Basic Energy Sciences

Funding Profile by Subprogram

(dollars in thousands)

	FY 2003 Comparable Appropriation	FY 2004 Original Appropriation	FY 2004 Adjustments	FY 2004 Comparable Appropriation	FY 2005 Request
Basic Energy Sciences					
Research					
Materials Sciences and Engineering	533,552	575,711	-3,355[a]	572,356	603,228
Chemical Sciences, Geosciences, and Energy Biosciences	211,898	220,914	-1,332[a]	219,582	228,422
Subtotal, Research	745,450	796,625	-4,687	791,938	831,650
Construction	256,491	219,950	-1,297[a]	218,653	231,880
Subtotal, Basic Energy Sciences	1,001,941	1,016,575	-5,984[a]	1,010,591	1,063,530
Use of Prior Year Balances	0	-2,291	0	-2,291	0
Total, Basic Energy Sciences	1,001,941[bcde]	1,014,284	-5,984[a]	1,008,300	1,063,530

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.

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[a] Excludes a rescission of $5,984,276 in accordance with the Consolidated Appropriations Act, 2004, as reported in conference report H. Rpt. 108-401 dated November 25, 2003.

[b] Excludes $437,000 transferred to Security Operations in FY 2004 for waste management activities at the New Brunswick Laboratory.

[c] Excludes $16,584,000 which was transferred to the SBIR program and $995,000 which was transferred to the STTR program.

[d] Excludes $6,654,740 for a rescission in accordance with the Consolidated Appropriations Resolution, FY 2003.

[e] Includes $2,806,481 for the Emergency Wartime Supplemental Appropriations for FY 2003.

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 and combat terrorism. 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 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. 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 goals:

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, to advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences, and to 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.

A key strategic emphasis of these subprograms is to lead the nanoscale science revolution, delivering 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 the development of advanced tools and instruments for x-ray, neutron, and electron diffraction, scattering, and imaging and for other advanced probes of matter for exploration and discovery in materials sciences and engineering; chemistry; earth, environmental, and geosciences; and plant and biosciences. 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 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 contributes to this goal by managing the Combustion Research Facility at Sandia National Laboratories in Livermore, California, an internationally recognized facility for the study of combustion science and technology.

Annual Performance Results and Targets

FY 2000 Results	FY 2001 Results	FY 2002 Results	FY 2003 Results	FY 2004 Targets	FY 2005 Targets
Program Goal 5.22.00.00 Advance the Basic Science for Energy Indpendence					
Materials Sciences and Engineering					
N/A	N/A	N/A	N/A	Improve Spatial Resolution: Demonstrate first measurement of spatial resolutions for imaging in the hard x-ray region of <115 nm and in the soft x-ray region of <19 nm, and spatial information limit for an electron microscope of 0.08 nm.	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 temporal resolution: Demonstrate first measurement of x-ray pulses that are <200 femtoseconds in duration and have an intensity of >5,000 photons per pulse.	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).
Chemical Sciences, Geosciences, and Energy Biosciences					
N/A	N/A	N/A	N/A	As a part of the Scientific Discovery through Advanced Computing (SciDAC) program, perform a three-dimensional combustion reacting flow simulation involving more than 44 reacting species and 500,000 grid points.	As a part of the SciDAC program, perform a three-dimensional combustion reacting flow simulation involving more than 44 reacting species and 7 billion grid points.

FY 2000 Results	FY 2001 Results	FY 2002 Results	FY 2003 Results	FY 2004 Targets	FY 2005 Targets
Materials Sciences and Engineering					
Scientific user facilities were maintained and operated to achieve an average at least 90 percent of the total scheduled operating time. [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90 percent of the total scheduled operating time. [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90 percent of the total scheduled operating time. [Met Goal]	Scientific user facilities were maintained and operated to achieve an average at least 90 percent of the total scheduled operating time. [Met Goal]	Maintain and operate the scientific user facilities to achieve an average at least 90 percent of the total scheduled operating time.	Maintain and operate the scientific user facilities to achieve an average at least 90 percent of the total scheduled operating time.
Construction					
Cost and timetables were maintained within 10 percent 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 percent 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 percent 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 percent of the baselines given in the construction project data sheets for all construction projects ongoing during the year. [Met Goal]	Meet the cost and timetables within 10 percent of the baselines given in the construction project data sheets for all ongoing construction projects.	Meet the cost and timetables within 10 percent 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, U.S. Department of Agriculture, Department of Interior, and National Institute 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 held to ensure technical progress, cost and schedule adherence, and responsiveness to program requirements.

Program Assessment Rating Tool (PART) Assessment

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 through which programs can assess their activities differently than through traditional reviews. The Basic Energy Sciences (BES) program has incorporated feedback from OMB into the FY 2005 Budget Request and has taken, or will take, the necessary steps to continue to improve performance.

In the PART review, OMB gave the Basic Energy Sciences (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. However, OMB noted concerns regarding the collection and reporting of performance data. To address these concerns, BES will work with its Advisory Committee to develop research milestones for the long-term performance goals, will include the long term research goals in grant solicitations, will work to improve performance reporting by grantees and contractors, and will work with the CFO to improve BES sections of the Department's performance documents. BES role in providing scientific research facilities is strongly supported by the Administration. OMB noted concerns regarding underutilization and poor performance reporting at some BES facilities. Funding is provided in FY 2005 to operate the program's main major scientific user facilities at maximum capacity. BES will continue to improve performance reporting and centralize management and planning of operations at its user facilities.

Funding by General and Program Goal

(dollars in thousands)

	FY 2003	FY 2004	FY 2005	$ Change	% Change
Basic Energy Sciences					
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	533,552	572,356	603,228	+30,872	+5.4%
Chemical Sciences, Geosciences and Energy Biosciences	211,898	219,582	228,422	+8,840	+4.0%
Construction	256,491	218,653	231,880	+13,227	+6.0%
Total, Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence	1,001,941	1,010,591	1,063,530	+52,939	+5.2%
Use of Prior Year Balances	0	-2,291	0	+2,291	+100.0%
Total, Basic Energy Sciences	1,001,941	1,008,300	1,063,530	+55,230	+5.5%

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 2003, the program funded research in more than 143 academic institutions located in 47 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; and on a 20-year roadmap for BES facilities. 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 at: http://www.sc.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 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 (1) the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document proposal actions and (2) the quality of the resulting portfolio, specifically the breadth and depth of portfolio elements and the national and international standing of the elements. The first reviews assessed the chemistry activities (FY 2002) and the materials sciences and engineering activities (FY 2003). In FY 2004, the activities associated with the management of the scientific user facilities will be assessed. The cycle will begin again in FY 2005, so that all elements of the BES program will be reviewed once every three years.

Planning and Priority Setting

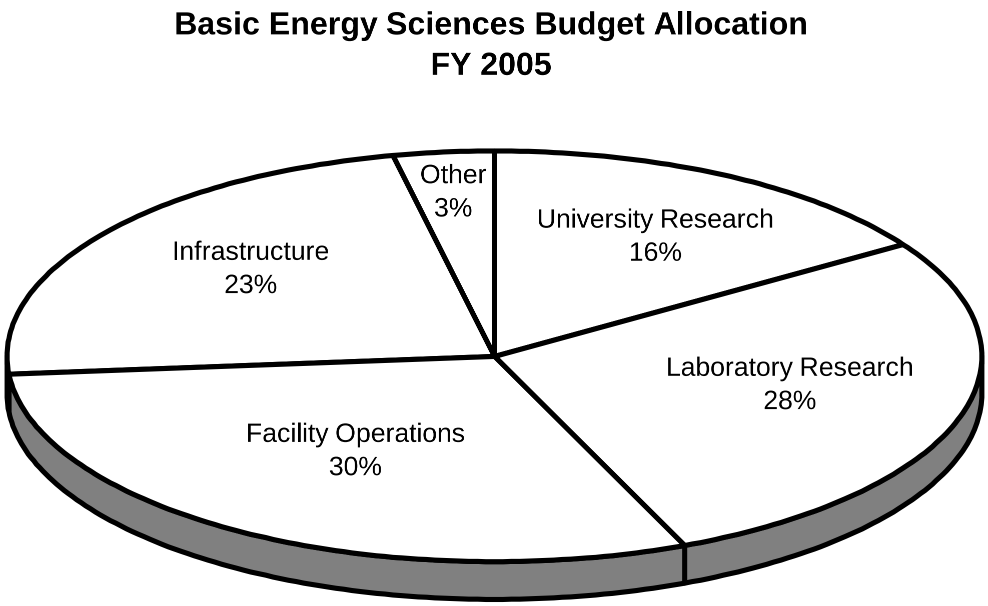
Because the BES program supports research covering a wide range of scientific disciplines as well as a large number of major scientific user facilities, planning is an ongoing activity. Many long-range planning exercises for elements of the BES program are performed under the auspices of BESAC. Prioritization 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; 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 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 2005 budget request continues priorities established in the past few years. Construction of the Spallation Neutron Sources continues in accord with the established baseline. A significant investment in the area of nanoscale science includes construction funding for four 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 is providing $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 funding is also provided for the Linac Coherent Light Source, a 4^{th} 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.

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, construction, and long-lead procurement remain significant budget components in FY 2005, including the Spallation Neutron Source, Nanoscale Science Research Centers, and the Linac Coherent Light Source.



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, which are not typically found at universities. Mission critical research is also sited at DOE laboratories when it is outside of the mainstream of research supported at universities, e.g., heavy-element chemistry or combustion chemistry. Research sited at DOE laboratories is very often collocated with and sometimes cofunded with research activities of the DOE technology offices, providing a synergism not available in universities. Finally, research that requires strong interdisciplinary interactions, large teams of closely collaborating researchers, or a large technical support staff is also well suited to DOE laboratories.

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

Significant Program Shifts

In FY 2005, Project Engineering Design (PED) and construction will proceed on four Nanoscale Science Research Centers (NSRCs) and funding will be continued for a Major Item of Equipment for the fifth NSRC. 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.

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."

NSRCs will be 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.

