting from an initial distribution of fluctuating temperatures at high pressure, the evolution of localized ignition sites was studied in a constant volume DNS with detailed hydrogen/air reaction kinetics. For the first time, numerical simulations revealed that flame front and spontaneous ignition propagation can coexist in this environment. The simulations showed that the local nature of the ignition propagation is primarily dependent upon the inverse of the local temperature gradient. Criteria were developed from the DNS data (e.g., speed of the ignition front and a critical temperature gradient at the front) to distinguish between the different modes of propagation.

- Charge Separation by Carbon Nanotube/Ferrocene Nanohybrids. Carbon nanotubes, which are chemically stable and electrically conducting, have been modified for the first time by attachment of electron donors, in this case, ferrocene molecules. When excited with visible light, these carbon nanotube-ferrocene hybrids exhibit intramolecular electron transfer to yield long-lived charge-separated species. The carbon nanotube serves as the electron acceptor in the donor-acceptor ensemble, distributing the charge over its extended π-electronic system. The separation of charge is sufficiently long lived to show promise for future development of solar photoelectrochemical cells based on modified carbon nanotubes.
- They Bend Before They Break: Fast Scission of Chemical Bonds. Bond-breaking reactions in liquid solution which are so fast that the rates could not previously be measured, have recently been studied at the new picosecond Laser-Electron Accelerator Facility (LEAF) at Brookhaven National Laboratory. A large class of molecules known as aryl halides was studied, in which a halogen atom, such as chlorine or bromine, dissociates from a sizable planar ring structure, breaking its bond. The newly measured rates can only be explained theoretically if the bond breaks by the halogen atom bending out of plane by about 30 degrees before bond breaking, in a bent transition state. Such fundamental knowledge of the reaction mechanism may lead to improvements in energy efficiency and fewer toxic by-products in large-scale industrial processing.
- Protein-Nanoparticle Hybrid Systems for Light Energy Conversion. Novel protein-nanoparticle hybrid assemblies have been developed that employ semiconductor nanoparticles for initial light-induced charge separation and biomolecules for subsequent chemical/electrical conversion. The end-to-end, wire-like nanorod structures are based on nanoscale metal oxide particles, in which the ability to systematically manipulate size and shape of the nanoparticles was exploited in synthesis of axially anisotropic tubes, cubes, rods, or stars. The nanoparticles were oriented into organized architectures using biolinkers, such as the biotin molecule, that bind strongly to the protein, avidin. Photoexcitation of the wire-like architecture resulted in charge separation originating at the tips of the nanorods: the photogenerated electrons being localized at the semiconductor, and holes at the protein. Thus, a rational design of protein-nanoparticle hybrid architectures enables coupling of photoinduced charge separation in nanocrystallites with the charge-transfer induced chemistry on proteins. The hybrid architectures and ensuing chemistries can either use or alter protein functionality, and could be used for construction of solar-based molecular machines.
- Reverting Carbon Dioxide into Valuable Chemicals. An inexpensive, low-temperature synthetic route for the conversion of carbon dioxide into useful chemicals and fuels is a long-standing

challenge. Despite extensive research, current catalysts still use expensive complexes of platinum-group metals. Recent work has led to a breakthrough in the catalytic addition of hydrogen to carbon dioxide to produce formic acid. Using sophisticated high-throughput techniques to rapidly search for promising catalytic structures, investigators have identified the broadest range to date of hydrogenation catalysts that can sustain high activity for many cycles. These structures consist of phosphine-complexes of copper, chromium, iron, indium, molybdenum, niobium, nickel, or tungsten, all of which are abundant and inexpensive metals. Detailed structural and mechanistic studies have led to even further improvement of the activity and durability by surrounding the metal centers with ligands designed to provide optimum electronic structure while protecting the metals from degradation. The new nickel, copper, and iron phosphine-cyano complexes carry out the production of formic acid at 40 bar and 50^{o}Celsius with limited deactivation for periods of days.

- Pure Hydrogen from Alcohol through Microsecond Catalysis. Researchers have recently shown that it is possible to selectively extract pure hydrogen from ethanol, a renewable fuel made from biomass, in a matter of microseconds. The process is based on a high-temperature ceramic catalyst containing rhodium metal and cerium oxide. At about 800^{o}C, wet ethanol, contacted with the catalyst for about one microsecond, undergoes oxidative dehydrogenation to hydrogen and carbon dioxide, with 95% conversion and 100% selectivity to hydrogen. This remarkable catalytic performance and the low-cost wet alcohol source could result in an economically feasible hydrogen production process for the future, especially as many of these very rapid oxidation reactions are self-sustaining even at 800^{o}C or higher and do not require external heat sources. Advances in this hydrogen production process might provide an alternative to steam reformation of hydrocarbons as a source of hydrogen.

- Benign Polymerization Chemistry Leads to New Polymers. The demand for polymeric materials continues to rise at an impressive rate and, in the near future, environmental conservation may become a major constraint in this expansion. Researchers have long pursued catalysts that take molecules derived from biomass, such as sugars, alcohols, and esters, and convert them with high yield and no waste into synthetic plastics, such as polyethers, polyesters, and polycarbonates, with controlled characteristics. Besides having appropriate thermal and mechanical properties, a significant fraction of future polymers should be biodegradable or biocompatible for use in large-scale packaging or in smaller-scale biomedical applications: drug release membranes, synthetic tissue, and sutures. Recently, investigators have successfully synthesized a family of metal alkoxide catalysts that produce polyesters and blends via ring-opening polymerization of cyclic esters derived from renewable sources. Examples are the synthesis of polylactides from lactides derived from corn and the formation of polycarbonates by ring-opening copolymerization of epoxides-oxiranes and carbon dioxide. The latter is a chemically benign alternative to the current technology for polycarbonate synthesis that uses phosgene, a highly poisonous gas. Through mechanistic, microstructural, and kinetic studies, these investigators are arriving at fundamentally new rules and new catalysts for transformations of oxygenated molecules that may dramatically change the landscape of polymerization chemistry.

- Fundamental Studies on Crown Ethers Benefit Cleanup of Nuclear Waste at Savannah River. Fundamental research has provided the foundation enabling innovative technology for nuclear-waste cleanup at the Savannah River Site (SRS). In early 2004, a large contract was awarded for the design, construction, and commissioning of the Salt Waste Processing Facility (SWPF) to clean up a major portion of some of the nation's most dangerous Cold War era nuclear waste stored at the SRS. Approximately 34 million gallons of waste from nuclear-weapons production are stored in tanks at the SRS. Over 31 million gallons of that waste is solid or dissolved salts in which the fission product cesium-137 comprises more than 98% of the total radioactivity in the salt. In 2001, the Office of Environmental Management chose the Caustic-Side Solvent eXtraction (CSSX) process developed at Oak Ridge National Laboratory for removing cesium-137 from the waste in the SWPF. The selection followed an intensive period of evaluating candidate technologies by a multi-site team of scientists and engineers over a four-year period. Selection was based on the ability of candidate technologies to meet difficult processing requirements, including the ability to remove 99.9975% of the cesium-137 from the waste. Such extraordinary performance requires extraordinary chemistry, which had its roots in fundamental research which focused on the principles of host-guest chemistry, emphasizing the synthesis of tailored molecules that selectively bind (or host) target species. The understanding of host-guest chemistry from this research led to the ability to design the synthesis of crown ethers with appropriate architecture to complex with alkali metal ions to effect extraction with high selectivity.

- Improved Analysis for the Next Generation of Electronic Devices. New research has shown that by covalent Fluorescent Labeling of Surface Species (FLOSS), the inherent sensitivity of fluorescence spectroscopy can be exploited to identify and quantify low concentration functional groups on surfaces. FLOSS enables the detection of surface chemical groups as low as 10^{11} molecules/cm^2 (0.01% of the surface) by specific covalent attachment of fluorescent chromophores to surface functionalities. Advances in electronics and sensors have been made by decreasing the size of the components making electronics faster and sensors more sensitive and selective. These advances provide an important step in our ability to control size and thickness of insulating layers for modern electronic devices. The technique used to develop these films is to expose the surface, such as silicon, to a long chained molecule, and allow it to self assemble on the surface. The length of these chains can then be reduced to control the resistivity by reaction with electrons or ozone, and the pattern they make on the surface can be controlled by ion or electron bombardment using a mask or laser ablation by rastering the beam across the surface. Understanding and controlling the chemistry of these reactions is critical to make the next generation of devices.

- Building Polar Actinide Materials. Compounds that adopt polar structures are able to exhibit a wide range of important technological properties such as second-harmonic generation (nonlinear optics), piezoelectricity, and pyroelectricity. One strategy for constructing polar structures is to use oxoanions containing heavy atoms such as selenium, tellurium, and iodine. These oxoanions share a common feature: they contain a nonbonding pair of electrons that can be aligned during crystal formation to create polar structures. These anions have been combined with the actinide elements uranium, neptunium, and plutonium to create novel polar actinide materials. Some of the neptunium compounds are further unusual in that the distance between neptunium atoms within the crystals can be controlled, allowing magnetic interactions to take place between the actinide elements. This work allows detailed structure-property relationships to be developed in polar actinide materials. These relationships elucidate the properties of 5f electrons, which contribute uniquely to the bonding in actinide materials and provide models for polar materials of nonradioactive transition metals.

- Plutonium Oxide Unraveled. A collaboration of research groups has developed sophisticated quantum chemistry software to model the electronic properties of actinide materials. These computational programs solve the first-principles, basic equations governing the quantum mechanics of electrons and nuclei, to yield predictions about conducting properties, equilibrium structure, and other electronic properties of materials like plutonium oxide (PuO_2). In a recent series of calculations on a cluster of high-performance computers, it was predicted for the first time that PuO_2 is an insulating material with a band gap of a few eV and with ferro- and anti-ferromagnetic phases in close energetic balance. These results are consistent with subsequent experimental data obtained by other researchers. A successful description of electronic properties of PuO_2 is a prerequisite for more elaborated modeling of the interaction of PuO_2 surfaces with water and other environmental species. Understanding these basic processes is essential to predict the long-term stability of PuO_2 when it is exposed to air, water, and other common substances.

- Bioelectrochemistry on Nanostructured Surfaces. A defining feature of modern bioelectrochemistry is extraction of functional biomolecules and their reconstitution on patterned surfaces in defined geometries. The bioelectrochemical process of solar energy absorption and subsequent conversion of light energy uses two molecular reaction centers operating in series, Photosystems I (PSI) and II (PSII). Photon absorption triggers electron transfer reactions that generate an electric voltage. It is this electrochemical potential that is the source of free energy for conversion of light energy into chemical energy. It has been demonstrated for the first time that PSI molecules can be oriented by elementary dipole forces that exist at the air-water interface and the dipole points predominantly towards the water. Orientation was demonstrated by measurement of the magnitude and sign of the electrostatic potential above the PSI-containing air-water interface. Bioreaction centers supported in nanoporous media enable the construction of bioelectrochemical systems for both basic and applied needs.
- Thermophysical Properties of Macromolecular Systems in Nanoscopic Structures. An important part of nanotechnology is to understand whether the properties of polymeric systems in nanoscopic structures are different from those of the bulk. Theoretical studies have established for the first time that nanometer-length structures of polymer glasses exhibit a glass transition temperature which is significantly lower than that of the corresponding bulk polymer. These studies also established that the elastic properties of the polymer in such structures are considerably “weaker” than those of the bulk. Finally, and perhaps most importantly, it has been demonstrated that the elastic moduli of nanoscopic polymeric samples are highly anisotropic, raising serious concerns about the applicability of continuum-mechanics computational approaches for study of such systems. These predictions indicate that the mechanical stability of features smaller than 50 nm is severely degraded. Extrapolation of current technology as applied in the microelectronics industry might not be possible.
- Structure of Electric Double Layer at the Rutile Surface from Molecular Dynamics Simulations. Rutile (α-TiO_2) is the protective surface phase that will cover the drip shields over the waste canisters at the Yucca Mountain waste repository. It is also an important mineral in the chemical and materials industries as a catalytic substrate, photocatalyst, pigment, and ceramic raw material. Molecular simulation of the structure of the relaxed rutile (110) crystal surface in contact with aqueous solutions were performed to determine the structure of water molecules near the interface, adsorption of ions, identification of several modes of binding of adsorbed ions with surface oxygens, and static and dynamic properties of the surface. Quantitative experimental data provided by synchrotron x-ray investigations determined the distribution of adsorbed water molecules and cations at the rutile (110) surface and verified the predictive capabilities of the computational approaches. Computational chemical physics demonstrated the utility of classical models of the macroscopic properties of the electric double layer. Solid-liquid surface properties (colloidal

stability, structure of micelles, membranes, metallurgy, chemical sensors, catalysis, and synthesis of nanophase materials) can now be linked to the atomic-level structural information.

- Water-Driven Structural Transformation in Nanoparticles at Room Temperature. Natural mineralogical nanoparticles exist at ambient temperature, pressure, and humidity in the geosphere. Research on nanoparticulate mineral phases provides understanding of the role of natural nanoparticles and in predicting what the future of "new" nanoparticles will be in the environment. Zinc sulphide nanoparticles (~3nm, 700 atoms) synthesized in methanol exhibited a reversible structural transformation accompanying methanol desorbtion. The binding of water to the as-formed particles at room temperature led to a dramatic structural modification, significantly reducing distortions of the surface and interior to generate a structure close to that of the mineral sphalerite. This shows one route for post-synthesis control of nanoparticles structure, and the potential use of the nanoparticles' structural state as an environmental sensor. The results also demonstrate that the structure and reactivity of natural nanoparticles will depend both on the particle size and on the nature of the surrounding molecules.
- A Molecular Switch Controls Cell Identity. Like its fuzzy, dwarf namesake from the "Star Wars" movie, the YODA (YDA) mutant in Arabidopsis is small but powerful. Recent molecular genetic experiments reveal that YODA acts as a negative regulator of plant cell fate decisions following asymmetric cell divisions. This regulation is essential for establishing normal cell patterns for stomata, tiny surface pores in leaves and shoots. Pore size is regulated by a pair of flanking guard cells that serve as gas valves controlling carbon dioxide and water vapor movement in or out of the leaf. Early in development these cells make an irrevocable decision on whether they will end up as epidermal cells, or undergo an asymmetric division and become guard cells. YODA's kinase activity sends the signal that decides this developmental fate, thus determining the number of stomates on a leaf surface. So as plants grow and form new leaves, they can adjust to factors such as carbon dioxide, and water and light availability by changing stomatal density and distribution. This illustrates how protein-gene interactions within complex regulatory feedback loops and pathways can be deciphered to understand how a group of cells can grow, develop, and adapt to an ever-changing environment in the coordinated form of a whole plant.
- Structural and Functional Analysis of a Minimum Plant Centromere. Every chromosome, the carrier of hereditary information in all living organisms, contains three essential elements: the telomere ends, the origin of replication that initiates copying of genetic information, and the centromeres that direct the partitioning of chromosomes during cell division. Scientists have made a startling discovery about the nature of these centromeres in rice plants. Their sequencing of the centromere of rice chromosome 8 revealed the presence of four active, expressed genes. This discovery refutes long-held scientific beliefs that centromeres contained only structural information for chromosome segregation, programmed within vast stretches of "junk DNA" consisting of repetitive, rearranged and noncoding sequence tracts. This work, significant for being the first completely sequenced plant centromere, complements the international effort to complete the sequence of the rice genome, and represents the first step toward achieving such practical applications as the creation of artificial chromosomes for precision plant engineering.
- The Glass Bead Game of Molecular Detection. A significant challenge in the study of biological systems is the ability to detect molecular interactions with sensitivity and accuracy. Scientists have developed a novel technique for detecting substrate binding to proteins embedded within cellular membranes. Their technique uses the fundamental qualities of colloidal particles, which self-

assemble into a variety of ordered phases in a manner driven by the pair interaction potential between particles. Colloidal suspensions of membrane lipids linked to a specific substrate were coated onto silica beads. When a protein binds to this immobilized substrate, it causes small perturbations on the membrane surface that result in visible reorganization of the colloid, such that the coated beads disperse. The ability to sense molecular interactions without the use of expensive fluorescent probes has practical implications for rapid, high-throughput screening of a variety of interactions between biological molecules.

Selected FY 2004 Facility Accomplishments

- The Combustion Research Facility (CRF)
  - Sample Preparation Laboratory Ready for Advanced Microscopy. A laboratory has been converted to a sample preparation space for the research activities in the Advanced Microscopy Laboratory. The new lab is equipped with instrumentation and supplies for preparing ultra-clean samples critical to single molecule imaging of biomolecules and nanomaterials.
  - Optically Accessible Engine Facility Established. The facility's new automotive-scale Homogeneous-Charge Compression-Ignition (HCCI) engine provides versatile optical access, accommodating the study of combustion via a laser-based investigation of in-cylinder processes. The facility is well suited for the examination of advanced fuel-air mixture preparation strategies that have been proposed as a way of achieving the strong potential of HCCI engines.
  - New Instrument Developed to Investigate Complex Reaction Processes. A new instrument consisting of an ion- and laser-beam surface analysis system coupled to time-of-flight and high-resolution Fourier Transform ion cyclotron resonance mass spectrometers has been built and tested. The instrument is used to investigate complex spatiotemporal reaction processes related to the aging of materials and biological processes at the cellular level.
  - New Laser Diagnostics Measure Diesel Particulate Emissions. Laser-induced incandescence (LII) and Laser-Induced Desorption with Elastic Laser Scattering (LIDELS) are new diagnostic techniques that provide previously unobtainable time-resolved measurements critical for the optimization of engine performance. Real-time measurements are particularly crucial for the development of regeneration strategies for lean NO_x catalysts and diesel particulate filters.

Detailed Program Justification

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
Chemical Sciences, Geosciences, and Energy Biosciences Research	**207,886**	**227,465**	**210,290**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**13,875**	**17,397**	**13,659**

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; and ultracold collisions and quantum condensates.

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

The knowledge and techniques developed in this activity have wide applicability. Results of this research provide new ways to use photons, electrons, and ions to probe matter in the gas and condensed phases. This has enhanced our ability to understand materials of all kinds and enables the full exploitation of the BES synchrotron light sources, electron beam 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 2006, major activities will include the interactions of atoms and molecules with intense laser pulses; 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. A reduction of $3,738,000 in AMO science funding reflects a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research on the physics of highly charged ions and ultracold molecular systems.

	FY 2004	FY 2005	FY 2006
▪ **Chemical Physics Research**	**31,311**	**34,276**	**32,063**

This activity supports experimental and theoretical investigations of gas phase chemistry and chemistry at surfaces. 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 at well characterized surfaces and the reactions of metal and metal oxide clusters leads 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 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 three fundamental research efforts: (1) chemically reacting flows; (2) the chemistry of unstable species and large molecules; and (3) actinide chemistry. 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 2006, there will be increased emphasis on chemical physics of condensed phase and interfacial chemistry, including the fundamental understanding of weak, non-covalent interactions and their relationship to chemical and physical properties of macroscopic systems. A reduction of $2,213,000 in chemical physics research reflects a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research in aspects of gas phase combustion chemistry.

	FY 2004	FY 2005	FY 2006
▪ **Photochemistry and Radiation Research**	**23,849**	**26,416**	**25,582**

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, 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 charge separation in molecule-based biomimetic assemblies should also be applicable in the future development of molecular optoelectronic devices. A strong interface with EE solar conversion programs exists at 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. Fundamental studies on radiation-induced processes complement collocated Nuclear Energy Research Initiative (NERI) and the Environmental Management Science Program (EMSP) projects.

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 2006, 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; and radiolytic processes at interfaces, radiolytic intermediates in supercritical fluids, and characterization of excited states by dual pulse radiolysis/photolysis experiments. The overall decrease for photochemistry and radiation research is attributable to an increase for research related to the hydrogen economy ($+394,000) offset by a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease for research in radiation chemistry ($-1,228,000).

	FY 2004	FY 2005	FY 2006
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	**13,000**	**13,746**	**13,469**

This activity supports fundamental research to characterize the molecular mechanisms involved in the conversion of solar energy to biomass, biofuels, bioproducts, and other renewable energy resources. Research supported includes the characterization of the energy transfer processes occurring during photosynthesis, the kinetic and catalytic mechanisms of enzymes involved in the synthesis of methane, the biochemical mechanisms involved in the synthesis and degradation of lignocellulosics, and the mechanisms of plant oil production. The approaches used include biophysical, biochemical, and molecular genetic analyses. The goal is to enable the future biotechnological exploitation of these processes and, also, to provide insights and strategies into the design of non-biological processes. This activity also encourages fundamental research in the biological sciences that interfaces with other traditional disciplines in the physical sciences.

In FY 2006, funding will continue studies on understanding the constituents and molecular-level interactions within natural photosynthetic systems. Exploiting and mimicking components of natural solar energy conversion will enable future strategies for the bio-inspired design of new energy capture systems. The overall decrease is attributable to an increase for research related to the hydrogen economy ($+186,000) offset by a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research on aspects of electron transfer in photosynthesis ($-463,000).

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
▪ **Metabolic Regulation of Energy Production**	**18,641**	**19,618**	**19,050**

This activity supports fundamental research in regulation of metabolic pathways and the integration of multiple pathways that constitute cellular function. The potential to synthesize an almost limitless variety of energy-rich organic compounds and polymers exists within the genetic diversity of plants and microbes. Understanding and realizing this potential is founded upon characterizing the genetic makeup of the organism and the regulation of these genes by physical and biological parameters. The research goal is to develop a predictive and experimental context for the manipulation and direction of metabolism to accumulate a desired product. Research supported includes the identification and characterization of genes and gene families within the context of metabolic pathways and their regulation by signaling pathways that can impact energy production; this includes understanding the transduction of signals received from physical sources (e.g. light, temperature, and solid surfaces) at the interface between the organism and its environment, as well as the transduction of signals received from biological sources (e.g. developmental programs, symbiotic or syntrophic relationships, and nutrient availability).

In FY 2006, funding will continue studies on Arabidopsis as a model system for the study of other plant systems with broader utility. Increased emphasis will be placed upon understanding interactions that occur within the nanoscale range; this includes signal reception at biological surfaces and membranes, catalytic and enzyme-substrate recognition, and how these molecules transfer within and between cellular components. This activity constitutes the fundamental biological advances needed to complement the chemical nanoscale catalysis activities. An emerging area will be the development of new imaging tools and methods to examine metabolic and signaling pathways and to visualize cellular architecture, at both the physical-spatial and temporal scale. In FY 2006, a reduction of $568,000 reflects a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction in research on the use of microbes and yeasts to convert energy and produce alternative fuels.

▪ **Catalysis and Chemical Transformation**...........	**34,756**	**39,121**	**38,890**

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

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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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 2006, 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 overall decrease for catalysis and chemical transformations research is attributable to an increase for research related to the hydrogen economy ($+588,000) offset by a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research in thermochemical properties ($-819,000).

▪ **Separations and Analyses**	**14,029**	**16,680**	**15,897**

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. 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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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 2006, 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) achieve high temporal resolution, so that changes can be monitored dynamically; and (3) enable multiple analytical measurements to be made simultaneously on systems such as fuel cell membranes, which have three percolation networks (proton, electron, and gas). The overall decrease for separations and analysis is attributable to an increase for research related to the hydrogen economy ($+310,000) offset by a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in modeling of separation systems at the engineering level ($-1,093,000).