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

Nanoscale Science Research Funding

	TEC	TPC	FY 2003	FY 2004	FY 2005
Research					
Materials Sciences and Engineering..			65,018	74,355	66,995
Chemical Sciences, Geosciences, and Biosciences......................			26,726	28,190	28,360
Capital Equipment					
Major Item of Equipment -- ANL, Center for Nanoscale Materials......			0	10,000	12,000
Nanoscale Science Research Centers					
PED – All sites..			11,850	2,982	2,012
Construction					
BNL, Center for Functional Nanomaterials.........................	79,700	81,000	0	0	18,465
LBNL, Molecular Foundry..........	83,700	85,000	0	34,794	32,085
ORNL, Center for Nanophase Materials Sciences..................	63,882	64,882	23,701	19,882	17,811
SNL/A and LANL, Center for Integrated Nanotechnologies.....	73,800	75,800	4,444	29,674	30,897
Total BES Nanoscale Science Funding...			131,739	199,877	208,625

In FY 2005, $29,183,000 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.er.doe.gov/production/bes/hydrogen.pdf. The 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 ten or more 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. The only hope of narrowing the gap significantly is 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. The areas targeted for increased funding, include: low-cost and efficient solar energy production of hydrogen, nanoscale catalyst design, biological, biomimetic, and bio-inspired materials and processes, complex hydride materials for hydrogen storage, nanostructured and other novel hydrogen storage materials, theory, modeling, and simulation of materials and molecular processes, low-cost, highly active, durable cathodes for low-temperature fuel cells, membranes and separations processes for hydrogen production and fuel cells, and analytical and measurement technologies. The new work is by its nature multidisciplinary and touches virtually all of the BES research activities. The work will be coordinated by a team of program managers and will have annual contractors' meetings to promote cohesion and rapid information exchange. This activity will be a part of the President's Hydrogen Initiative and will be coordinated with the DOE technology programs and with other Federal agencies through the Office of Science and Technology Policy's Hydrogen R&D Task Force.

President's Hydrogen Initiative

	FY 2003	FY 2004	FY 2005
Materials Sciences and Engineering Research	3,025	3,063	14,761
Chemical Sciences, Geosciences, and Biosciences	4,615	4,674	14,422
Total Hydrogen Initiative	7,640	7,737	29,183

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: characterizing chemically reacting flows as exemplified by combustion and 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 molecular where the physical descriptions are discrete in nature to 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. In the past year, 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 level of operations will be equal to that in FY 2004. 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 2001 Actual*	FY 2002 Actual*	FY 2003 Actual*	FY 2004 Estimate	FY 2005 Estimate
All Facilities					
Maximum Hours	36,800	36,800	36,800	36,800	36,800
Scheduled Hours	27,563	31,215	31,400	31,350	35,450
Unscheduled Downtime	4%	4%	9%	<10%	<10%
Number of Users	6,982	7,603	8,218	8,280	8,530
Advanced Light Source					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	5,468	5,236	5,530	5,700	5,700
Unscheduled Downtime	4%	7%	5%	<10%	<10%
Number of Users	1,163	1,385	1,662	1,500	1,600
Advanced Photon Source					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	5,000	4,856	4,912	5,700	5,700
Unscheduled Downtime	4%	3%	3%	<10%	<10%
Number of Users	1,989	2,299	2,767	2,400	2,500
National Synchrotron Light Source					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	5,556	5,818	5,570	5,700	5,700
Unscheduled Downtime	0%	3%	6%	<10%	<10%
Number of Users	2,523	2,413	2,206	2,500	2,500
Stanford Synchrotron Radiation Laboratory					
Maximum Hours	5,300	5,300	5,300	5,300	5,300
Scheduled Hours	4,781	4,706	2,841	2,000	5,000
Unscheduled Downtime	5%	5%	3%	<10%	<10%
Number of Users	907	1,023	867	1,000	1,000

* Scheduled hours for FY 2001, FY 2002, and FY 2003 show actual number of hours delivered to users.

	FY 2001 Actual*	FY 2002 Actual*	FY 2003 Actual*	FY 2004 Estimate	FY 2005 Estimate
High Flux Isotope Reactor					
Maximum Hours	6,100	6,100	6,100	6,100	6,100
Scheduled Hours	8	4,111	5,256	5,000	6,100
Unscheduled Downtime	0%	3%	20%	<10%	<10%
Number of Users....................................	38	76	218	400	400
Intense Pulsed Neutron Source					
Maximum Hours	4,700	4,700	4,700	4,700	4,700
Scheduled Hours	3,868	4,308	4,274	4,250	4,250
Unscheduled Downtime	0%	0%	7%	<10%	<10%
Number of Users	240	243	229	280	280
Manuel Lujan, Jr. Neutron Scattering Center					
Maximum Hours	3,600	3,600	3,600	3,600	3,600
Scheduled Hours	2,882	2,180	3,017	3,000	3,000
Unscheduled Downtime	18%	12%	21%	<10%	<10%
Number of Users	122	164	269	200	250

Cost and Schedule Variance

	FY 2001 Actual	FY 2002 Actual	FY 2003 Actual	FY 2004 Estimate	FY 2005 Estimate
Spallation Neutron Source					
Cost Variance...................................	+0.4%	-0.3%	+0.5%		
Schedule Variance	-6.7%	-1.8%	-1.4%		
Major (Levels 0 and 1) Milestones Completed or Committed to	None	Linac Design Completed	Front End Beam Available to Linac Target Design Complete Linac Tunnel Beneficial Occupancy Ring Tunnel Beneficial Occupancy	None	Instrument Systems Design Complete Linac Beam Available to Ring

* Scheduled hours for FY 2001, FY 2002, and FY 2003 show actual number of hours delivered to users.

	FY 2001 Actual	FY 2002 Actual	FY 2003 Actual	FY 2004 Estimate	FY 2005 Estimate
Linac Coherent Light Source (SLAC)					
Cost Variance	N/A	N/A	N/A		
Schedule Variance	N/A	N/A	N/A		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 0 – Mission Need	None	Approved Critical Decision 1 – Preliminary Baseline Range Approved Critical Decision 2a – Long-Lead Procurement Budget	Approve Critical Decision 2b – Performance Baseline	
Center for Nanophase Materials Sciences (ORNL)					
Cost Variance	N/A	N/A	0%		
Schedule Variance	N/A	N/A	0%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 0 – Mission Need	Approved Critical Decision 1 – Preliminary Baseline Range Approved Critical Decision 2 – Performance Baseline	Approved Critical Decision 3 – Start of Construction	Approve Critical Decision 4a – Initial Start of Operations	
Center for Integrated Nanotechnologies (SNL/LANL)					
Cost Variance	N/A	N/A	-0.4%		
Schedule Variance	N/A	N/A	-2.9%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 0 – Mission Need	Approved Critical Decision 1 – Preliminary Baseline Range	Approved Critical Decision 2 – Performance Baseline	Approve Critical Decision 3a – Start Utility Construction Approve Critical Decision 3b – Start of Full Construction	None

	FY 2001 Actual	FY 2002 Actual	FY 2003 Actual	FY 2004 Estimate	FY 2005 Estimate
The Molecular Foundry (LBNL)					
Cost Variance	N/A	N/A	+1.0%		
Schedule Variance	N/A	N/A	+1.4%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Critical Decision 0 – Mission Need	Approved Critical Decision 1 – Preliminary Baseline Range	Approved Critical Decision 2 – Performance Baseline	Approve Critical Decision 3 – Start Construction	None
Center for Nanoscale Materials (ANL)					
Cost Variance	N/A	N/A	N/A		
Schedule Variance	N/A	N/A	N/A		
Major (Levels 0 and 1) Milestones Completed or Committed to			Approved Critical Decision 0 – Mission Need Approved Critical Decision 1 – Preliminary Baseline Range	Approve Critical Decision 2 – Performance Baseline Approve Critical Decision 3 – Start Construction	None
Center for Functional Nanomaterials (BNL)					
Cost Variance	N/A	N/A	N/A		
Schedule Variance	N/A	N/A	N/A		
Major (Levels 0 and 1) Milestones Completed or Committed to		Approved Critical Decision 0 – Mission Need	Approved Critical Decision 1 – Preliminary Baseline Range	Approve Critical Decision 2 – Performance Baseline	Approve Critical Decision 3 – Start Construction
SSRL SPEAR3 Upgrade					
Cost Variance	+0.3%	+2.0%	0%		
Schedule Variance	-7.8%	-1.6%	0%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Approved Preliminary Safety Assessment Document	Completed RF System Production Completed Magnet Production	Approved Final Safety Assessment Document Completed Vacuum System Production	Complete Accelerator Readiness Review Start Commission-ing	None

	FY 2001 Actual	FY 2002 Actual	FY 2003 Actual	FY 2004 Estimate	FY 2005 Estimate
			Completed Raft Assemblies	Approve Critical Decision 4 – Start Operations	
			Completed Major Installation		

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 2005 budget authority is requested to continue R&D, procurement, and installation of equipment for instrument systems. The extraction dump, high-energy beam transport, and accumulator ring will be commissioned; and installation and testing for the ring-target beam transport system will be performed. Preparation for the ring-target beam transport system accelerator readiness review will begin. Installation and testing will be completed and preparation for the accelerator readiness review will start for target systems. Conventional facilities construction will be completed. Procurement, installation, and testing will continue for integrated control systems.

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.

Linac Coherent Light Source (LCLS) Project

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 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 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. 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 preliminary Total Estimated Cost (TEC) is in the range of $220,000,000 to $260,000,000. FY 2005 Project Engineering Design (PED) funding of $20,075,000 is requested for Title I and Title II design work and $4,000,000 is requested for research and development. Additional information on the LCLS Project is provided in the LCLS PED data sheet, project number 03-SC-002.

In addition, FY 2005 Long-lead Procurement (LLP) funding of $30,000,000 is requested for selected components of the gun laser, the electron injector, and the linac system. Additional information on the LLP is provided in the LCLS construction datasheet, project number 05-R-320.

Nanoscale Science Research Centers (NSRCs)

Funds are requested for Project Engineering Design (PED) and construction of NSRCs located at Oak Ridge National Laboratory, 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-312, 03-R-313, 04-R-313, and 05-R-321; in the Project Engineering Design (PED) data sheet, project number 02-SC-002; and in the Materials Sciences and Engineering subprogram.

Stanford Synchrotron Radiation Laboratory (SSRL) Upgrade

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade was undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The upgrade increased injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decreased beam emittance by a factor of 7 to increase beam brightness; increased operating current from 100 mA to 200 mA to increase beam intensity; and maintained long beam life time (>25 hr). The increased photon flux will greatly improve performance in a variety of applications including powder and thin film diffraction, topographic studies, surface microcontamination studies, x-ray tomographic analysis, x-ray absorption studies, and protein crystallography. The magnets and associated vacuum chambers of the existing SPEAR storage ring were replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC was $29,000,000; DOE and NIH equally funded the upgrade with a total Federal cost of $58,000,000. NIH provided $14,000,000 in FY 1999, $14,000,000 in FY 2000, and $1,000,000 in FY 2001.