	FY 2004	FY 2005	FY 2006
▪ **Heavy Element Chemistry**	**10,359**	**9,912**	**9,547**

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

The heavy element chemistry program, with its genesis in the Manhattan project, has explored the chemical properties of the transuranium and transactinide elements, the latter using techniques developed for isotopes that have half-lives on the order of seconds to tens of seconds. In recent years the emphasis of the program returned to the chemistry of the lighter transuranium elements and fission products, driven by the necessity to identify species found in the waste tanks at the Hanford and Savannah River sites. Knowledge of the molecular speciation of actinide and fission products materials under tank conditions is necessary to treat these complex mixtures. Accidental release of actinide and fission product materials to the environment also requires molecular speciation information in order to predict their fate under environmental conditions. This activity is closely coupled to the BES separations and analysis activity and to the actinide and fission product chemistry efforts in DOE's Environmental Science Program.

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 based at the national laboratories because of the special licenses and facilities needed to obtain and safely handle

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

radioactive materials. However, research in heavy element chemistry is supported at universities, and collaborations between university and laboratory programs are encouraged. The training of graduate students and postdoctoral research associates is viewed as 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 for synchrotron light source experiments to safely handle the actinides.

In FY 2006, 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. 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. A $365,000 decrease reflects a decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction in activities in the role of transuranic elements on the properties of materials.

▪ **Geosciences Research**	**21,356**	**22,599**	**20,423**

The Geosciences activity supports long-term basic research in geochemistry and geophysics. Geochemical research focuses on subsurface solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand physical properties of fluids, rocks, and minerals. 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 high pressure work and scattering, and for experimental, field, and computational capabilities.

In FY 2006, 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. A reduction of $2,176,000 reflects a decrease due to one-time funding of research in geochemistry and geophysics and discontinued research in high resolution imaging of the earth’s crust and the flow of fluids in porous media.

▪ **Chemical Energy and Chemical Engineering**....	**10,837**	**10,492**	**4,244**

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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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 2006, 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 ($-6,248,000).

	FY 2004	FY 2005	FY 2006
▪ **General Plant Projects (GPP)**..............................	**11,380**	**12,800**	**13,408**

GPP funding is increased in FY 2006 for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems principally at the Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the BES stewardship responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Facilities Operations justification in both the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. The total estimated cost of each GPP project will not exceed $5,000,000.

	FY 2004	FY 2005	FY 2006
▪ **General Purpose Equipment (GPE)**	**4,493**	**4,408**	**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.

	FY 2004	FY 2005	FY 2006
Facility Operations..	**5,892**	**6,169**	**6,169**

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

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
Combustion Research Facility..	5,892	6,169	6,169

	FY 2004	FY 2005	FY 2006
	(dollars in thousands)		
SBIR/STTR..	**0**	**5,841**	**5,342**

In FY 2004 $4,825,000 and $579,000 were transferred to the SBIR and STTR programs, respectively. The FY 2005 and FY 2006 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

	FY 2004	FY 2005	FY 2006
Total, Chemical Sciences, Geosciences, and Energy Biosciences..	**213,778**	**239,475**	**221,801**

Explanation of Funding Changes

	FY 2006 vs. FY 2005 ($000)
Chemical Sciences, Geosciences, and Energy Biosciences Research	
▪ **Atomic, Molecular, and Optical (AMO) Science**	
Decrease for atomic, molecular, and optical science because of a one-time funding increase in FY 2005 for all portfolio elements and a reduction for the physics of highly charged ions and ultracold molecular systems..	-3,738
▪ **Chemical Physics Research**	
Decrease for chemical physics research because of a one-time funding increase in FY 2005 for all portfolio elements and a reduction in aspects of gas phase combustion chemistry..	-2,213
▪ **Photochemistry and Radiation Research**	
Overall decrease for photochemistry and radiation research because of increase in research related to the hydrogen economy ($+394,000) and decrease due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction for research in radiation chemistry ($-1,228,000)...	-834
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	
Overall decrease in molecular mechanisms of natural solar energy conversion because of increase for research related to the hydrogen economy ($+186,000) and reduction due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction for research in aspects of electron transfer related to photosynthesis ($-463,000)	-277
▪ **Metabolic Regulation of Energy Production**	
Decrease in metabolic regulation of energy production research due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction in the area of production of alternate fuels by yeasts and microbes..	-568

	FY 2006 vs. FY 2005 ($000)
▪ **Catalysis and Chemical Transformation**	
Overall decrease in catalysis and chemical transformations for research because of increase for research related to the hydrogen economy ($+588,000) and reduction due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research in thermochemical properties ($-819,000)	-231
▪ **Separations and Analyses**	
Overall decrease in separations and analyses because of increase for research related to the hydrogen economy ($+310,000) and reduction due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research for modeling systems at the engineering level ($-1,093,000)	-783
▪ **Heavy Element Chemistry**	
Decrease for heavy element chemistry due to a one-time funding increase in FY 2005 for all portfolio elements and a decrease in research on the role of transuranics on the properties of materials	-365
▪ **Geosciences Research**	
Decrease in geosciences research due to a one-time funding increase in FY 2005 for all portfolio elements and a reduction in the areas of high resolution imaging of the earth's crust and the flow of fluids in porous media	-2,176
▪ **Chemical Energy and Chemical Engineering**	
Decrease in chemistry and chemical engineering because of reduction in research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research.	-6,248
▪ **General Plant Projects**	
Increase in general plant projects intended to help alleviate recurring maintenance costs by improving infrastructure ($+258,000) and an FY 2005 transfer between GPP and GPE ($+350,000)	+608
▪ **General Purpose Equipment**	
Decrease due to FY 2005 transfer between GPE and GPP	-350
SBIR/STTR	
Decrease in SBIR/STTR funding because of a decrease in operating expenses	-499
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	**-17,674**

Construction

Funding Schedule by Activity

(dollars in thousands)

	FY 2004	FY 2005	FY 2006	$ Change	% Change
Construction					
Spallation Neutron Source (ORNL)	123,865	79,891	41,744	-38,147	-47.7%
Project Engineering Design, Nanoscale Science Research Centers	2,982	1,996	0	-1,996	-100.0%
Project Engineering Design, Linac Coherent Light Source (SLAC)	7,456	19,914	2,544	-17,370	-87.2%
Linac Coherent Light Source (SLAC)	0	29,760	83,000	+53,240	+178.9%
Center for Functional Nanomaterials (BNL)	0	18,317	36,553	+18,236	+99.6%
The Molecular Foundry (LBNL)	34,794	31,828	9,606	-22,222	-69.8%
Center for Nanophase Materials Science (ORNL)	19,882	17,669	0	-17,669	-100.0%
Center for Integrated Nanotechnologies (SNL/LANL)	29,674	30,650	4,626	-26,024	-84.9%
Total, Construction	218,653	230,025	178,073	-51,952	-22.6%

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, radiation 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 Spallation Neutron Source, the four Nanoscale Science Research Centers, and the Linac Coherent Light Source – 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 2004	FY 2005	FY 2006
▪ **Spallation Neutron Source (SNS)**	**123,865**	**79,891**	**41,744**

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 completed in 2006, the SNS will be significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence – ISIS at the Rutherford Laboratory in England. 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 will consist 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 2004	FY 2005	FY 2006

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 $7,387,000 in FY 2004, $7,643,000 in FY 2005, and $8,079,000 in FY 2006. 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.

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.

FY 2005 budget authority was requested to continue R&D, procurement, and installation of equipment for instrument systems. Commissioning of Linac Systems will be completed. Commissioning of the high-energy beam transport and accumulator ring will begin; installation and testing for the ring-target beam transport system will be performed. Installation and testing will be performed and preparation for the read, mess review will start for target systems. The remaining major construction contracts will be completed. Procurement, installation, and testing will continue for integrated control systems.

FY 2006 budget authority is requested to 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 remains constant at $1,411,700,000, and the construction schedule continues to call for project completion by mid-2006. Additional information on the SNS Project is provided in the SNS construction project data sheet, project number 99-E-334.

	FY 2004	FY 2005	FY 2006
▪ **Project Engineering and Design, Nanoscale Science Research Centers**....................................	**2,982**	**1,996**	**0**

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 will be 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.

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006
▪ **Project Engineering and Design, Linac Coherent Light Source**..	**7,456**	**19,914**	**2,544**

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

	FY 2004	FY 2005	FY 2006
	(dollars in thousands)		

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.

FY 2006 Project Engineering Design (PED) funding of $2,544,000 is requested for 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 2004	FY 2005	FY 2006
▪ **Linac Coherent Light Source**	**0**	**29,760**	**83,000**

FY 2005 budget authority was requested 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. The Total Estimated Cost (TEC) is $315,000,000 and the Total Project Cost is $379,000,000.

FY 2006 budget authority is requested to initiate 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.

	FY 2004	FY 2005	FY 2006
▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, Brookhaven National Laboratory**	**0**	**18,317**	**36,553**

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 2006 funding is requested to continue 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 follows later in construction project data sheet 05-R-321.

	FY 2004	FY 2005	FY 2006
▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL**	**34,794**	**31,828**	**9,606**

The Molecular Foundry, a BES Nanoscale Science Research Center, will focus its research on the interface between soft materials like 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,

	(dollars in thousands)		
	FY 2004	FY 2005	FY 2006

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 funding continued construction and equipment procurement, and FY 2006 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 follows later in construction project data sheet 04-R-313.

	FY 2004	FY 2005	FY 2006
▪ **Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL**	**19,882**	**17,669**	**0**

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 to be located at Oak Ridge National Laboratory. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet.

	FY 2004	FY 2005	FY 2006
▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, Sandia National Laboratories/Los Alamos National Laboratory**	**29,674**	**30,650**	**4,626**

The Center for Integrated Nanotechnologies (CINT), a BES Nanoscale Science Research Center, will focus on exploring the path from scientific discovery to the integration of nanostructures into the micro- and macro-worlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. CINT will be jointly administered by Los Alamos National Laboratory 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 2004	FY 2005	FY 2006
	(dollars in thousands)		

FY 2004, and FY 2005 funding was requested for the construction for the Center for Integrated Nanotechnologies managed jointly by Sandia National Laboratories and Los Alamos National Laboratory. FY 2006 funding is requested to complete this construction. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information follows later in construction project data sheet 03-R-313.

Total, Construction	**218,653**	**230,025**	**178,073**

Explanation of Funding Changes

	FY 2006 vs. FY 2005 ($000)
▪ **Spallation Neutron Source**	
Decrease in funding for construction of the Spallation Neutron Source at ORNL, representing the scheduled ramp down of activities.	-38,147
▪ **Project Engineering and Design, Nanoscale Science Research Centers**	
Decrease in Project Engineering and Design (PED) for Nanoscale Science Research Centers at ORNL, LBNL, SNL, and BNL, representing the scheduled change in PED funding profiles.	-1,996
▪ **Project Engineering and Design, Linac Coherent Light Source**	
Decrease in funding for Project Engineering Design (PED) related to design-only activities for the Linac Coherent Light Source (LCLS) at SLAC, representing the scheduled decrease in activities.	-17,370
▪ **Linac Coherent Light Source**	
Increase in funding to initiate construction for the LCLS project.	+53,240
▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, Brookhaven National Laboratory**	
Increase in funding for construction of the Center for Functional Nanomaterials at BNL.	+18,236
▪ **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.	-22,222

	FY 2006 vs. FY 2005 ($000)
▪ **Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL**	
Decrease in funding for construction of the Center for Nanophase Materials Sciences at ORNL, representing the scheduled ramp down of activities.	-17,669
▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies Sandia National Laboratories/Los Alamos National Laboratory**	
Decrease in funding for construction of the Center for Integrated Nanotechnologies at SNL/LANL, representing the scheduled ramp down of activities.	-26,024
Total Funding Change, Construction	**-51,952**

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 2004	FY 2005	FY 2006	$ Change	% Change
Major User Facilities					
Advanced Light Source at Lawrence Berkeley National Laboratory	43,937	45,600	42,367	-3,233	-7.1%
Advanced Photon Source at Argonne National Laboratory	95,740	99,950	98,000	-1,950	-2.0%
National Synchrotron Light Source at Brookhaven National Laboratory	37,398	37,400	37,400	0	0.0%
Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.	29,670	30,654	28,300	-2,354	-7.7%
High Flux Isotope Reactor at Oak Ridge National Laboratory.	40,284	46,930	40,032	-6,898	-14.7%
Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	6,100	4,500	0	-4,500	-100.0%
Intense Pulsed Neutron Source at Argonne National Laboratory.	16,768	17,055	17,055	0	0.0%
Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	9,844	10,053	10,300	+247	+2.5%
Spallation Neutron Source at Oak Ridge National Laboratory.	18,397	33,100	106,872	+73,772	+222.9%
Combustion Research Facility at Sandia National Laboratories/California.	5,892	6,169	6,169	0	0.0%
Center for Nanoscale Materials at Argonne National Laboratory	0	0	3,894	+3,894	—
Molecular Foundry at Lawrence Berkeley National Laboratory	0	0	8,554	+8,554	—
Center for Nanophase Materials Sciences at Oak Ridge National Laboratory	0	0	18,086	+18,086	—
Center for Integrated Nanotechnologies at Sandia National Laboratories/Albuquerque and Los Alamos National Laboratory	0	0	12,709	+12,709	—
Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center	0	0	3,500	+3,500	—
Linac for LCLS	0	0	30,000	+30,000	—
Total, Major User Facilities	304,030	331,411	463,238	+131,827	+39.8%

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 2004	FY 2005	FY 2006	$ Change	% Change
General Plant Projects	12,958	14,387	13,830	-557	-3.9%
Accelerator Improvement Projects	6,100	9,255	9,259	+4	+0.0%
Capital Equipment	83,795	87,993	99,362	+11,369	+12.9%
Total, Capital Operating Expenses	102,853	111,635	122,451	+10,816	+9.7%

Construction Projects

	(dollars in thousands)					
	Total Estimated Cost (TEC)	Prior Year Appro-priations	FY 2004	FY 2005	FY 2006	Unappro-priated Balances
05-R-320, SLAC, Linac Coherent Light Source	315,000[a]	0	0	29,760	83,000	166,240
05-R-321, BNL, Center for Functional Nanomaterials	79,700[b]	0	0	18,317	36,553	18,864
04-R-313, LBNL, The Molecular Foundry	83,700[c]	0	34,794	31,828	9,606	257
03-SC-002, PED, SLAC, Linac Coherent Light Source	36,000	5,925	7,456	19,914	2,544	161
03-R-312, ORNL, Center for Nanophase Materials Sciences	63,740[d]	23,701	19,882	17,669	0	0
03-R-313, SNL, Center for Integrated Nanotechnologies	73,800[e]	4,444	29,674	30,650	4,626	247
02-SC-002 PED, Nanoscale Science Research Centers	19,828	14,850	2,982	1,996	0	0
99-E-334, ORNL, Spallation Neutron Source	1,192,700	947,200	123,865	79,891	41,744	0
Total, Construction			218,653	230,025	178,073	185,769

[a] Includes $36,000,000 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 2004	FY 2005	FY 2006	Acceptance Date
ANL Center for Nanophase Materials	72,500[a]	36,000	0	10,000	12,000	14,000	FY 2006
SNS Instrumentation[b] ...	50–75,000	50–75,000	5,635	7,387	7,643	8,079	FY07–11 est.
Transmission Electron Aberration Corrected Microscope	25– 30,000	11,200–13,500	0	0	0	2,000	TBD
Total, Major Items of Equipment.....................				17,387	19,643	24,079	

[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.

05-R-320, Linac Coherent Light Source, Stanford Linear Accelerator Center, Menlo Park, California

(Changes from FY 2005 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

The scope of work in FY 2005 has been expanded to include modification of existing facilities at the Stanford Linear Accelerator Center for testing of the long-lead equipment items.

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost[a] ($000)	Total Project Cost[a] ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 2005 Budget Request *(Preliminary Estimate)*................	2Q 2003	4Q 2006	1Q2006	4Q2008	260,000	315,000
FY 2006 Budget Request *(Performance Baseline)*..............	2Q 2003	4Q 2006	3Q2006	2Q2009	315,000	379,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering Design			
2003	5,925 [b]	5,925 [b]	3,644
2004	7,456 [b]	7,456 [b]	9,670
2005	19,914 [b]	19,914 [b]	17,664
2006	2,544 [b]	2,544 [b]	4,861
2007	161 [b]	161 [b]	161
Construction			
2005	29,760[cd]	29,760[cd]	25,280
2006	83,000	83,000	78,625
2007	105,740[d]	105,740[d]	99,800
2008	50,500	50,500	62,320
2009	10,000	10,000	12,975

[a] The full project TEC and TPC, established at Critical Design 2b (Approved Performance Baseline), are $315,000,000 and $379,000,000, respectively.

[b] PED funding was reduced by $75,000 as a result of the FY 2003 general reduction and rescission, by $44,000 as a result of the FY 2004 rescission, and by $161,000 as a result of the FY 2005 rescission. This total reduction is restored in FY 2005, FY 2006, and FY 2007 to maintain the TEC and project scope.

[c] FY 2005 funding in FY 2005 President's Request was for long-lead procurements. The scope of work in FY 2005 has been expanded to include modification of existing facilities at the Stanford Linear Accelerator Center for testing of the long-lead equipment items.

[d] Construction funding was reduced by $240,000 as a result of the FY 2005 rescission. This total reduction is restored in FY 2007 to maintain the TEC and project scope.

3. Project Description, Justification and Scope

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 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 revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray Free Electron Laser (FEL) in the 1.5 - 15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems described below. This will be the world's first such facility.

The LCLS is based on the existing SLAC linac. The SLAC linac can accelerate electrons or positrons to 50 GeV for colliding beam experiments and for nuclear and high-energy physics experiments on fixed targets. At present, the first two-thirds of the linac is being used to inject electrons and positrons into PEP-II, and the entire linac is used for fixed target experiments. When the LCLS is completed, the latter activity will be limited to 25 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 75 percent of the available beam time. For the LCLS, the linac will produce high-brightness 5 - 15 GeV electron bunches at a 120 Hertz repetition rate. When traveling through the new 120 meter long LCLS undulator, these electron bunches will amplify the emitted x-ray radiation to produce an intense, coherent x-ray beam for scientific research.

The LCLS makes use of technologies developed for SLAC and the next generation of linear colliders, as well as the progress in the production of intense electron beams with radiofrequency photocathode guns. These advances in the creation, compression, transport, and monitoring of bright electron beams make it possible to base this next generation of x-ray synchrotron radiation sources on linear accelerators rather than on storage rings.

The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called "table-top" x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing 10^{11} x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific application in the chemical, material, and biological sciences.

The LCLS Project requires a 135 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 undulator and associated equipment. Two new buildings, the Near Experimental Hall and the Far Experimental Hall, will be constructed and connected by the beam line tunnel. A Central Laboratory and Office Building will be constructed to provide laboratory and office space for LCLS users and serve as a center of excellence for basic research in x-ray physics and ultrafast science.

The combined characteristics (spectral content, peak power, pulse duration, and coherence) of the LCLS beam are far beyond those of existing light sources. The demands placed on the x-ray instrumentation and optics required for scientific experiments with the LCLS are unprecedented. The LCLS experimental program will commence with: measurements of the x-ray beam characteristics and tests of the capabilities of x-ray optics; instrumentation; and techniques required for full exploitation of the scientific potential of the facility. For this reason, the project scope includes a comprehensive suite of instrumentation for characterization of the x-ray beam and for early experiments in atomic, molecular, and optical physics. The experiments include x-ray multiphoton processes with isolated atoms, simple molecules, and clusters. Also included in the scope of the LCLS Project are the instrumentation and infrastructure necessary to support research at the LCLS, such as experiment hutches and associated interlock systems; computers for data collection and data analysis; devices for attenuation and collimation of the x-ray beam; prototype optics for manipulation of the intense x-ray beam; and synchronized pump lasers.

Beyond the scope of the LCLS construction project, an instrument development program has been implemented in order to qualify and provide instruments for the LCLS. Instrument proposals will undergo a scientific peer review process to evaluate technical merit; those concepts that are accepted may then establish interface agreements with the LCLS Project. Expected funding sources include appropriated funds through the Department of Energy and other Federal agencies, private industry, and foreign entities. These instruments will all be delivered after completion of the LCLS line item project. The LCLS Scientific Advisory Committee, working in coordination with the broad scientific community, has already identified a number of high priority initial experiments that are summarized in the document, *LCLS: The First Experiments*. Five specific areas of experimentation are: fundamental studies of the interaction of intense x-ray pulses with simple atomic systems; use of LCLS to create warm dense matter and plasmas; structural studies on single nanoscale particles and biomolecules; ultrafast dynamics in chemistry and solid-state physics; and studies of nanoscale structure and dynamics in condensed matter. The combination of extreme brightness and short pulse length will make it possible to follow dynamical processes in chemistry and condensed matter physics in real time. It may also enable the determination of the structure of single biomolecules or small nanocrystals using only the diffraction pattern from a single moiety. This application has great potential in structural biology, particularly for important systems, such as membrane proteins, which are virtually uncharacterized by x-ray crystallography because they are nearly impossible to crystallize. Instrument teams will form to propose instruments to address these and other scientific areas of inquiry.

Construction funding requested in FY 2005 is for selected long-lead items, and the necessary refurbishment of existing space to provide for a magnet measurement facility for the testing of the long-lead equipment. Early acquisition of selected critical path items will support pivotal schedule and technical aspects of the project. These include acquisition of the 135 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 systems required to produce electron beams meeting the stringent requirements of the LCLS FEL. Early acquisition of the 135 MeV injector is required in order that first tests of the FEL can begin. Acquisition of the undulators in FY 2005 will allow delivery in FY 2007, which in turn will enable achievement of performance goals in FY 2009. The main linac magnets and radiofrequency systems must be ready for operation shortly after the linac has reached its performance goals.

The FY 2006 funding is requested to initiate 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.

4. Details of Cost Estimate

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	18,200	18,500
Design Management costs (1.6% of TEC)	5,000	5,000
Project Management costs (1.6% of TEC)	5,100	5,000
Total Design Costs	28,300	28,500
Construction Phase		
Improvements to Land	9,000	8,000
Buildings	54,100	36,300
Other Structures	6,600	1,800
Special Equipment	105,800	98,000
Inspection, design and project liaison, testing, checkout and acceptance	8,000	4,500
Construction Management (2.9% of TEC)	9,000	6,000
Project Management	15,700	11,700
Total, Construction Costs	208,200	166,300
Contingencies		
Design Phase (2.4% of TEC)	7,700	7,500
Long Lead Procurements (2.1% of TEC)	6,500	6,000
Construction Phase (20.4% of TEC)	64,300	51,700
Total, Contingencies (24.9% of TEC)	78,500	65,200
Total, Line Item Costs (TEC)	315,000	260,000

5. Method of Performance

A Conceptual Design Report (CDR) for the project has been completed and reviewed. Key design activities are being specified in the areas of the injector, undulator, x-ray optics and experimental halls to reduce schedule risk to the project and expedite the startup. Also, the LCLS management systems are being put in place and tested during the Project Engineering Design (PED) phase. These activities are managed by the LCLS Project Office at SLAC, with additional portions of the project being executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL). The design of technical systems is being accomplished by the three collaborating laboratories. The conventional construction design aspect (experimental halls, tunnel connecting the halls, and a Central Laboratory and Office Building) was contracted to an experienced Architect/Engineering (A/E) firm to perform Title I and II design. Title I design was completed in FY 2004. Title II design began in FY 2005.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2004	FY 2005	FY 2006	Outyears	Totals
Facility Cost						
PED	3,644	9,670	17,664	4,861	161	36,000
Long-Lead Procurements	0	0	25,280	4,720	0	30,000
Construction	0	0	0	73,905	175,095	249,000
Total, Line Item TEC	3,644	9,670	42,944	83,486	175,256	315,000
Other project costs						
Research & Development	0	1,750	4,250	0	0	6,000
Conceptual Design	1,470	0	0	0	0	1,470
NEPA documentation costs	30	0	0	0	0	30
Pre-operations	0	0	0	3,500	45,000	48,500
Spares	0	0	0	0	8,000	8,000
Total, Other Project Costs	1,500	1,750	4,250	3,500	53,000	64,000
Total Project Cost (TPC)	5,144	11,420	47,194	86,986	228,256	379,000

7. Related Annual Funding Requirements

(FY 2010 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs	$50,000	$50,000
Total related annual funding	$50,000	$50,000

FY 2010 is expected to be the first full year of LCLS facility operations. The current estimate is preliminary and based on historical experience with operating similar types and sizes of facilities. This estimate will be refined as the LCLS Project matures.