BES provides funding for general plant projects (GPP) and general plant equipment (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 8,000 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 2001	FY 2002	FY 2003	FY 2004 Enacted	FY 2005 Request
# University Grants	1,094	1,071	1,100	1,200	1,270
Average Size ($ thousands/yr)	134	140	145	145	150
# Permanent Ph.D.s	3,780	3,650	3,800	3,970	4,050
# Postdocs	1,090	1,050	1,100	1,150	1,200
# Grad Students	1,780	1,700	1,750	1,800	1,900

Materials Sciences and Engineering

Funding Schedule by Activity

(dollars in thousands)

	FY 2003	FY 2004	FY 2005	$ Change	% Change
Materials Sciences and Engineering					
Materials Sciences and Engineering Research	252,539	263,929	275,543	+11,614	+4.4%
Facilities Operations	281,013	294,517	312,854	+18,337	+6.2%
SBIR/STTR	0	13,910	14,831	+921	+6.6%
Total, Materials Sciences and Engineering	533,552	572,356	603,228	+30,872	+5.4%

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.

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 is 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 2003 Research Accomplishments

- *Towards an Exciton Condensate – A New Form of Matter*. A Bose-Einstein condensate, a form of matter heretofore observed only in atoms chilled to less than a millionth of a degree above absolute zero, may now have been observed at temperatures in excess of one Kelvin in excitons, the bound pairs of electrons and holes that enable semiconductors to function as electronic devices. Researchers have observed excitons in a macroscopically ordered electronic state, indicating the formation of a condensate. The observations were made by shining laser light on specially designed nano-sized structures called quantum wells, which were grown at the interface between two semiconductors – gallium arsenide and aluminum gallium arsenide. These quantum wells allow electrons and electron holes (spaces in the crystal that are positively charged) to move freely through the two dimensions parallel to the quantum well plane, but not through the perpendicular dimension. Under photoluminescence, the macroscopically ordered exciton state appeared against a black background as a bright ring that had been fragmented into a chain of circular spots extending out to one millimeter in circumference. Just as the Nobel prize-winning creation of Bose-Einstein condensate atoms offered scientists a new look into the hidden world of quantum mechanics, so, too, will the creation of Bose-Einstein condensate excitons provide scientists with new possibilities for observing and manipulating quantum mechanical properties. The observation also holds potential for ultrafast digital logic elements and quantum computing devices.
- *Magnetic Nanocomposites*: *The Next Little Thing*. Magnetic materials are indispensable to a modern industrial society; however, it is no longer possible to squeeze significantly better performance out of today's most advanced magnets. A new approach is to create a composite material of two magnetic materials combined on the nanoscale to create a material with better performance than either taken separately. The boundary between the two magnetic materials is exceedingly important. Studies of bilayers of magnetically-hard and magnetically-soft magnetic materials have revealed that diffusion between the two materials alters the interface between them, resulting in improved magnetic properties. Theoretical modeling confirms that interfacial modification can enhance interlayer magnetic coupling. The results reveal the potential of careful interfacial control for improving magnets through manipulation of the material at the nanoscale.
- *Tuning the Properties of Materials at the Nanoscale*. As the size of silicon electronic devices shrinks toward the nanometer scale, the properties of the nanometer-thick silicon thin film in the devices depart from those of the bulk form of silicon. Nanostressors will be able to tune the properties of such thin films. For example, germanium islands grown on silicon act as nanostressors to shape the silicon film. The induced bending of the silicon film modifies the local electronic and optical properties of silicon. This ability to "tune" the properties of solid thin films is expected to become more prominent as semiconductor devices shrink to ever smaller scales.
- *New Nanoscale Structures Form where Grain Boundaries Meet Surfaces*. A newly discovered nanoscale "defect" may be connected to unusual behavior of metal catalysts and thin films, which are critical to the chemical and electronic industries. A distinct channel with a V-shaped cross section has been observed along the intersection of a grain boundary with an external surface. Atomic-resolution observations of gold surfaces in combination with atomic-scale simulations show that this channel has a different crystal structure than the remainder of the material. One implication is that when the grains become sufficiently small, these channel regions may dominate the surface and

result in very different reactivity and catalytic activity than expected based on the bulk structure. These channel defects may also pin grain boundaries, slowing or preventing their motion and affecting the processing of thin films for microelectronics. Furthermore, the channels can be thought of as naturally occurring nanoscale wires along the surface of a material, whose arrangement could be controlled by appropriate processing.

- *Imaging Single, Individual Molecules*. By using a tightly focused beam of electrons less than a nanometer in diameter and by reconstructing images from the electron scattering data, the exact atomic positions in an individual carbon nanotube have been determined. Images of high resolution and high contrast can be obtained as has been shown by solving the structure of a single, double-walled carbon nanotube – a very complicated problem involving one tube nested in another. The technique has the potential to allow imaging of atomic arrangements in individual non-periodic structures such as biological macromolecules.
- *Nanofluids Improve Heat Transfer*. Suspensions of nanoscale metal particles or carbon nanotubes in fluids exhibit unusual enhancements in thermal conductivity. Picosecond measurements using laser techniques have been used to make the first quantitative measurements of heat transfer at the solid/fluid interface. Very large improvements for thermal conductivity are expected based on simple theory for carbon-nanotubes, but are not observed. The picosecond data shows that the thermal coupling between the nanotube and the surrounding matrix is weak, greatly impeding heat transfer in the carbon-nanotube composite. The results also indicate that the thermal conductance at the particle/fluid interface is highly sensitive to both structure and chemistry.
- *Silicon: From Information Age to an Efficient Light Emitter?* Silicon is the bedrock on which the information age is built, but it is a notoriously poor light emitter. The holy grail of silicon technology is to make silicon an efficient light emitter so that digital information can be converted to light for the ultimate transmission speed across optical fiber networks. New calculations have shown that a novel impurity superlattice structure of thin-layer oxide could do precisely that by altering silicon electronic charge characteristics to couple directly to light. This breakthrough opens the door so that the light-emitting efficiency of silicon could be drastically enhanced. This discovery will dramatically impact the microelectronics industry by significantly reducing the cost and complexity associated with the integration of optoelectronics into silicon-chip products.
- *Synchrotron Light Sources Help Reveal Secrets of Welding.* Welding is a critical metal joining technology used worldwide in the energy, automotive, aerospace, construction, and chemicals industries. Rapid cooling during welding induces numerous phase changes in the metal. Theories have been developed to describe this, but they have never been verified experimentally. Time-resolved x-ray diffraction using synchrotron radiation has now been used for the first time to monitor in-situ phase evolution of a multi-component steel weld during melting and subsequent solidification. The results show that equilibrium theories applied to rapid cooling conditions are not valid for steel welds containing fast diffusing (carbon) and slow diffusing (aluminum) atoms. This new ability to observe the competition of multi-component phases at the microstructural level will make it possible to design stronger and tougher welds, chemically tailored for optimum performance.
- *Ultrathin, Laminar Films for Instantaneous Computer Boot-up.* A new technique has been developed to deposit metal atoms onto thin oxide layers. This technique will help next-generation computers boot up instantly by making entire memories immediately available for use. The method anchors ultrathin metallic cobalt layers on sapphire by using a surface chemical reaction that overcomes an island formation problem that has long plagued researchers. The new, inexpensive trick to prevent

island formation is as simple as exposing thin oxide films to water vapor before depositing the metal layer. The thin metal layer achieves crystallinity after the deposition of only a few atomic layers. This process should be applicable to a wide range of metals on metal oxides.

- *Novel Synthesis of Shape-Controlled Nanostructures.* Fabricating shape-controlled nanostructures such as nanowires and nanodots plays a central role in nanoscale science and technology. A novel electrodeposition process has been developed to self-assemble an array of nanostructures on flat surfaces. The new technique is based on the application of an electric field to ions on graphite substrates immersed in an aqueous solution. A large variety of voltage-controlled nanostructures have been grown such as cubes, pyramids, pentagons, hexagons, nanowires and snowflakes in superconductors and ferromagnets as well as in emerging application systems such as catalytic silver and hydrogen-sensing palladium. These unique nanostructures provide a new theater to explore shape effects on quantum confinement and present new opportunities for nanoelectronic applications.
- *Biomolecular Route to Photovoltaic and Semiconductor Nanocrystals.* Biology exhibits a remarkable ability to control the nanostructures of materials, such as the exquisitely shaped microscopic shells of diatoms and radiolarians, with a precision that far exceeds the capability of present human engineering. Now, the biomolecular mechanism that directs the nanofabrication of silica in living organisms has been harnessed to direct the synthesis of photovoltaic and semiconductor nanocrystals of such materials as titanium dioxide, gallium oxide, and zinc oxide -- materials that biology has never used in structures before. Proteins from a marine sponge – and their counterparts produced from cloned, recombinant DNA – were used to catalyze and structurally direct the growth of the inorganic semiconductors at low temperature and under mild conditions, in marked contrast to the need for elevated temperatures and caustic chemicals presently required by conventional manufacturing methods. The nanocrystallites of gallium oxide formed in this process show a preferential alignment directed by the underlying proteins, revealing a template-like structure-directing activity of the biomolecules. Furthermore, the proteins working at low temperature produce and stabilize crystal forms of gallium oxide and titanium dioxide normally seen only at very high temperatures. Such biomolecular routes may lead to new, environmentally benign routes to semiconductor and photovoltaic materials with improved control over both nanostructure and performance, as well as improved interfaces between optoelectronic devices and living systems.
- *The Impact of a Single Atom.* Never before has it been possible to identify single atoms within bulk materials and determine the influence of a single atom on its surroundings. Isolated atoms can significantly modify the physical properties of many of the technologically most relevant and scientifically interesting materials. While it has long been known that in semiconductors, for example, the presence of a single dopant atom among 1019 host elements drastically modifies the macroscopic properties, the possibility of identifying, localizing, and even measuring the electronic properties of single atoms becomes of fundamental importance in the nanotechnology era. We now have that capability. The aberration-corrected scanning transmission electron microscope allows not only the imaging of individual atoms inside a crystal, but their chemical identification. This remarkable improvement in sensitivity reaches the quantum limit of information, the ability to probe the electronic environment of a single atom.
- *Molecular Cages under Pressure.* The isolation, removal, and entombment of radioactive waste are challenging scientific problems. Structural data from high-pressure x-ray powder diffraction has demonstrated that cage-like zeolites can potentially separate toxic waste from the environment. Using reversible superhydration -- the selective absorption of excess water under pressure into fully hydrated zeolites — the immobilization of commonly occurring radioisotopes such as 90Sr, 137Cs

and 60Co via a “trap-door mechanism” may be realized. By exchanging ions at high pressures, the holes of the zeolites will expand due to the excess water entering the zeolite cages. After pressure release these holes contract again, essentially closing the trap door and sealing the waste inside the zeolite for good.