The estimate includes LCLS facility operations only. It does not include SLAC linac operations which is funded by HEP in FY 2005 and prior, but begins 3-4 year transition to BES funding beginning in FY 2006. Operation of the SLAC Linac is essential to the operation of the LCLS.

05-R-321, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York

(Changes from FY 2005 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

While advancing Project Engineering Design and establishing project baseline, the Center for Functional Nanomaterials (CFN) Laboratory/Office building has been increased from approximately 85,000 gross square feet to 94,500 gross square feet, to optimize clean room space and building performance. There is no increase to the Total Project Cost (TPC).

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($000)	Total Project Cost ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 2005 Budget Request *(Preliminary Estimate)*	4Q 2003	4Q 2004	3Q 2005	2Q 2008	79,700	81,000
FY 2006 Budget Request *(Performance Baseline)*	4Q 2003	4Q 2004	3Q 2005	3Q 2008	79,700	81,000

2. Financial Schedule

(Dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering & Design (PED)			
2003	988[a]	988[a]	733
2004	2,982[a]	2,982[a]	2,721
2005	1,996[ab]	1,996[b]	2,152
2006	0	0	360
Construction			
2005	18,317[ab]	18,317[ab]	13,801
2006	36,553[a]	36,553[a]	34,983
2007	18,864[b]	18,864[b]	23,371
2008	0	0	1,579

[a] PED funding was reduced by $12,000 as a result of the FY 2003 general reduction and rescission, and by $18,000 as a result of the FY 2004 rescission. This total reduction is restored in FY 2005 and FY 2006 to maintain the TEC and project scope.

[b] PED funding was reduced by $16,000 and construction funding by $148,000 as a result of the FY 2005 rescission. This reduction is restored in FY 2007 to maintain the project scope and TEC.

3. Project Description, Justification and Scope

This project will establish a Nanoscale Science Research Center (NSRC) at BNL. The scientific theme of the BNL Center for Functional Nanomaterials (CFN) is "atomic tailoring of functional nanomaterials to achieve a specific response." The CFN will be a user facility designed to provide a wide range of tools for the preparation and characterization of nanomaterials. The CFN will seek to integrate these unique capabilities with other BNL facilities, including the broad range of synchrotron characterization techniques available at the National Synchrotron Light Source (NSLS).

The CFN will be a new building, located across the street from the existing NSLS. Siting of the CFN will take advantage of close proximity to the Instrumentation Division and the Departments of Physics, Materials Science, and NSLS, which are key interdisciplinary participants in nanoscience research.

The design and scope of the CFN will fulfill DOE mission needs and incorporate input from potential users, gained through many channels including outreach efforts such as workshops. An essential component of the project is to establish an organizational infrastructure open to external users based on peer review. In this way a truly national nanomaterials effort can create breakthrough opportunities. The laboratory areas are organized into seven facility themes established to provide the necessary primary user service. Facility theme functions cover a wide range of physical and chemical synthesis and characterization. They are designated Nanopatterning, Ultrafast Optical Sources, Electron Microscopy, Materials Synthesis, Proximal Probes, Theory and Computing, and CFN Endstations at NSLS. The CFN will allow users to control processes, tailoring the properties of materials structured on the nanoscale. Some of these materials, all relevant to the BES mission, include piezoelectrics, ferroelectrics, organic films and conductors, magnetic nanocomposites, and catalysts.

This effort began with preliminary engineering (Title I) and detailed engineering design (Title II) necessary to construct a BNL Center for Functional Nanomaterials. The engineering effort includes all engineering phase activities, including field investigation, preliminary design, specifications and drawings for conventional construction, final design, preparation of procurement documents for experimental equipment, and construction/equipment procurement estimates.

The completed design will enable construction of a new two-story Laboratory/Office building of approximately 94,500 gross square feet. The facility will include clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be some of the equipment necessary to explore, manipulate and fabricate nanoscale materials and structures. Also included are individual offices and landscape office areas, seminar area, transient user space for visiting collaborators with access to computer terminals, conference areas on both floors, and vending/lounge areas. In addition it will include circulation/ancillary space, including mechanical equipment areas, corridors, and other support spaces.

Technical procurement for the project will include an initial suite of laboratory equipment for the CFN laboratory themes: Nanopatterning, Ultrafast Optical Sources, Electron Microscopy, Materials Synthesis, Proximal Probes, and Theory and Computing as well as for the CFN Endstations at NSLS.

The FY 2005 funds for the CFN will be used to complete project engineering and design, and begin conventional construction and technical equipment procurement. FY 2006 funds will be used to continue conventional construction and technical equipment procurement.

The building will incorporate human factors into its design to encourage peer interactions and collaborative interchange by BNL staff and CFN users and visitors. In addition to flexible office and laboratory space it will provide "interaction areas" including a seminar room and a lunch room for informal discussions. This design approach is considered state-of-the-art in research facility design as it leverages opportunities for the free and open exchange of ideas essential to creative research processes.

4. Details of Cost Estimate

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications at $2,708K)	3,283	3,105
Project Management costs (2.4% of TEC)	1,921	1,820
Design Management Costs (0.5% of TEC)	361	415
Total, Design Costs (7.0% of TEC)	5,565	5,340
Construction Phase		
Technical Facilities		
Equipment	25,821	29,480
Inspection, design & project liaison, testing, checkout and acceptance	218	330
Project Management (0.1% of TEC)	58	135
Total, Technical Costs	26,097	29,945
Conventional Facilities		
Improvements to Land	865	945
Building Construction	28,457	23,465
Site Utilities	4,527	4,420
Standard Equipment	903	920
Inspection, design & project liaison, testing, checkout and acceptance	542	875
Project Management (1.9% of TEC)	1,477	1,725
Total, Construction Costs	36,771	32,350
Contingencies		
Design Phase (0.5% of TEC)	401	642
Construction Phase (13.6% of TEC)	10,866	11,423
Total Contingencies	11,267	12,065
Total, Line Item Costs (TEC)	79,700	79,700

5. Method of Performance

Design and inspection of the facilities and equipment will be by the operating contractor and A/E subcontractor as appropriate. Technical construction will be competitively bid, lump sum contracts. To the extent feasible, construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Years	FY 2004	FY 2005	FY 2006	Outyears	Total
Project Cost						
Facility Cost						
Design	733	2,721	2,152	360	0	5,966
Construction	0	0	13,801	34,983	24,950	73,734
Total, Line Item TEC	733	2,721	15,953	35,343	24,950	79,700
Other Project Costs						
Conceptual design cost [a]	280	0	0	0	0	280
NEPA Documentation Costs	10	0	0	0	0	10
Other project-related costs	10	0	0	0	1,000	1,010
Total, Other Project Costs	300	0	0	0	1,000	1,300
Total, Project Cost (TPC)	1,033	2,721	15,953	35,343	25,950	81,000

7. Related Annual Funding Requirements

(FY 2009 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs	18,500	18,500
Total annual operating funding	18,500	18,500

[a] Experimental research will begin at the time of beneficial occupancy of the facility. These research costs are not part of the TPC and are funded by BES.

04-R-313, Molecular Foundry
Lawrence Berkeley National Laboratory, Berkeley, California

(Changes from the FY 2005 Congressional Budget Request denoted with a vertical line in the left margin)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($000)	Total Project Cost ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 2004 Budget Request *(Preliminary Estimate)*	3Q 2002	1Q 2004	2Q 2004	2Q 2006	83,700	85,000
FY 2005 Budget Request *(Performance Baseline)*	3Q 2002	1Q 2004	2Q 2004	1Q 2007	83,700	85,000
FY 2006 Budget Request...............	3Q 2002	1Q 2004	2Q 2004	1Q 2007	83,700	85,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering And Design (PED)			
2002	500	500	38
2003	6,715[a]	6,715[a]	5,263
2004	0	0	1,896
2005	0	0	18
Construction			
2004	34,794[b]	34,794[b]	11,583
2005	31,828[ac]	31,828[ac]	34,013
2006	9,606[b]	9,606[b]	29,052
2007	257[c]	257[c]	1,837

[a] PED funding was reduced by $85,000 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission was restored in the FY 2005 request to maintain the TEC and project scope.
[b] Construction funding was reduced by $207,000 as a result of the FY 2004 rescission. This reduction is restored in the FY 2006 request to maintain the TEC and project scope.
[c] Construction funding was reduced by $257,000 as a result of the FY 2005 rescission. This reduction is restored in the FY 2007 request to maintain the TEC and project scope.

3. Project Description, Justification and Scope

The proposed Molecular Foundry at LBNL will be a new structure near the National Center for Electron Microscopy. The project includes an approximately 89,000 gross square foot research building, a separate approximately 6,000 gross square foot utility center, and an initial set of special equipment to support nanoscale scientific research. The research building will be an advanced facility with state-of-the-art clean rooms for the design, modeling, synthesis, processing, fabrication and characterization of novel molecules and nanoscale materials. Space in the new facility will support studies in nanostructures by providing offices and laboratories for materials science, physics, chemistry, biology, and molecular biology. These laboratories, equipped with advanced instrumentation and staffed by full-time, dedicated staff scientists and technicians, will be user facilities, available to scientists from universities, industry, and government laboratories whose research proposals will have been peer reviewed by a Proposal Study Panel. This combination of advanced equipment, collaborative staff, and breadth across disciplines will allow users to explore the frontiers of nanoscience.

The goals and operation of the Molecular Foundry are consistent with DOE guidance and address the research challenges described in the reports *Nanoscale Science, Engineering and Technology Research Directions* and *Complex Systems: Science for the 21st Century.* The Foundry's laboratories will be designed and constructed to facilitate collocation of research activities in a wide variety of fields, as required for progress in this new area of science. The Foundry will support a broad research effort focusing on both "hard" nanomaterials (nanocrystals, tubes, and lithographically patterned structures) and "soft" nanometer-sized materials (polymers, dendrimers, DNA, proteins, and whole cells), as well as design, fabrication, and study of multi-component, complex, functional assemblies of such materials.

By functioning as a "portal" to Lawrence Berkeley National Laboratory's established major user facilities, the Foundry will also leverage existing nanoscience research capabilities at the Advanced Light Source, the National Center for Electron Microscopy, and the National Energy Research Scientific Computing Center. The research program will, as an additional benefit, provide significant educational and training opportunities for students and postdoctoral fellows as the "first true generation" of nanoscientists.

FY 2004 funding is being used to initiate construction to complete site preparation, and for equipment procurement. FY 2005 and FY 2006 funding will be used to continue conventional construction and equipment procurement.

4. Details of Cost Estimate[a]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary Design & Final Design	5,010	4,877
Design Management costs (2.6% of TEC)	2,205	1,570
Total, Design Costs (8.6% of TEC)	7,215	6,447
Construction Phase		
Building & Improvements to land	49,444	47,450
Special Equipment[b]	15,056	15,000
Inspection, design and project liaison, check out	2,057	2,446
Construction Management & Project Management (2.2% of TEC)	1,806	2,106
Total, Construction Costs	68,363	67,002
Contingencies		
Design Phase (0.0% of TEC)	0	768
Construction Phase (9.7% of TEC)	8,122	9,483
Total, Contingencies (9.7% of TEC)	8,122	10,251
Total, Line Item Costs (TEC)	83,700	83,700

5. Method of Performance

An Architect Engineering firm (AE) with appropriate multi-disciplinary design experience has prepared a building program and design criteria with the support of the LBNL Facilities Department. The AE also prepared Title I and II design and is providing technical oversight during Title III construction. A Construction Management (CM) contractor performed cost, schedule, and constructability reviews during design. Selection of the CM contractor during the design phases was based on competitive bidding of the Construction General Conditions. The CM contract has an option for management of the construction process. At the completion of design, the CM contractor bid out the design to subcontractors. The University has exercised its option to proceed with the CM contractor. Construction subcontract(s) are awarded on a competitive basis using best value source selection criteria that include price, safety, and other considerations.

[a] This cost estimate is based on Title II design. The annual escalation rates assumed in the FY 2004 estimate for FY 2003 through FY 2007, are 2.1%, 2.5%, 2.9%, 2.8% and 2.6% respectively.
[b] Initial research equipment.

6. Schedule of Project Funding

	(dollars in thousands)					
	Prior Years	FY 2004	FY 2005	FY 2006	Outyears	Total
Facility Cost						
PED	5,301	1,896	18	0	0	7,215
Construction	0	11,583	34,013	29,052	1,837	76,485
Total, Line Item TEC	5,301	13,479	34,031	29,052	1,837	83,700
Other Project Costs						
Conceptual design cost	730	0	0	0	0	730
NEPA Documentation Costs	40	0	0	0	0	40
Other project-related costs[a]	162	0	0	368	0	530
Total, Other Project Costs	932	0	0	368	0	1,300
Total, Project Costs (TPC)	6,233	13,479	34,031	29,420	1,837	85,000

7. Related Annual Funding Requirements

	(FY 2007 dollars in thousands)	
	Current Estimate	Previous Estimate
Annual facility operating costs	18,500	18,000
Total related annual funding	18,500	18,000

[a] Includes tasks such as safety documentation, ES&H monitoring, operations and maintenance support, readiness assessment, and preoperational start-up. Experimental research will begin at the time of beneficial occupancy of the facility. These research costs are not part of the TPC and will be funded by the BES program.

03-SC-002, Project Engineering Design (PED), Linac Coherent Light Source, Stanford Linear Accelerator Center

(Changes from the FY 2005 Congressional Budget Request are denoted with a vertical line in the left margin.)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost[a] ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete	
FY 2003 Budget Request *(Preliminary Estimate)*	1Q 2003	2Q 2005	N/A	N/A	33,500
FY 2004 Budget Request	1Q 2003	4Q 2006	N/A	N/A	36,000
FY 2005 Budget Request	2Q 2003	4Q 2006	N/A	N/A	36,000
FY 2006 Budget Request *(Performance Baseline)*	2Q 2003	4Q 2006	N/A	N/A	36,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2003	5,925[b]	5,925[b]	3,644
2004	7,456[b]	7,456[b]	9,670
2005	19,914[b]	19,914[b]	17,664
2006	2,544[b]	2,544[b]	4,861
2007	161[b]	161[b]	161

3. Project Description, Justification and Scope

These funds allow the Linac Coherent Light Source (LCLS), located at the Stanford Linear Accelerator Center (SLAC), to proceed from conceptual design into preliminary design (Title I) and definitive design (Title II). The design effort will be sufficient to assure project feasibility, define the scope, provide detailed estimates of construction costs based on the approved design, working drawings and specifications, and provide construction schedules including procurements. The design effort will ensure that construction can physically start or long-lead procurement items can be initiated to support the baseline LCLS schedule.

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 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.

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[a] The full project TEC and TPC, established at Critical Design 2 (Approved Performance Baseline), are $315,000,000 and $379,000,000, respectively.

[b] PED funding was reduced as a result of the FY 2003 general reduction and rescission by $75,000, as a result of the FY 2004 rescission by $44,000, as a result of the FY 2005 rescission by $161,000. This total reduction is restored in FY 2005, FY 2006, and FY 2007 to maintain the TEC and project scope.

Synchrotrons revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray free-electron-laser (FEL) in the 1.5 – 15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems. This will be the world's first such facility.

The LCLS is based on the existing SLAC linac. The SLAC linac can accelerate electrons or positrons to 50 GeV for colliding beam experiments and for nuclear and high-energy physics experiments on fixed targets. At present, the first two-thirds of the linac is being used to inject electrons and positrons into PEP-II, and the entire linac is used for fixed target experiments. When the LCLS is completed, the latter activity will be limited to 25 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 75 percent of the available beam time. For the LCLS, the linac will produce high-brightness 5 - 15 GeV electron bunches at a 120 Hz repetition rate. When traveling through the new 120-meter long LCLS undulator, these electron bunches will amplify the emitted x-ray radiation to produce an intense, coherent x-ray beam for scientific research.

The LCLS makes use of technologies developed for the SLAC and the next generation of linear colliders, as well as the progress in the production of intense electron beams with radiofrequency photocathode guns. These advances in the creation, compression, transport, and monitoring of bright electron beams make it possible to base this next generation of x-ray synchrotron radiation sources on linear accelerators rather than on storage rings.

The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called "table-top" x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing over 10^{11} x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific applications in the chemical, material, and biological sciences. The LCLS Scientific Advisory Committee, working in coordination with the broad scientific community, identified high priority initial experiments that are summarized in the document, *LCLS: The First Experiments*. These first five areas of experimentation are: fundamental studies of the interaction of intense x-ray pulses with simple atomic systems; use of the LCLS to create warm dense matter and plasmas; structural studies on single nanoscale particles and biomolecules; ultrafast dynamics in chemistry and solid-state physics; and studies of nanoscale structure and dynamics in condensed matter.

The experiments fall into two classes. The first follows the traditional role of x-rays to probe matter without modifying it, while the second utilizes the phenomenal intensity of the LCLS to excite matter in fundamentally new ways and to create new states in extreme conditions. The fundamental studies of the interactions of intense x-rays with simple atomic systems are necessary to lay the foundation for all interactions of the LCLS pulse with atoms embedded in molecules and condensed matter. The structural studies of individual particles or molecules make use of recent advances in imaging techniques for reconstructing molecular structures from diffraction patterns of non-crystalline samples. The enormous photon flux of the LCLS may make it feasible to determine the structure of a *single* biomolecule or small nanocrystal using only the diffraction pattern from a single moiety. This application has enormous potential in structural biology, particularly for important systems such as membrane proteins, which are virtually uncharacterized by x-ray crystallography because they are nearly impossible to crystallize. The last two sets of experiments make use of the extremely short pulse of the LCLS to follow dynamical processes in chemistry and condensed matter physics in real time. The use of ultrafast x-rays will open up entire new regimes of spatial and temporal resolution to both techniques.

The LCLS Project requires a 135 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 undulator and associated equipment. Two new buildings, the Near Experimental Hall and the Far Experimental Hall will be constructed and connected by a beam line tunnel. A Central Laboratory and Office Building will be constructed to provide laboratory and office space for LCLS users and serve as a center of excellence for basic research in x-ray physics and ultrafast science.

4. Details of Cost Estimate[a]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	25,900	26,000
Design Management costs (13.9% of TEC)	5,000	5,000
Project Management costs (14.2% of TEC)	5,100	5,000
Total Design Costs (100% of TEC)	36,000	36,000
Total, Line Item Costs (TEC)	36,000	36,000

5. Method of Performance

A Conceptual Design Report (CDR) for the project was completed and reviewed in FY 2002. Key design activities are being specified in the areas of the injector, undulator, x-ray optics and experimental halls to reduce schedule risk to the project and expedite the startup. Also, the LCLS management systems are being put in place and tested during the Project Engineering Design (PED) phase. These activities are managed by the LCLS Project Office at SLAC, with additional portions of the project being executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL).

The design of technical systems is being accomplished by the three collaborating laboratories. The conventional construction design aspect (experimental halls, tunnel connecting the halls, and a Central Laboratory and Office Building) was contracted to an experienced Architect/Engineering (A/E) firm to perform Title I and II design. Title I design was completed in FY 2004. Title II design began in FY 2005.

[a] This cost estimate includes design phase activities only. Construction funding is requested as an individual line item under Construction Project 05-R-320.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2004	FY 2005	FY 2006	Outyears	Total
Facility Cost						
PED	3,644	9,670	17,664	4,861	161	36,000
Other project costs						
Conceptual design costs	1,470	0	0	0	0	1,470
Research and development costs	0	1,750	4,250	0	0	6,000
NEPA documentation costs	30	0	0	0	0	30
Total, Other Project costs	1,500	1,750	4,250	0	0	7,500
Total, Project Cost (TPC)	5,144	11,420	21,914	4,861	161	43,500

03-R-313[a], The Center for Integrated Nanotechnologies (CINT) Facility, Sandia National Laboratories Albuquerque, New Mexico, and Los Alamos National Laboratory, Los Alamos, New Mexico

(Changes from FY 2005 Congressional Budget Request are denoted with a vertical line in the left margin.)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($000)	Total Project Cost ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 2004 Budget Request *(Preliminary Estimate)*	3Q 2002	2Q 2004	3Q 2004	3Q 2007	73,800	75,800
FY 2005 Budget Request *(Performance Baseline)*	4Q 2002	2Q 2004	1Q 2004	3Q 2007	73,800	75,800
FY 2006 Budget Request	4Q 2002	2Q 2004	1Q 2004	3Q 2007	73,800	75,800

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering and Design (PED)			
2002	1,000	1,000	167
2003	3,159[b]	3,159[b]	3,319
2004	0	0	592
2005	0	0	81
Construction			
2003	4,444[c]	4,444[c]	0
2004	29,674[d]	29,674[d]	11,222
2005	30,650[bce]	30,650[bce]	40,527
2006	4,626[d]	4,626[d]	15,376
2007	247[e]	247[e]	2,516

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[a] This project was submitted in the FY 2004 President's Request as project 04-R-314. In FY 2003 Congress appropriated construction funds for this project (after the FY 2004 Request was submitted to Congress) under project 03-R-313.

[b] PED funding was reduced $41,000 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission was restored in the FY 2005 request to maintain the TEC and project scope.

[c] Construction funding was reduced by $56,000 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission was restored in the FY 2005 request to maintain the TEC and project scope.

[d] Construction funding was reduced by $176,000 as a result of the FY 2004 rescission. This rescission is restored in FY 2006 to maintain the TEC and project scope.

[e] Construction funding was reduced by $247,000 as a result of the FY 2005 rescission. This rescission is restored in FY 2007 to maintain the TEC and project scope.

3. Project Descriptions, Justification and Scope

This project provides materials and services required to design and construct the proposed Center for Integrated Nanotechnologies (CINT) Facility. CINT is one of the five BES/Office of Science Nanoscale Science Research Centers (NSRCs). It will be operated jointly by Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL). The Center for Integrated Nanotechnologies (CINT) is a U.S. Department of Energy (DOE) line item project that is being carried out as a partnership between Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL) to design and build a world-class user facility for research in nanoscale science. The partnership between two world-class DOE laboratories, each with significant technical expertise and capability in nanoscale research, will provide the best possible facility to the nanoscience research community.