- *Biocompatible Lasers for Ultrasensitive Detection.* A highly sensitive quantum optics device using a biocompatible semiconductor laser microcavity has been devised that can analyze and characterize spore simulants. This device is based on recent advances in the surface chemistry of semiconductors and the concept of quantum squeezing of light emitted through a spore flowing at high speed in the laser’s microcavity. This light squeezing enables even tiny spores to generate a very large signal which, when analyzed, yields critical biological information including the spore’s protein coat morphology, shape, intracellular granularity, protein density, and uniformity. This field-deployable biolaser should be able to identify different types of spores (for example, anthrax) within a large population of harmless spores rapidly and effectively.
- *Electrocatalyst Design for Fuel Cells.* Electrocatalytic fuel cells at ambient temperature require materials with high catalytic activity and high tolerance to poisons such as carbon monoxide and sulfur. The use of alloys presents inherent limitations including a random distribution of the constituent elements and their propensity to segregate. The use of ordered intermetallics provides stable ordered phases. Based on studies of model systems, it is predicted that the ordered intermetallic bismuth-platinum (BiPt) should exhibit high catalytic activity and greatly reduced poisoning from carbon monoxide. These predictions, based on electronic and geometric effects, respectively, were borne out by experiments. BiPt catalyzes the oxidation of formic acid and is a better material than pure platinum in some ways; moreover, it exhibits catalytic currents about 30 times those on platinum and is virtually immune to carbon monoxide poisoning. Although the focus has been on anode materials, this new design paradigm has clear implications in the design of cathodes as well as reformer catalysts and could usher a new era in fuel cell R&D.

Selected FY 2003 Facility Accomplishments

- The Advanced Light Source (ALS)
  - *Record Low Vertical Emittance Demonstrated.* The emittance is a key parameter that describes the circulating particle beam in a storage ring. Accelerator scientists have reduced the ALS vertical emittance to 5 picometer-radians during accelerator physics experiments. This is the lowest emittance value ever realized in any storage ring. While this emittance is a factor of 20 lower than the value normally used in ALS operation for users, it will be especially important for future spectroscopy studies in which the highest possible resolution is important.
  - *Femtosecond R&D Program Launched.* The study of ultrafast dynamical processes on the time scale of fundamental processes, such as a molecular vibration, is one of the most active areas of modern science. An ALS R&D program was initiated that aims to produce ultrafast x-ray pulses by means of a technique known as electron-beam slicing. To generate x-rays from soft to hard x-ray energies with the maximum intensity, the first narrow-gap in-vacuum undulator will be installed in the ALS.
  - *Beamline Devoted to Study of Soft X-Ray Coherent Science.* Exploitation of the coherence of undulator light has not kept pace with that of other properties, such as brightness. To address this issue at the ALS, a branchline dedicated to coherence has been added to an existing undulator beamline that will produce microwatts of tunable coherent soft x rays. This new capability will allow users to carry out a wide range of experiments in both scattering and fundamental optics.

- *Next-Generation Detector for Synchrotron Radiation Developed.* The brightness of third-generation synchrotron radiation sources often generates huge signal rates that overwhelm the capabilities of existing detector systems. Often, the detector saturation problem both prevents the fullest utilization of the synchrotron light and limits the realization of certain new types of experiments. To overcome this bottleneck, the ALS has developed and successfully tested a high speed (more than 1 GHz), next-generation detector based on high-energy physics technology.

▪ The Advanced Photon Source (APS)

- *A Bull's Eye for Storage Ring Beam Orbit Stability.* Stable x-ray beams are critical for all users of x-ray facilities, particularly those users who microfocus x-rays onto small samples. X-ray beam-position monitors developed for the APS insertion device beamlines are providing beam stability that is now equivalent to firing a stream of bullets through the bull's eye of a target from several miles away.

- *New Information from APS Could Lead to Improved Data Storage.* A surface twisted magnetic state predicted 15 years ago has, for the first time, been confirmed using a new experimental technique at the BES-funded X-ray Operation and Research sector 4 at the APS. Twisted magnetic states of materials have important ramifications for applications in the development of improved magnetic memory.

- *EPICS Collaboration Helps APS and the World.* EPICS (Experimental Physics and Industrial Control System) software developed at two DOE national laboratories is being used worldwide to control complex mechanical systems, from accelerators that reveal the nature of subatomic particles, to observatory telescopes that view distant galaxies, to industrial control processes such as semiconductor wafer manufacturing.

- *Optics Capabilities at the APS Enable New Dynamical Studies of Liquids and Solids.* Inelastic x-ray scattering (IXS) is a synchrotron x-ray tool that opens new vistas for the study of high-temperature materials. The x-ray optics capabilities of the APS have reached a level that makes possible implementation of an IXS spectrometer with exceptional resolving power.

- *A Breath of Fresh Air for Insect Physiology.* A technique that couples phase-enhanced x-ray imaging to the intensity of APS x-ray beams has revealed a previously unknown insect breathing mechanism. Further development of this technique could have important implications for human health care and afford the potential for a wide variety of other materials-related applications, including detecting and studying cracks, voids, and other boundaries inside optically opaque structures; studying fluid flow in rocks and soils for oil exploration and recovery; and characterizing advanced materials, such as ceramics and fiber composites.

▪ The National Synchrotron Light Source (NSLS)

- *High Gain Harmonic Generation (HGHG) FEL Reaches Saturation in Ultraviolet.* The NSLS is pioneering the development of laser seeded Free Electron Lasers (FEL). The HGHG FEL makes uses of a Ti-Sapphire seed laser to produce fully coherent 266 nm light. This marks the first HGHG FEL to successfully reach saturation in the ultraviolet regime and thereby obtaining sub-picosecond pulses with energy in excess of 100 microjoules.

- *New Powder and Single Crystal Diffraction Beamline Completed.* A new bending magnet beamline, X6B, has been completed. The beamline was constructed to meet the increasing demand of nanoscience users for powder and single crystal x-ray diffraction. The beamline consists of a Si(111) monochromator, tunable from 5 keV to 20 keV, and a double focusing mirror. The beamline is designed to perform (a) time-resolved powder diffraction, (b) combined x-ray spectroscopy and x-ray diffraction, (c) single crystal diffraction, and (d) measurement of electron density of excited states.

- *Superconducting Wiggler Beamline Upgraded.* The X17 superconducting wiggler beamline is the only high-energy x-ray insertion device at the NSLS. It serves a large and very productive earth science and high-pressure user community. In FY 2003, two new experimental hutches were constructed so that a materials science instrument, a large volume press instrument, and a diamond anvil cell instrument will each have a dedicated experimental hutch. All three programs will be able to operate simultaneously, thus significantly increasing the amount of beam time available to these user communities.
- *Low-Energy X-Ray Beamline Upgraded.* The low-energy x-ray region is important because it covers the K absorption edges of Si, S, P, Cl, and L edges of 4d transition metals. X-ray spectroscopy and x-ray resonant scattering in this energy range are valuable tools in catalysis, environmental science, magnetism, and bio-materials. A new monochromator was designed and installed in FY 2003 to improve the cooling of the monochromator crystals in X19A beamline. The new design has led to better energy and intensity stability of the beamline.

▪ The Stanford Synchrotron Radiation Laboratory (SSRL)

- *First Beam from the Sub-Picosecond Pulse Source (SPPS) is Achieved.* Ultrafast pulses of x-rays are key tools for probing the electronic and structural changes in materials during fast chemical reactions and phase changes. To this end, the SPPS was installed in the SLAC Final Focus Test Beam Facility, which generates pulses of 8-10 keV x-rays with 10^7 photons/pulse at a pulse rate of 10 pulses per second. The peak brightness of these x-ray pulses exceeds that of any existing x-ray source. The SPPS is planned to operate 3-4 months per year through 2005, when it will be displaced by the construction of the Linac Coherent Light Source, a much more intense source of short x-ray pulses.
- *SSRL's Final Run with SPEAR2 Ends on a Perfect Note.* SSRL's most recent experimental run prior to the decommissioning of SPEAR2 ended very successfully with SPEAR delivery of scheduled beam time to users at the 100% mark during the last week of operations. Even though the FY 2003 run was shortened by about 4 months due to the beginning of the SPEAR3 installation, a total of 813 users came to SSRL during the run to conduct experiments on 32 stations. The up time average for the entire FY 2003 run was 96.8%.
- *SPEAR3 Installation Program Proceeding on Schedule.* The SPEAR3 Installation Program began on schedule on March 31, 2003. The Installation Program involves three phases: demolition of SPEAR2, modification of the facilities to meet SPEAR3 needs, and finally the actual installation of SPEAR3 technical systems and components. Each phase is a complex procedure that is planned in great detail with overall completion by the end of October 2003.
- *New Experimental Station Developed on BL11.* A new experimental station that will be used for both materials scattering and macromolecular crystallography has been commissioned on BL11. This new station will help relieve the significant over subscription on BL7-2 for users performing x-ray structural studies of thin films as well as provide for single- or multi-wavelength anomalous dispersion (SAD and MAD) experiments to be carried out at the Se edge for macromolecular crystallography applications.