CINT will be a distributed Center that is jointly operated by SNL and LANL. Its primary objective is to develop the scientific principles that govern the performance and integration of nanoscale materials, thereby building the foundations for future nanotechnologies. The distinguishing characteristic of the Center is its focus on exploring the path from scientific discovery to the integration of nanostructures into the micro and macro worlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. This Center works closely with the other NSRCs to ensure that their discoveries are evaluated in the context of integrated functional systems. This approach offers a unique role for the DOE in support of the National Nanotechnology Initiative.

The managements of the Los Alamos and Sandia National Laboratories are committed to develop CINT as a DOE national resource for the advancement of nanoscience and technology. Through its laboratory partnership, CINT will leverage expertise and facilities from both SNL and LANL and make those resources available to the user community. In order to provide a strong central focus for the user community while also providing extraordinary leverage and access to existing laboratory capabilities, the CINT project, in conjunction with its user community, has developed a unique Core/Gateway structure.

The Core Facility (approximately 95,000 gross square feet), which will be constructed in Albuquerque, will be the single point of entry for the CINT user community and will provide the multi-disciplinary research environment needed to explore scientific challenges associated with nanoscience integration. In order to assure open access to the user community, the Core Facility is being constructed on DOE property outside of the Kirtland Air Force Base (KAFB).

In addition to developing the Core Facility, the CINT user community strongly recommended that the CINT project also provide access to the deep and broad resources of both SNL and LANL. The Gateway Facilities at both SNL and LANL are designed to provide the user community with direct access to existing DOE/SC and DOE/NNSA programmatic investments at each laboratory.

The Gateway to Sandia Facility is housed within an existing space in a NNSA building located on the main campus within the KAFB. The Gateway to Sandia, which will provide office and laboratory space for CINT users, is co-located with many of Sandia's existing facilities for nanoscale science research and Sandia's world-class microfabrication facilities. No new construction is required for the Gateway to Sandia since it will utilize existing NNSA space. (While the NNSA facility that houses the Gateway to Sandia is within the KAFB boundaries, it is located outside classified restricted boundaries and is therefore open for general user access).

Development of the Gateway to Los Alamos Facility (approximately 34,000 gross square feet) involves the construction of a new building on the Los Alamos campus providing the user community direct access to existing nanoscale materials science and bioscience capabilities. The Gateway to Los Alamos Facility is located in the center of the Los Alamos materials science complex which is in an open security environment and will facilitate easy access to these existing nanoscale materials science and bioscience resources. Traditionally, materials science and bioscience have been viewed as separate activities and are housed primarily in separate parts of the Los Alamos campus. The Gateway to Los Alamos will provide a unique research environment for CINT users by combining nanoscale materials science and biosciences capabilities and expertise under one roof surrounded by supporting resources accessible to CINT users.

The CINT project is building a unified community around its Core Facility and two Gateway Facilities (one each at SNL and LANL). The CINT project is using public workshops, presentations at scientific forums, web-based communications, and one-on-one interactions with CINT scientists to help build its user community with significant participation from university, industrial, and laboratory researchers. Input and advice from the user community is used to help define and refine the proper tools and scientific focus to address the challenges of nanoscale science and technology. CINT is focused on *integration* because it is the key factor in the scientific development and application of nanoscience. The tools and resources of CINT will be available at no cost to university, industrial, and laboratory researchers through a peer-reviewed process. The external scientific community has been and will continue to be a vital partner in developing CINT so that it is successful in achieving its vision.

The initial technical focus of the Center will be on the following five thrusts:

- Nanophotonics and Nanoelectronics
- Complex Functional Nanomaterials
- Nanomechanics
- Nanoscale and Bio-Microinterfaces
- Theory and Simulation

This proposed laboratory and office space complex will house state-of-the-art clean rooms and equipment for nanolithography, atomic layer deposition, and materials characterization along with general purpose chemistry and electronics labs and offices for Center staff and collaborators.

The CINT Core Facility will include class 1,000 clean room space for nanofabrication and characterization equipment and class 100 clean room space for lithography activities. This facility will also require general purpose chemistry/biology laboratories, electronic and physical measurement laboratories, office and meeting room space.

The scope of this project is to construct the CINT Core and Gateway to Los Alamos. The engineering effort includes preliminary and final design of both buildings. The project also includes procurement of an initial set of experimental capital equipment and construction of facilities. FY 2003 and FY 2004 construction funds were used for conventional construction and equipment procurement. FY 2005 and FY 2006 construction funds will be used to continue these activities.

4. Details of Cost Estimate [a]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs	2,489	2,507
Design Management Costs (1.2% of TEC)	916	806
Project Management Costs (1.0% of TEC)	754	710
Total, Design Costs (5.6% of TEC)	4,159	4,023
Construction Phase		
Buildings	37,902	34,415
Improvements to Land	1,430	1,430
Utilities	1,722	1,777
Special Equipment[b]	11,667	16,645
Standard Equipment	2,194	2,178
Inspection, Design and Project Liaison, Testing, Checkout and Acceptance	3,022	3,151
Construction and Project Management (3.4% of TEC)	2,512	1,212
Total, Construction Costs	60,449	60,808
Contingencies		
Design Phase (0.0% of TEC)	0	136
Construction Phase (12.5% of TEC)	9,192	8,833
Total, Contingencies (12.5% of TEC)	9,192	8,969
Total, Line Item Costs (TEC)	73,800	73,800

5. Method of Performance

Contracted Architect-Engineering (AE) support was used for development of the design concept and associated narrative and supporting material for the Conceptual Design Report. Design Criteria and other documents required during the conceptual phase for the Core Facility were done by SNL personnel with external support as needed. Title I and II design for the Core Facility was provided by contracted A-E support. The construction contractor was selected using a competitive best value process. The process considered the contractors' qualifications and experience and the quoted price. The resultant contract is fixed price.

Performance specifications have been prepared by LANL staff with contracted support for the Gateway to Los Alamos Facility. A design-build contract was awarded to a construction contractor selected using a competitive best value process. The process considered the contractors' qualifications, experience, and the quoted price.

SNL and LANL personnel are providing project management, design management, and project controls support.

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[a] This cost estimate is based on direct field inspection and historical cost estimate data, coupled with parametric cost data and completed conceptual studies and designs. Escalation rates are taken from the DOE construction project and operating expense escalation rate assumptions (as of January 27, 2002).

[b] Initial research equipment including testing and acceptance.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Years	FY 2004	FY 2005	FY 2006	Outyears	Total
Project Cost						
Facility Cost						
Design	3,486	592	81	0	0	4,159
Construction	0	11,222	40,527	15,376	2,516	69,641
Total, Line item TEC	3,486	11,814	40,608	15,376	2,516	73,800
Other Project Costs						
Conceptual design cost	330	0	0	0	0	330
NEPA documentation costs	199	0	0	0	0	199
Other project-related costs [a]	271	150	500	550	0	1,471
Total, Other Project Costs	800	150	500	550	0	2,000
Total, Project Costs (TPC)	4,286	11,964	41,108	15,926	2,516	75,800

7. Related Annual Funding Requirements [b]

(FY 2008 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs	18,500	18,500
Total related annual funding	18,500	18,500

[a] Includes tasks such as Safety documentation, ES&H Monitoring, Operations and Maintenance Support, Readiness Assessment, and Pre-operational Start-up. Experimental research will begin at the time of beneficial occupancy of the facilities. These research costs are not part of the TPC and will be funded by the BES program.

[b] These costs are preliminary and based on the conceptual design.

99-E-334, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Changes from FY 2005 Congressional Budget Request are denoted with a vertical line in the left margin.)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($000)	Total Project Cost ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 1999 Budget Request *(Preliminary Estimate)*	1Q 1999	4Q 2003	3Q 2000	4Q 2005	1,138,800	1,332,800
FY 2000 Budget Request	1Q 1999	4Q 2003	3Q 2000	1Q 2006	1,159,500	1,360,000
FY 2001 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,220,000	1,440,000
FY 2001 Amended Budget Request (*Performance Baseline*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2006 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700

2. Financial Schedule [a]

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
1999	101,400	101,400	37,140
2000	100,000	100,000	105,542
2001	258,929	258,929	170,454
2002	276,300	276,300	253,059
2003	210,571	210,571	276,887
2004	123,865[b]	123,865[b]	205,884
2005	79,891[bc]	79,891[bc]	96,090
2006	41,744[c]	41,744[c]	47,644

3. Project Description, Justification and Scope [d]

The purpose of the Spallation Neutron Source (SNS) Project is to provide a next-generation short-pulse spallation neutron source for neutron scattering and related research in broad areas of the physical, chemical, materials, and biological sciences. The SNS will be a national facility with an open user policy

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[a] Beyond the 5 instruments included in the SNS line item project, a broad instrument development program is being executed over the next several years to qualify and provide instruments for the remaining 19 neutron beam lines (the target station is designed to accommodate a total of 24 instruments). Instrument proposals undergo a scientific peer review process to evaluate technical merit; those concepts that are accepted may then establish interface agreements with the SNS Project. Expected funding sources include appropriated funds through the Department of Energy and other Federal agencies, private industry, and foreign entities. These instruments will all be delivered after completion of the SNS line item project. The instruments listed below have been initiated with the identified funding sources. As indicated, five of these instruments have been grouped together for the sake of management efficiency to form the "SNS Instruments – Next Generation" (SING) project, which is budgeted in the Basic Energy Sciences program as a Major Item of Equipment.

1. Cold Neutron Chopper Spectrometer – Basic Energy Sciences grant to Pennsylvania State University;
2. Wide Angle Chopper Spectrometer – Basic Energy Sciences grant to California Institute of Technology;
3. High Pressure Diffractometer – Basic Energy Sciences (SING);
4. High Resolution Chopper Spectrometer – Basic Energy Sciences (SING);
5. Single Crystal Diffractometer – Basic Energy Sciences (SING);
6. Hybrid Spectrometer – Basic Energy Sciences (SING);
7. Disordered Materials Diffractometer – Basic Energy Sciences (SING);
8. Fundamental Physics Beam Line – Nuclear Physics;
9. Engineering Diffractometer – the Canada Foundation for Innovation (CFI); and
10. Neutron Spin Echo – Forsehungszentrum Julich Gmbh (FZJ).

The final 9 SNS instruments will be selected under this process and identified when they are approved and funded.

[b] Construction funding was reduced by $735,000 as a result of the FY 2004 rescission. The reduction is restored in FY 2005 to maintain the TEC and project scope.

[c] Construction funding was reduced by $644,000 as a result of the FY 2005 rescission. The reduction is restored in FY 2006 to maintain the TEC and project scope.

[d] As part of the development of Oak Ridge National Laboratory, other buildings may be located on Chestnut Ridge, which is the site of the SNS and is located just across Bethel Valley Road from improvements planned for the main ORNL campus. For example, the Center for Nanophase Materials Sciences (CNMS) is being built on Chestnut Ridge, because research activities at the CNMS will integrate nanoscale science research with: neutron science; synthesis; and theory, modeling, and simulation. The CNMS is adjacent to the SNS Laboratory – Office Building and is connected to it by a walkway. See construction project datasheet 03-R-312 for further information on the CNMS.

attractive to scientists from universities, industries, and federal laboratories. It is anticipated that the facility, when fully operating, will be used by 1,000-2,000 scientists and engineers each year and that it will meet the national need for neutron science capabilities well into the 21st Century.

The scientific justification and need for a new neutron source and instrumentation in the U.S. were established by numerous studies by the scientific community since the 1970s. These include the 1984 National Research Council study *Major Facilities for Materials Research and Related Disciplines* (the Seitz-Eastman Report), which recommended the immediate start of the design of both a steady-state source and an accelerator-based pulsed spallation source. More recently, the 1993 DOE Basic Energy Sciences Advisory Committee (BESAC) report *Neutron Sources for America's Future* (the Kohn Panel Report) again included construction of a new pulsed spallation source with SNS capabilities among its highest priorities. This conclusion was even more strongly reaffirmed by the 1996 BESAC Report (the Russell Panel Report), which recommended the construction of a 1 megawatt (MW) spallation source that could be upgraded to significantly higher powers in the future.

Neutron scattering enables the determination of the positions and motions of atoms in materials, and it has become an increasingly indispensable scientific tool. Over the past decade, it has made invaluable contributions to the understanding and development of many classes of new materials, from high temperature superconductors to fullerenes, a new form of carbon. The information that neutron scattering provides has wide impacts. For example, chemical companies use neutrons to make better fibers, plastics, and catalysts; drug companies use neutrons to design drugs with higher potency and fewer side effects; and automobile manufacturers use the penetrating power of neutrons to understand how to cast and forge gears and brake discs in order to make cars run better and more safely. Furthermore, research on magnetism using neutrons has led to higher strength magnets for more efficient electric generators and motors and to better magnetic materials for magnetic recording tapes and computer hard drives.

Based on the recommendations of the scientific community obtained via the Russell Panel Report, the SNS is required to operate at an average power on target of at least 1 megawatt (MW); although the designers had aimed for 2 MW, current projections fall between 1 to 2 MW. At this power level, the SNS will be the most powerful spallation source in the world-many times that of ISIS at the Rutherford Laboratory in the United Kingdom. Furthermore, the SNS is specifically designed to take advantage of improvements in technology, new technologies, and additional hardware to permit upgrades to substantially higher power as they become available. Thus, the SNS will be the nation's premiere neutron facility for many decades.

The importance of high power – and consequently high neutron intensity – cannot be overstated. The properties of neutrons that make them an ideal probe of matter also require that they be generated with high flux. (Neutrons are particles with the mass of a proton, with a magnetic moment, and with no electrical charge.) Neutrons interact with nuclei and magnetic fields; both interactions are extremely weak, but they are known with great accuracy. Because they have spin, neutrons have a magnetic moment and can be used to study magnetic structure and magnetic properties of materials. Because they weakly interact with materials, neutrons are highly penetrating and can be used to study bulk phase samples, highly complex samples, and samples confined in thick-walled metal containers. Because their interactions are weak and known with great accuracy, neutron scattering is far more easily interpreted than either photon scattering or electron scattering. However, the relatively low flux of existing neutron sources and the small fraction of neutrons that get scattered by most materials, mean that most measurements are limited by the source intensity.

The pursuit of high-flux neutron sources is more than just a desire to perform experiments faster, although that, of course, is an obvious benefit. High flux enables broad classes of experiments that cannot be done with low-flux sources. For example, high neutron intensity enables studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions.

The SNS will consist of a linac-ring accelerator system that delivers short (microsecond) pulses to a target/moderator system where neutrons are produced by a nuclear reaction process called spallation. The process of neutron production in the SNS consists of the following: negatively charged hydrogen ions are produced in an ion source and are accelerated to approximately 1 billion electron volts energy in a linear accelerator (linac); the hydrogen ion beam is injected into an accumulator ring through a stripper foil, which strips the electrons off of the hydrogen ions to produce a proton beam; the proton beam is collected and bunched into short pulses in the accumulator ring; and, finally, the proton beam is injected into a heavy metal target at a frequency of up to 60 Hz. The intense proton bursts striking the target produce pulsed neutron beams by the spallation process. The high-energy neutrons so produced are moderated (i.e., slowed down) to reduce their energies, typically by using thermal or cold moderators. The moderated neutron beams are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations.

The primary objectives in the design of the site and buildings for the SNS are to provide optimal facilities for the DOE and the scientific community for neutron scattering well into the 21st Century and to address the mix of needs associated with the user community, the operations staff, security, and safety.

A research and development (R&D) program is required to ensure technical feasibility and to determine physics design of accelerator and target systems that will meet performance requirements.

The objectives stated above will be met by the technical components described earlier (ion source; linac; accumulator ring; target station with moderators; beam transport systems; and initial experimental equipment necessary to place the SNS in operation) and attendant conventional facilities. As the project design and construction progresses, value engineering analyses and R&D define changes that are applied to the technical baseline to maximize the initial scientific capability of the SNS within the currently established cost and schedule. The SNS project will be considered complete when all capital facilities necessary to achieve the initial baseline goals have been installed and certified to operate safely and properly. In addition, to the extent possible within the Total Project Cost, provisions will be made to facilitate a progression of future improvements and upgrades aimed at keeping SNS at the forefront of neutron scattering science throughout its operating lifetime. Indeed, the current design contains a number of enhancements (e.g. superconducting radiofrequency (RF) acceleration, best-in-class instruments, more instrument stations, and higher energy ring) that provide higher performance than the conceptual design that was the basis of initial project approval.

The scientific user community has advised the DOE Office of Basic Energy Sciences that the SNS should keep pace with developments in scientific instruments. Since the average cost for a state-of-the-art instrument has roughly doubled in recent years, SNS reduced the number of instruments provided within the project TEC. Although this translated into an initial suite of five rather than the ten instruments originally envisioned, the cumulative scientific capability of the SNS has actually increased more than ten-fold. In order to optimize the overall project installation sequence and early experimental operations, three of these instruments will be installed as part of the project; procurement of components for the other two will be completed, with installation occurring during initial low power operations following project completion. As with all scientific user facilities such as SNS, additional and even more capable instruments will be installed over the course of its operating lifetime.

Funds appropriated in FY 2004 were used to continue instrument R&D, design, and procurement. The drift tube linac and coupled cavity linac subsystems were installed and commissioning activities were continued in the linac. Cryogenic refrigerator installation and system cool down were completed, and cryogenic transfer line installation and testing were completed. Cryogenic module fabrication and installation were continued. Ring fabrication and assembly activities were continued. Target fabrication and assembly activities were continued. Most buildings were completed with the exception of ongoing construction work in the target building and the central laboratory and office building.

FY 2005 budget authority will be used to continue R&D, procurement, and installation of equipment for instrument systems. Commissioning of Linac systems will be completed. Installation of accumulator ring and high-energy beam transport systems will continue. Installation and testing of target systems will be performed along with starting preparations for the target systems readiness review. The remaining major construction contracts will be completed. Procurement, installation, and testing will continue for integrated control systems.

FY 2006 budget authority is requested to complete the SNS Project. Procurement and installation of equipment for instrument systems will be performed. Accelerator readiness reviews will be completed, and ring and target systems will be successively commissioned. All requirements to begin operations will be met and all SNS facilities will be turned over to operations.

4. Details of Cost Estimate [a]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 20% of construction costs	160,500	160,500
Construction management at approximately 2% of construction costs	15,900	15,900
Project management at approximately 13% of construction costs	104,700	104,700
Total, Design Costs (23.6% of TEC)	281,100	281,100
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	31,500	31,500
Buildings	250,624	239,800
Utilities (electrical, water, steam, and sewer lines)	20,900	20,900
Technical Components	524,040	520,600
Total, Construction Costs	827,064	812,800
Standard Equipment	17,500	17,500
Major computer items	5,500	5,500
Design and project liaison, testing, checkout and acceptance	31,000	31,000
Subtotal	1,162,164	1,147,900
Contingencies at approximately 3% of above costs [b]	30,536	44,800
Total, Line Item Costs (TEC)	1,192,700	1,192,700

5. Method of Performance

The SNS project is being carried out by a partnership of six DOE national laboratories, led by Oak Ridge National Laboratory, as the prime contractor to DOE. The other five laboratories are Argonne, Brookhaven, Lawrence Berkeley, and Los Alamos National Laboratories and Thomas Jefferson National Accelerator Facility. Each laboratory is assigned responsibility for accomplishing a well defined portion of the project's scope that takes advantage of their technical strengths: Argonne – Instruments; Brookhaven – Accumulator Ring; Lawrence Berkeley – Ion Source; Los Alamos – Normal conducting Linac and RF power systems; TJNAF – Superconducting Linac; Oak Ridge - Target. Project execution is the responsibility of the SNS Associate Laboratory Director with the support of a central SNS Project Office at ORNL, which provides overall project management, systems integration, ES&H, quality assurance, and commissioning support. The SNS Associate Laboratory Director has authority for directing the efforts at all six partner laboratories and exercises financial control over all project activities. ORNL has subcontracted to an Industry Team that consists of an Architect-Engineer for the conventional facilities design and a Construction Manager for construction installation, equipment

[a] The project is using the appropriated funds included in the TEC to meet or exceed the project performance baseline. The project is also accepting transferred surplus materials and equipment to the extent possible. Examples of the transferred items include ring pumps, lead bricks, concrete blocks, trailers and furniture. The net book value of the surplus materials will be far less than one percent of the TEC over the life of the project. All such transferred materials will be appropriately recorded as non-fund cost and capitalized.

[b] The current baselined contingency level, expressed as a percentage of the remaining effort to complete the line item project, is approximately 20%.

procurement, testing and commissioning support. Procurements by all six laboratories are being accomplished, to the extent feasible, by fixed price subcontracts awarded on the basis of competitive bidding.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2004	FY 2005	FY 2006	Total
Project Cost					
Facility Cost [a]					
Line Item TEC	843,082	205,884	96,090	47,644	1,192,700
Other project costs					
R&D necessary to complete project [b]	81,846	1,188	614	0	83,648
Conceptual design cost [c]	14,397	0	0	0	14,397
NEPA Documentation costs [d]	1,928	0	0	0	1,928
Other project-related costs [e]	32,201	17,951	36,847	30,925	117,924
Capital equipment not related construction [f]	911	130	62	0	1,103
Total, Other project costs	131,283	19,269	37,523	30,925	219,000
Total project cost (TPC)	974,365	225,153	133,613	78,569	1,411,700

7. Related Annual Funding Requirements

	(FY 2007 dollars in thousands) Current Estimate	Previous Estimate
Facility operating costs	45,700	45,700
Facility maintenance and repair costs	24,800	24,800
Programmatic operating expenses directly related to the facility	47,700	47,700
Capital equipment not related to construction but related to the programmatic effort in the facility	14,100	14,100
GPP or other construction related to the programmatic effort in the facility	1,000	1,000
Utility costs	19,400	19,400
Accelerator Improvement Modifications (AIMs)	7,300	7,300
Total related annual funding (4Q FY 2006 will begin operations)	160,000	160,000

[a] Construction line item costs included in this budget request are for providing Title I and II design, inspection, procurement, and construction of the SNS facility for an estimated cost of $1,192,700,000.
[b] A research and development program at an estimated cost of $83,648,000 is needed to confirm several design bases related primarily to the accelerator systems, the target systems, safety analyses, cold moderator designs, and neutron guides, beam tubes, and instruments. Several of these development tasks require long time durations and the timely coupling of development results into the design is a major factor in detailed task planning.
[c] Costs of $14,397,000 are included for conceptual design and for preparation of the conceptual design documentation prior to the start of Title I design in FY 1999.
[d] Costs of $1,928,000 are included for completion of the Environmental Impact Statement.
[e] Estimated costs of $117,924,000 are included to cover pre-operations costs.
[f] Estimated costs of $1,103,000 to provide test facilities and other capital equipment to support the R&D program.

During conceptual design of the SNS project, the annual funding requirements were initially estimated based on the cost of operating similar facilities (e.g., ISIS and the Advanced Photon Source) at $106,700,000. The operating parameters, technical capabilities, and science program are now better defined and the key members of the ORNL team that will operate SNS are now in place. Based on these factors, the SNS Project developed a new estimate of annual operating costs, which was independently reviewed by the Department, and provides the basis of the current estimate indicated above. FY 2007 will be the first full year of operations and this estimate is generally representative of the early period of SNS operations. If proposed upgrades and instrumentation plans are carried out in the future, the annual funding requirements will increase by an additional 10-15 percent.