- The Intense Pulsed Neutron Source (IPNS)
  - *Upgrades of IPNS Instruments Continue.* IPNS continues to make major instrument upgrades and source improvements to maintain world class science capabilities for U.S. users: 1) an upgrade project for a powder diffractometer, GPPD, has been completed putting the instrument on a par with the fastest powder instruments in the world; 2) installation of a guide on QENS, a quasi-elastic spectrometer boosted flux on sample by a factor of five; 3) redesigning the moderator/reflector assembly resulted in a gain of 60% neutrons-on-sample for small angle scattering applications.
  - *Outstanding Operations at IPNS Continues.* For the sixth consecutive year, the IPNS has exceeded its goal of offering at least 95% reliable operations, achieving a figure of 97% in FY 2002. This reliability assures users that experiments can be performed as planned and offers additional evidence that pulsed neutron sources can be run in a reliable manner.
  - *IPNS Hosts the National Neutron and X-Ray Scattering School.* During the two-week period of August 10-24, 2003, 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 143 applications for the 60 positions available in 2003.
- The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE)
  - *First Results with the 11-T Magnet at Lujan Center.* The newly commissioned 11-T superconducting magnet provided Lujan Center users with the first results of an intensity image (reflection) of neutron data collected from an antiferromagnetic material on the new Asterix instrument. Significantly, the mass of material contributing to the reflection is only about 100 micrograms. Moreover, exceedingly good thermal stability was achieved during the measurements.
  - *Upgraded NPDF Produces 300 Data Sets.* The Neutron Powder Diffractometer (NPDF) opened its shutter for the first time and produced over 300 experimental data sets during the run cycle. Promising results obtained during the run cycle not only put NPDF at the cutting edge of local-structure determination but also served as a development platform for a new structure-analysis tool based on pair-distribution functions in disordered and nanostructured materials.
  - *Upgrades to SPEAR Improve Reflectivity Measurements.* Upgrades to SPEAR have simplified the operation of the instrument and provided more precise and reproducible reflectivity measurements. SPEAR is a time-of-flight neutron spectrometer ideally suited to study thin organic and inorganic layers in a variety of environments. A recent experiment on SPEAR provided fundamental information about the stability of model biomembranes in the presence of large electric fields.
  - *Upgrades to LQD Enables More Sophisticated Small-Angle Scattering Experiments.* Small-angle scattering has been improved at the Lujan Center to keep apace with the significantly increased cold-neutron flux available to LQD (Low-Q Diffractometer), which has been increased by approximately a factor of five. These upgrades will allow more measurements, higher-quality data, and the ability to perform more sophisticated experiments.

- The High Flux Isotope Reactor (HFIR)
  - *World-Class Triple-Axis Spectrometers Installed at HFIR.* These spectrometers, designated HB-1, HB-1A, and HB-3, are exceeding performance goals and are equal to the highest intensity instruments of their kind in the world. The installation of three additional world-class instruments is under way at the HB-2 shielding tunnel, which was completed in March 2003. The first of the new instruments should be available in early fall 2003 with the other two to follow by the end of 2003.
  - *Construction of the Small Angle Neutron Scattering (SANS) Guide Hall Completed.* The high bay guide hall will house the new 40m and 35m SANS instruments and supporting lab space. It will provide a research environment away from the reactor building that will be used by numerous facility users for physical and biological material studies.

Detailed Justification

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
Materials Sciences and Engineering Research....	**252,539**	**263,929**	**275,543**
▪ **Structure and Composition of Materials.........**	**28,915**	**32,954**	**32,183**

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, and corrosion susceptibility.

In FY 2005, major activities 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. One aspect of this will be research towards an optimal platform for Transmission Electron Aberration-corrected Microscopy. This effort is intended to dramatically extend electron scattering capabilities for three-dimensional tomography, local spectroscopy, and *in-situ* sample manipulation and processing. An additional $975,000 is provided for novel

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

analytical technologies to access hydrogen storage materials. State-of-the-art electron microscopy and spectroscopy approaches will be used to monitor atomic-level processes in such materials. Observing these processes under realistic experimental conditions is required to determine basic mechanisms of hydrogen storage and release.

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

The overall decrease for structure and composition of materials is attributable to an increase for research related to hydrogen economy ($+975,000) offset by a decrease in capital equipment for electron microscopy activities ($-1,746,000).

	FY 2003	FY 2004	FY 2005
▪ **Mechanical Behavior and Radiation Effects**...	**13,323**	**13,600**	**13,600**

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.

In FY 2005, major activities will include continued development of experimental techniques and methods for the characterization of mechanical behavior including mechanical behavior of matter with nanoscale dimensions, the development of a universal model for mechanical behavior that includes all length scales from atomic through nanoscale to bulk dimensions, and the continued advancement of computer simulations for modeling mechanical behavior and radiation induced degradation.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

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

▪ **Physical Behavior of Materials**.........................	**20,262**	**20,500**	**22,450**

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 field, chemical environment, and proximity of surfaces or interfaces. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the superconducting properties for high-temperature superconductors; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures encountered in energy conversion processes; and diffusion and transport of ions in ceramic electrolytes for improved performance in batteries and fuel cells.

Research underpins the 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.

In FY 2005, major activities will continue fundamental studies of corrosion resistance and surface degradation; semiconductor performance based on organic and inorganic materials; high-temperature superconductors; and the interactions, and transport of defects in crystalline matter. An additional $1,950,000 is provided for basic research on the storage of hydrogen using a broad class of complex hydrides. The emphasis will be on understanding the fundamental factors governing bond strength, kinetics, absorption and desorption behavior, and degradation with hydrogen uptake/release cycles. This information will be used to modify the performance of known hydrogen storage materials and to identify new classes of materials. Research on efficient solar energy production of hydrogen using organic photovoltaics with quantum-size organic semiconductors also will be performed. Systematic experimental approaches coupled with theory, modeling, and simulation will be applied to both research areas.

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.

▪ **Synthesis and Processing Science**	**11,839**	**12,000**	**12,975**

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.

The 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 2005, major activities 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. An additional $975,000 is provided for research on the design, synthesis, and processing of nanomaterials for the storage and release of hydrogen. By changing the structure of a given chemical compound at the nano-level, materials with different behavior are obtained which can be optimized for hydrogen storage behavior.

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

	FY 2003	FY 2004	FY 2005
▪ **Engineering Research**	**15,297**	**14,038**	**13,500**

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. FY 2005 activity will continue laser based generation and

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

characterization of phonons in solids with application to needs in heat transfer, thermoelectric energy conversion, and non-destructive early-warning of impending failure and remaining safe lifetime predictive capabilities. This activity will also support fundamentals of granular systems (which are utilized for powder and particular matter preparation and conveyance, in fluidized bed reactors, and in certain heat transfer applications).

The decrease of funding for Engineering Research is attributable to a decreased emphasis on fluid dynamics of multi-component systems ($-538,000).

▪ **Neutron and X-ray Scattering**	**37,821**	**41,877**	**42,058**

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.

In FY 2005, with an additional $2,437,000, research in the area of nanostructured and novel hydrogen storage media will be performed 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.

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

The overall increase for Neutron and X-ray Scattering is attributable to an increase in Neutron and X-ray Scattering Research for instrumentation related to hydrogen ecology ($+2,437,000) offset by a decreased emphasis on core research ($-2,256,000).

▪ **Experimental Condensed Matter Physics**	**37,205**	**40,500**	**42,449**

This activity supports condensed matter physics with emphasis in the areas of electronic structure, surfaces/interfaces, and new materials. Research includes measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This activity includes the design and synthesis of new materials with new and improved properties. The materials examined 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 can be 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. Research in superconductivity is coordinated with the technology programs in Energy Efficiency and Renewable Energy (EE/RE). Research on magnetism and magnetic materials focuses on hard magnet materials, such as those used for permanent magnets and in motors. This activity provides direct research assistance to the technology programs in EE/RE (photovoltaics, superconductivity, power sources, thermoacoustics, and thermoelectrics), and in the National Nuclear Security Administration (NNSA) (photoemission, positron research, electronic and optical materials, advanced laser crystals, and weapons-related materials). In addition, it supports several DOE technologies and the strategically important information technology and electronics industries through its results 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 2005, major activities will include 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. The potential impacts of understanding the physics are very significant. For example, nanoscale structures provide a path toward the next generation of powerful permanent magnets for more efficient electric motors, better thermoelectric materials, and materials for more efficient solar energy conversion. An additional $1,949,000 is provided for the development of nanomaterials (structure and phase dimensions of 1-100 nanometer) for both energy conversion and hydrogen energy storage, which exhibit size-dependent properties that are not seen in macroscopic solid state materials. Examples include both carbon-based materials, such as nanotubes, nanohorns, fullerenes, and non-carbon-based materials such as semiconductors. Enhanced electrical, thermal, mechanical, optical, and chemical properties have shown that these new materials 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.

	FY 2003	FY 2004	FY 2005
▪ **Condensed Matter Theory**	**16,993**	**17,000**	**17,975**

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; ceramics; modeling oxidation processes at surfaces and interfaces; excited state electronic structure and response functions; polymers at interfaces; and quantum transport in molecular and nanoscale systems.

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

In FY 2005, this activity will provide support for theory, modeling, and large-scale computer simulation to explore new nanoscale phenomena and the nanoscale regime. Support for the Computational Materials Sciences Network will be continued with new topical areas as they evolve. An additional $975,000 is provided to advance theoretical understanding of critical processes and reactions in hydrogen systems, which will provide a fundamental basis for new materials design.

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

	FY 2003	FY 2004	FY 2005
▪ **Materials Chemistry**..	**40,563**	**42,000**	**44,437**

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 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

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

biological approaches may yield materials for advanced separations and energy storage.

In FY 2005, this activity 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. An additional $2,437,000 is provided for research on hydrogen production (by biomolecular materials), storage (in complex hydrides, nanocomposites, nanotubes), and fuel cells (novel electrode and membrane materials and processes).

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

▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)**....................	**11,722**	**7,673**	**7,673**

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, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Mexico, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, and the Commonwealth of Puerto Rico. The states of Delaware, Tennessee and Rhode Island, and the U.S. Virgin Islands may also become eligible for the EPSCoR program in FY 2005. The work supported by the EPSCoR program includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, fossil energy sciences, and energy efficiency and renewable energy sciences. The following table shows EPSCoR distribution of funds by state.

EPSCoR Distribution of Funds by State

	(dollars in thousands)		
	FY 2003	FY 2004 Estimate	FY 2005 Estimate
Alabama	946	815	510
Alaska[a]	0	0	0
Arkansas	205	140	0
Hawaii[b]	0	0	0
Idaho	100	0	102
Kansas	881	560	560
Kentucky	1,224	355	224
Louisiana	287	0	198
Maine	0	0	0
Mississippi	685	535	535
Montana	580	515	375
Nebraska	1,155	300	0
Nevada	1,146	250	0
New Mexico[b]	0	0	0
North Dakota	137	0	139
Oklahoma	339	140	135
Puerto Rico	435	375	375
South Carolina	781	140	266
South Dakota	0	0	0
Vermont	1,064	857	709
West Virginia	1,405	360	201
Wyoming	130	0	130
Technical Support	222	100	110
Other	0	2,231 [c]	3,104 [c]
Total	11,722	7,673	7,673

[a] Alaska became eligible for funding in FY 2001.

[b] Hawaii and New Mexico became eligible for funding in FY 2002.

[c] Uncommitted funds in FY 2004 and 2005 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**	**3,564**	**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)**	**0**	**2,000**	**4,000**

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.

▪ **Nanoscale Science Research Centers**	**100**	**400**	**600**

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.

▪ **SPEAR3 Upgrade**	**9,300**	**0**	**0**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) was undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The upgrade increased injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decreased beam emittance by a factor of 7 to increase beam brightness; increased operating current from 100 mA to 200 mA to increase beam intensity; and maintained long beam life time (>25 hr). The increased photon flux will greatly improve performance in a variety of applications including powder and thin film diffraction, topographic studies, surface microcontamination studies, x-ray tomographic analysis, x-ray absorption studies, and protein crystallography. The magnets and associated vacuum chambers of the existing SPEAR storage ring were replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC was $29,000,000; DOE and NIH equally funded the upgrade with a total Federal cost of $58,000,000. NIH provided $14,000,000 in FY 1999, $14,000,000 in FY 2000, and $1,000,000 in FY 2001. This MIE project was completed on schedule and within budget. The SPEAR3 is now being commissioned.

▪ **The Center for Nanoscale Materials**	**0**	**10,000**	**12,000**

Funds are provided for a major item of equipment with a total estimated cost of $36,000,000 for instrumentation, including clean rooms, for the Center for Nanoscale Materials at Argonne National Laboratory. The instrumentation will be contained in a new building, which 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

	FY 2003	FY 2004	FY 2005
	(dollars in thousands)		

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.

	FY 2003	FY 2004	FY 2005
▪ **Instrumentation for the Spallation Neutron Source**	**5,635**	**7,387**	**7,643**

Funds are provided for a major item of equipment with a total estimated cost in the range $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 following completion of Title I design and an External Independent Review in FY 2004. It is anticipated that these five instruments will be installed at the SNS on a phased schedule between FY 2007 – 2011.

	FY 2003	FY 2004	FY 2005
Facilities Operations	**281,013**	**294,517**	**312,854**
▪ **Operation of National User Facilities**	**281,013**	**294,517**	**312,854**

The facilities included in Materials Sciences and Engineering are: Advanced Light Source, Advanced Photon Source, National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory, High Flux Isotope Reactor, Intense Pulsed Neutron Source, and Manuel Lujan, Jr. Neutron Scattering Center. Research and development in support of the construction of the Spallation Neutron Source is also included. 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 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.

	FY 2003	FY 2004	FY 2005
	(dollars in thousands)		

Facilities

	FY 2003	FY 2004	FY 2005
	(dollars in thousands)		
Advanced Light Source	42,844	43,205	42,200
Advanced Photon Source	90,894	93,410	97,400
National Synchrotron Light Source	36,950	38,325	38,400
Stanford Synchrotron Radiation Laboratory	25,903	30,305	28,100
High Flux Isotope Reactor	36,838	37,805	39,832
Radiochemical Engineering Development Center	6,515	6,305	6,300
Intense Pulsed Neutron Source	16,714	16,655	17,222
Manuel Lujan, Jr. Neutron Scattering Center	9,914	10,110	10,300
Spallation Neutron Source	14,441	18,397	33,100
Total, Facilities	281,013	294,517	312,854

	FY 2003	FY 2004	FY 2005
SBIR/STTR	**0**	**13,910**	**14,831**

In FY 2003, $11,897,000 and $714,000 were transferred to the SBIR and STTR programs, respectively. The FY 2004 and FY 2005 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

	FY 2003	FY 2004	FY 2005
Total, Materials Sciences and Engineering	**533,552**	**572,356**	**603,228**

Explanation of Funding Changes

	FY 2005 vs. FY 2004 ($000)
Materials Sciences and Engineering Research	
▪ Overall decrease for structure and composition of materials research because of increase for research related to the hydrogen economy ($975,000) and decrease because of reduction in capital equipment for electron microscopy activities ($-1,746,000)	-771
▪ Increase for physical behavior of materials research for research related to the hydrogen economy.	+1,950
▪ Increase in synthesis and processing science research for research related to the hydrogen economy.	+975

	FY 2005 vs. FY 2004 ($000)
▪ Decrease in engineering research because of decreasing emphasis on fluid dynamics of multicomponent systems.	-538
▪ Overall increase in neutron and x-ray scattering research for instrumentation related to hydrogen economy ($2,437,000). Research is decreased ($-2,256,000) to fund the MIE for the ANL Center for Nanoscale Materials and the increase for instrumentation for the Spallation Neutron Source.	+181
▪ Increase in experimental condensed matter physics for research related to the hydrogen economy.	+1,949
▪ Increase in condensed matter theory for research related to the hydrogen economy.	+975
▪ Increase in materials chemistry for research related to the hydrogen economy.	+2,437
▪ Increase for research and development for the Linac Coherent Light Source.	+2,000
▪ Increase for other project costs per schedule associated with the Nanoscale Science Research Centers.	+200
▪ Increase for MIE for the ANL Center for Nanoscale Materials.	+2,000
▪ Increase for Instrumentation for the Spallation Neutron Source.	+256
Total, Materials Sciences and Engineering Research	+11,614
Facilities Operations	
▪ Decrease for operations of the Advanced Light Source as a result of a one-time FY 2004 capital equipment increment for new components of the beamline for nanoscience spectroscopy and diffraction..	-1,005
▪ Increase for operations for the Advanced Photon Source.	+3,990
▪ Increase for operations of the National Synchrotron Light Source.	+75
▪ Decrease for operations of the Stanford Synchrotron Radiation Laboratory as a result of a one-time FY 2004 capital equipment increment for a new insertion device for the nanomagnetism beamline	-2,205
▪ Increase for operations for the High-Flux Isotope Reactor	+2,027
▪ Decrease for operations for the Radiochemical Engineering and Development Center	-5
▪ Increase for operations for the Intense Pulsed Neutron Source.	+567
▪ Increase for operations of the Manuel Lujan, Jr. Neutron Scattering Center.	+190
▪ Increase in the Spallation Neutron Source Other Project Costs per FY 2004 project datasheet for the operations.	+14,703
Total, Materials Sciences and Engineering Facilities Operations	+18,337

	FY 2005 vs. FY 2004 ($000)
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in total operating expense funding	+921
Total Funding Change, Materials Sciences and Engineering	+30,872

Chemical Sciences, Geosciences, and Energy Biosciences

Funding Schedule by Activity

(dollars in thousands)

	FY 2003	FY 2004	FY 2005	$ Change	% Change
Chemical Sciences, Geosciences, and Energy Biosciences					
Chemical Sciences, Geosciences, and Energy Biosciences Research.................	205,963	208,221	216,743	+8,522	+4.1%
Facilities Operations	5,935	5,967	6,169	+202	+3.4%
SBIR/STTR	0	5,394	5,510	+116	+2.2%
Total, Chemical Sciences, Geosciences, and Energy Biosciences	211,898	219,582	228,422	+8,840	+4.0%

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 2003 Research Accomplishments

- *Emergence from the Primordial Soup.* Fifty years ago, Miller and Urey (Science, 1953) showed that simple inorganic molecules presumed present in the early earth atmosphere could yield amino acids after exposure to an electric discharge. Subsequent models of the chemical origin of life were complicated by the requirement to explain the asymmetric (chiral) nature of DNA and its components. Both of these elements are addressed in recent work using advanced mass spectrometric tools to study amino acid aggregation and reaction products in the gas phase. The simple amino acid serine is the commonly accepted product of formaldehyde and glycine, both known to exist in interstellar space. Using sonic-spray ionization with mass spectrometric detection, researchers have shown that certain especially stable clusters of serine are homochiral, that is, exclusively one of the possible symmetries. Furthermore, in reactions of the cluster with other important biological molecules, the asymmetry is passed on to the reaction products. These observations rationalize a model of prebiotic chemistry beginning with the assembly of homochiral serine octamers. Following selection of a particular homochiral cluster by an unknown asymmetric species, reactions with other biologically relevant molecules could pass on the asymmetry as further chemical reaction led to the formation of chiral, self replicating, life forms.

- *Designer Solvents.* Ionic liquids have already replaced volatile, polluting hydrocarbon solvents in some industrial processes, and progress is being made in using ionic liquids for inherently safe processing of nuclear fuel and radioactive waste. It is important to understand how chemical reaction patterns are influenced by the unusual environment of ionic liquids. New studies have explored fast reactions in ionic liquids by pulse radiolysis and have shown that charged species, such as a bare electron surrounded by solvent, move more slowly in ionic liquids in comparison to neutral species, just the opposite of what is seen in normal solvents. Also discovered was a reactive and highly mobile form of the electron that exists for only a few trillionths of a second in normal solvents but persists thousands of times longer in ionic liquids.

- *Reactivity within Nanovessels.* The elusive challenge of attaining chemical selectivity close to 100 percent for reactions in aqueous solution may eventually be achieved by mimicking Nature's most selective catalysts – enzymes. Researchers are attempting just that by synthesizing stable and semi-rigid inorganic cage structures that are able to sequester organometallic catalysts in their interior. By using the restrictive environment of the nanovessel cavity, they have shown reactant-selective organic transformations. As a dramatic demonstration of reactant selectivity, they have shown that these encapsulated complexes react with aldehydes with rates that depend on the size of the molecule, unlike the same complexes in solution, which cannot discriminate among aldehydes of different length.

- *Fundamental Studies of Water*. It is difficult to identify a quantity more fundamental to chemistry than the O–H bond dissociation energy of water. Its importance arises from its ubiquity, which ranges from elementary reactions to those in complex environments such as flame chemistry or atmosphere chemistry. A joint experimental/ theoretical study recently revised the value of this bond dissociation energy by a small amount. Although a relatively small change, the impact of this correction is enormous. It will cause changes in the gas-phase acidity of water, several proton affinities, all R-OH bond dissociation energies, reaction enthalpies of all OH reactions, and heats of formation computed relative to H2O or OH bond dissociation energies.
- *Storing Energy in Dendrimer Trees.* Dendrimers are nanoscale molecules constructed from branches connected to a central core. If a dendrimer is built with an electron acceptor in the core and electron donors on the branches, the molecule can capture and temporarily store energy from light by moving electrons from the branches to the core. Further chemistry can then be used to capture the energy permanently before it is dissipated by electron transfer back to the branches. A dendrimeric system has been designed that functions as an electron antenna, absorbing several photons to create a core with a long lifetime. The stored energy can be lost if the electron returns to the "hole" it left behind. However, for dendrimers with branches long enough to allow their tips to touch, the holes are trapped on pairs of molecules at the tips, and the charge-separated state lasts for a long period of time.
- *Coherent Surface Plasmons in Nanoscale Systems.* One of the great promises of nanotechnology is the localization of phenomena on the nanoscale. Theoreticians have recently described the nanoscale analog of a laser in which coherent optical-frequency radiation fields are confined and amplified in nanosystems. They show that quantum generation of surface plasmons for a nanoscale v-shaped metal or semiconductor pattern can lead to stimulated emission and gain for certain highly localized plasmon modes. Such a device has been christened a SPASER, for Surface Plasmon Amplification by Stimulated Emission of Radiation. If realized, the SPASER has enormous potential applications in nanotechnology, including optical detection and information processing.
- *Triple-Action Catalytic Polymerization.* Catalysts that involve multiple functions working in concert at the molecular level offer dramatic advantages over single-function catalysts by reducing intermediate separation steps and achieving unusual reaction selectivity by controlling the competitive interplay of catalytic sites and the various molecular species present in the solution. Triple functions were synthesized on a complex catalytic compound that is active for ethylene polymerization. The terfunctional catalyst produces branched polyethylene with regular structures that cannot be obtained with a single catalyst or a pair of catalysts working in tandem. The extent and type of branching exhibited by the polymers, and therefore the chemical, mechanical, and optical properties of those materials, can be controlled by adjusting the ratios of the different functionalities.
- *Multidimensional Chemical Analysis of Attomole Sample.* Modern applications of chemical analysis, ranging from pollution studies to homeland security, increasingly require the ability to interrogate extremely small sample sizes. These mass-limited situations might arise because the sample is incredibly expensive, unusually toxic (biothreat agents), or inherently difficult to obtain in large quantities (intracellular signaling molecules). Conventional instrumentation is challenged, because their requirement for large sample volumes leads to extremely diluted samples. Researchers are developing solutions to this conundrum by exploiting the special electrokinetic flow properties of tiny cylindrical capillaries to create multilayer chemical instrumentation capable of addressing samples as small as 1,000,000 molecules and below. Because the capillaries are less than 100

nanometers in diameter, they can control fluid flow among layers of microchannels, thereby making it possible to sequentially link separate chemical manipulations. For example, scientists recently demonstrated the use of a nanocapillary molecular gate to detect and capture a 100 attomole (10-16 moles) band from a chip-based electrophoretic separation, establishing a new low for preparative chromatography of mass-limited samples.

- *DNA Transport through a Single Carbon Nanotube.* Carbon nanotubes have been proposed as useful media for a variety of applications such as hydrogen storage, chemical separation, and ultrasensitive sensors. A common research theme among these applications is the need to understand mass transport through such nanoporous materials. In a dramatic demonstration of its separations capability, a single, multiwalled carbon nanotube has been immobilized within an electrophoretic membrane test chamber and the passage of single DNA molecules has been monitored by fluorescence microscopy. Individual DNA molecules having a diameter smaller than the nanotube's opening were observed to readily pass through, whereas larger DNA molecules exhibited behavior consistent with trapping and hindered passage. Because of the simple structure of the nanotubes, modeling can yield insight into the mass transport properties of its very small pores.
- *Actinide Supramolecular Chemistry: Giant Rings for Heaviest Atoms.* Supramolecular chemistry is the controlled formation of large molecular aggregates from smaller subunits. The formation is controlled in order to achieve or optimize specific chemical properties. Actinide ions, the largest metal ions, have unique electron configurations and represent materials that can be extremely useful or extremely dangerous. Supramolecular assemblies called helicates have been created where six thorium ions are encapsulated in a "box" (cluster) that self-assembles from eight smaller assemblies, that will now be investigated for their ability to remove toxic ions such as the actinides from the body.
- *Targeted Recognition of Actinide Ions.* Fundamental research on the selective complexation of specific ions of radioactive elements with disk-like complexants has led to simple and sensitive detection of these ions. Several classes of disk-like complexants create strong bonds between actinide ions, all of which are radioactive, and nitrogen atoms in the cages. These bonds cause transitions in electronic and vibrational spectra that result in visible color changes that occur only when specific actinide ions, in particular ions of neptunium and plutonium, are present. These colored complexes are important because of the changes they cause in electronic and vibrational structure and because they represent opportunities for detection of potentially hazardous radioactive ions that could be released into the environment – or to reassure first-line responders and the public that such species have not been released.
- *Life Cycle of a Water Molecule on an Electrode.* Technological progress towards a future hydrogen economy relies on understanding molecular-level phenomena governing conversion hydrogen formation at the electrodes in electrolyzers and fuel cells. Ruthenium dioxide is unsurpassed at enhancing catalytic activities in room-temperature fuel cell anodes, and it is a very promising electrocatalyst. Using synchrotron x-ray studies, fascinating sequential rearrangements of surface water molecules were discovered, evolving from a loose hydrogen-bonded water layer, to a hydroxide layer, and to a dense form of water, which exist on the ruthenium dioxide surface at different applied potentials. These interfacial forms of water may be the intermediates long suspected to be responsible for promoting oxidation of hydrogen and methanol in the fuel-cell environment as well as promoting the oxygen-evolution reaction. These previously unavailable molecular-level details of the energy-conversion processes provide scientific impetus for a more rational design of high performance electrocatalysts. This first-of-its-kind study was possible

because of the unprecedented level of sensitivity afforded by the high brilliance of today's synchrotron radiation light sources.

- *Identification and Structural Determination of a Novel Protein Motif.* The protein machinery within a biological cell is manufactured via a complex assembly line that stretches from decoding DNA into RNA and translates the message into a polypeptide chain. Subsequent assembly into larger complexes and covalent linkage of the peptide chain with other carbohydrate or lipid components may also occur to provide additional chemical reactivity or specificity. The photosynthetic machinery that captures light energy and turns it into chemical energy is assembled in just such a fashion, with both large and small subunits of the carbon-fixing enzyme, Rubisco, undergoing methylation on lysine residues. A novel protein motif called the SET domain that carries out the methylation of Rubisco has been identified and its structure determined. The SET domain has been found in many other enzymes in a variety of biological contexts ranging from enzyme substrate recognition to scaffolding and stabilizing DNA. The common function of recognizing a molecular structure for subsequent covalent modification may lead to a common code for deciphering regulatory mechanisms of catalysis and molecular recognition.
- *First measurement of how much energy is required to insert a single new protein into a chloroplast.* The presence of internal organelles within the plant cell poses numerous challenges for the coordinated synthesis and trafficking of new proteins, which often must be synthesized in one part of the cell and directed to another sub-cellular compartment. The latter process necessitates the movement of the new protein across one or more membranes. Plant chloroplasts represent a unique opportunity to study the energetics of a mixed transport system that incorporates the cellular challenges of both eukaryotes and microbes. The energetic cost of this process is a fundamental unanswered question in plant biology, since the majority of photosynthetic apparatus proteins are continuously synthesized and imported into the chloroplast, then rapidly degraded. DOE/BES support has led to the first measurement of how much energy is required to insert a single new protein—an astonishingly high proton flux that is equivalent to the energy stored within 10,000 ATP molecules! Thus approximately 3% of the total energy output of the chloroplast from photosynthesis is devoted to maintaining the photosynthetic machinery. This knowledge provides the foundation for future strategies for more efficient light-harvesting applications for renewable energy.

Selected FY 2003 Facility Accomplishments:

- The Combustion Research Facility (CRF)
  - *New Capability Developed for Three-Dimensional Measurements in Turbulent Flames.* Lasers and digital camera systems for imaging of laser-induced fluorescence in two intersecting planes were added to existing systems for line-imaging measurements of temperature and major species in turbulent flames. The combination yields information on the magnitude and effects of three-dimensional scalar dissipation, which is a central quantity in combustion theory and modeling.
  - *Station Established to Generate Periodically Poled Lithium Niobate (PPLN).* A station has been designed and built to pole lithium niobate at the CRF. PPLN is a quasi-phase-matched crystal that is significantly more efficient and tunable than conventional crystals. Recent major advances in nonlinear optical materials have opened up many new possibilities for chemical sensing. In particular, the development of PPLN has sparked the advent of broadly tunable, compact, highly efficient infrared laser sources. This technology could be applied to problems such as medical monitoring or transient molecule detection.

- *Picosecond Lasers Constructed.* Continued progress in understanding combustion processes relies on developing increasingly sophisticated laser diagnostics for detailed understanding of collisional phenomena. To meet this need, CRF scientists have developed three new tunable, short-pulse lasers optimized for pump-probe experiments. These sources are custom-built distributed-feedback dye lasers with sufficient resolution for studying most intermolecular collisional processes.
- *Time- and Frequency-Resolved Fluorescence Microscopy.* Researchers at the CRF have constructed a time- and frequency-resolved photon detection system with fluorescence microscopy to simultaneously measure fluorescence lifetime and spectra. With such correlated time and spectral information, scientists can characterize the fluorescence emission from a microscopic sample in more detail than previously possible, thereby unraveling the uncertainties associated with measuring the fluorescence lifetime and frequency separately.

Detailed Program Justification

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
Chemical Sciences, Geosciences, and Energy Biosciences Research	**205,963**	**208,221**	**216,743**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**13,379**	**13,401**	**13,401**

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.

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.

In FY 2005, major activities will include the interactions of atoms and molecules with intense electromagnetic fields that are produced by collisions with highly charged ions or short 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.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

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.

▪ **Chemical Physics Research**	**32,097**	**30,334**	**31,617**

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 optical diagnostics such as degenerate four-wave mixing, cavity ring-down spectroscopies, high-resolution optical spectroscopy, and ion-imaging techniques have been developed to characterize gas phase processes. 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 percent 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: chemically reacting flows, the chemistry of unstable species and large molecules; and 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.

In FY 2005 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 $667,000 in chemical physics research funding will result in a decreased effort in the study of aspects of gas phase chemistry. An additional $1,950,000 is provided for the following activities: the development of quantum chemical and density functional theories for the predictive, molecular-level modeling of

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

catalytic reaction mechanisms relevant to hydrogen production; use of first-principles dynamical calculations to investigate the interaction of hydrogen with storage materials; development of new analytical tools for probing natural hydrogen biocatalysts; and application of molecular modeling capabilities for predictive development of biomimetic catalysts for hydrogen production.

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

▪ **Photochemistry and Radiation Research**	**24,853**	**28,502**	**29,477**

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.

In FY 2005, major activities 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. An additional $975,000 is provided for synthesis and characterization of inexpensive, nanostructured semiconductor materials for conversion of solar radiation to electricity and efficient and direct photocatalytic splitting of water to produce hydrogen through discovery of improved catalytic materials.

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.

	FY 2003	FY 2004	FY 2005
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	**11,797**	**12,133**	**13,108**

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 2005, an additional $975,000 is provided for fundamental research to improve the efficiency and decrease the cost of solar hydrogen production. Exploiting and mimicking components of natural hydrogen-producing systems will enable key improvements in efficiency and reduction in the cost of solar hydrogen production. Capital equipment is included in this request.

	FY 2003	FY 2004	FY 2005
▪ **Metabolic Regulation of Energy Production**	**18,665**	**19,195**	**18,695**

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 2005, studies will continue 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

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

between cellular components. This new 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.

▪ **Catalysis and Chemical Transformation**............	**33,854**	**34,453**	**36,402**

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 chloroflurocarbons into environmentally acceptable refrigerants. Research supported by this program also provides the basis and impetus for creating a broad range of new materials, such as mesoporous solids that can act as improved catalysts.

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.

In FY 2005, the activity 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. An additional $1,949,000 is provided for fundamental research into the nature of catalytic processes on designed nanoscale catalysts. 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.

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.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
▪ **Separations and Analyses**	**14,547**	**13,517**	**16,441**

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 315 million barrels of oil. It has been estimated that separation processes account for more than five percent of 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.

In FY 2005, major activities 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. An additional $2,924,000 is provided for research to improve separations with membranes (1) to invent membranes that can enhance the efficiency of gas separations to produce ultra-pure hydrogen; (2) to develop thermally robust inorganic membranes that will enable thermal water splitting cycles for hydrogen production; (3) to improve gas permeability while retaining high proton conductivity of membranes for fuel cells; and (4) to innovate novel high-temperature fuel cells with advanced polymeric and inorganic-ion-conducting membranes. Chemical analysis research will be initiated (1) to study hydrogen-separation materials and processes under realistic environmental conditions, rather than in high vacuum; (2) to achieve high temporal resolution, so that changes can be monitored dynamically; and (3) to enable multiple analytical measurements to be made simultaneously on systems such as fuel cell membranes, which have three percolation networks (proton, electron, and gas).

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

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
▪ **Heavy Element Chemistry**	**9,974**	**9,375**	**9,375**

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 Management Science Program.

This activity represents the Nation's only funding for basic research in the chemical and physical principles of actinide and fission product materials. The program is primarily based at the national laboratories because of the special licenses and facilities needed to obtain and safely handle 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.

In FY 2005, major activities will 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.

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.

▪ **Geosciences Research**	**20,322**	**20,491**	**20,332**

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

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

approaches to understand physical properties of fluids, rocks, and minerals. It seeks fundamental understanding of the physics of wave propagation in complex media ranging from single crystals to the scale of the earth's crust. This activity has pioneered the application of x-ray and neutron scattering to geochemical and geophysical studies.

These studies provide the fundamental science base for new capabilities to locate and monitor oil and gas reservoirs, contaminant migration, and for characterizing disposal sites for energy related wastes. This activity provides the majority of individual investigator basic research funding for the federal government in areas with the greatest impact on unique DOE missions such as high-resolution Earth imaging and 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.

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.

▪ **Chemical Energy and Chemical Engineering**....	**9,779**	**10,637**	**10,687**

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

Knowledge of bulk behavior of chemicals and mixtures based on molecular properties is required for the design of energy efficient chemical processes in all aspects of plant design across the entire spectrum of industrial activities. The thermophysical and thermochemical properties of molecules provide the basis for developing equations of states and parameters for fluid models that are necessary for the development of engineering designs that maximize the efficiency of all energy production, storage, and consumption devices. These engineering designs are also an essential component of safety and risk assessment and environmental protection.

In the area of energy storage, coordination of fundamental and applied research efforts across the government is accomplished by participation in the Interagency Power Working Group. Close coordination with the Battery and Fuel Cell programs in Energy Efficiency and Renewable Energy's Transportation Technologies program is accomplished through joint program meetings, workshops, and strategy sessions.

In FY 2005, major activities will include research to expand the ability to control electrode structures on the nanometer scale. Preliminary studies have shown that this has a great impact on the electrochemical efficiency of electrode processes and the rate at which they respond to electrochemical potentials. An additional $975,000 is provided for research to understand: the nature of proton transport in high temperature polymer electrolyte membranes; the interaction of complex aqueous, gaseous, and solid interfaces in gas diffusion electrode assemblies; and the origin of the

	FY 2003	FY 2004	FY 2005

(dollars in thousands)

performance-robbing over potential for fuel cell cathodes for hydrogen use. Research in aspects of electrochemical energy storage is reduced by $925,000.

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

	FY 2003	FY 2004	FY 2005
▪ **General Plant Projects (GPP)**..............................	**11,614**	**11,700**	**13,150**

GPP funding is increased in FY 2005 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 Basic Energy Sciences 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 2003	FY 2004	FY 2005
▪ **General Purpose Equipment (GPE)**	**4,382**	**4,483**	**4,058**

GPE funding is provided for Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the Basic Energy Sciences stewardship responsibilities for these laboratories for general purpose equipment that supports multipurpose research. Increased 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 2003	FY 2004	FY 2005
▪ **SPEAR3 Upgrade**	**700**	**0**	**0**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) was undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The upgrade increased injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decreased beam emittance by a factor of 7 to increase beam brightness; increased operating current from 100 mA to 200 mA to increase beam intensity; and maintained long beam life time (>25 hr). The increased photon flux will greatly improve performance in a variety of applications including powder and thin film diffraction, topographic studies, surface microcontamination studies, x-ray tomographic analysis, x-ray absorption studies, and protein crystallography. The magnets and associated vacuum chambers of the existing SPEAR storage ring were replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC was $29,000,000; DOE and NIH equally funded the upgrade with a total Federal cost of $58,000,000. NIH provided $14,000,000 in FY 1999, $14,000,000 in FY 2000, and $1,000,000 in FY 2001. This MIE project was completed on schedule and within budget. The SPEAR3 is now being commissioned.

	FY 2003	FY 2004	FY 2005
Facility Operations...	**5,935**	**5,967**	**6,169**

The facility operations budget request, which includes operating funds, capital equipment, and general plant projects is described in a consolidated manner later in this budget. This subprogram funds the

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

Combustion Research Facility. 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.

Facilities

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
Combustion Research Facility	5,935	5,967	6,169

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
SBIR/STTR	**0**	**5,394**	**5,510**

In FY 2003, $4,687,000 and $281,000 were transferred to the SBIR and STTR programs, respectively. The FY 2004 and FY 2005 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**211,898**	**219,582**	**228,422**

Explanation of Funding Changes

	FY 2005 vs. FY 2004 ($000)
Chemical Sciences, Geosciences, and Energy Biosciences Research	
▪ Overall increase for chemical physics research because of increase for research related to the hydrogen economy ($+1,950,000) and decrease because of decreased emphasis on gas phase chemistry ($-667,000)	+1,283
▪ Increase for photochemistry and radiation research for research related to the hydrogen economy	+975
▪ Increase in molecular mechanisms of natural solar energy conversion for research related to the hydrogen economy.	+975
▪ Decrease in metabolic regulation of energy production research because of decreases in microbial research.	-500
▪ Increase in catalysis and chemical transformations for research related to the hydrogen economy	+1,949

	FY 2005 vs. FY 2004 ($000)
▪ Increase in separations and analyses for research related to the hydrogen economy..	+2,924
▪ Decrease in geosciences research because of decreased research in geophysics........	-159
▪ Overall increase for chemistry and chemical engineering because of increase for research related to the hydrogen economy ($+975,000) and decreases because of decreases in aspects of electrochemical energy storage ($-925,000)..........................	+50
▪ Increase in general plant projects intended to help alleviate recurring maintenance costs by improving infrastructure..	+1,450
▪ Decrease in general purpose equipment because of one time need in FY 2004	-425
Total, Chemical Sciences, Geosciences, and Energy Biosciences Research	+8,522
Facilities Operations	
Increase for operations of the Combustion Research Facility.	+202
SBIR/STTR	
Increase in SBIR/STTR funding because of an increase in operating expenses	+116
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences ..	+8,840

Construction

Funding Schedule by Activity

(dollars in thousands)

	FY 2003	FY 2004	FY 2005	$ Change	% Change
Construction					
SNS	210,571	123,865	80,535	-43,330	-35.0%
Project Engineering Design, NSRCs	11,850	2,982	2,012	-970	-32.5%
Project Engineering Design, LCLS	5,925	7,456	20,075	+12,619	+169.2%
Linac Coherent Light Source (SLAC)	0	0	30,000	+30,000	--
Center for Functional Nanomaterials (BNL)	0	0	18,465	+18,465	--
The Molecular Foundry (LBNL)	0	34,794	32,085	-2,709	-7.8%
Center for Nanophase Materials Science (ORNL)	23,701	19,882	17,811	-2,071	-10.4%
Center for Integrated Nanotechnologies (SNL/LANL)	4,444	29,674	30,897	+1,223	+4.1%
Total, Construction	256,491	218,653	231,880	+13,227	+6.0%

Description

Construction is needed to support the research in each of the subprograms in the Basic Energy Sciences 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 2003	FY 2004	FY 2005
Construction	**256,491**	**218,653**	**231,880**
▪ **Spallation Neutron Source (SNS)**	**210,571**	**123,865**	**80,535**

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 takes 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. 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 $5,635,000 in FY 2003, $7,387,000 in FY 2004, and $7,643,000 in FY 2005. 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 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

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

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, and installation activities, and to begin system commissioning. The ion source will be commissioned, and the drift tube linac will be installed and commissioning begun. Installation of other linac components will proceed, and installation of ring components will begin. Target building construction and equipment installation will continue in concert with each other. Numerous conventional facilities, including the klystron, central utilities, and ring service buildings as well as the linac and ring tunnels, will be completed. All site utilities will be available to support linac commissioning activities.

FY 2004 budget authority will continue instrument R&D, design, and procurement. The drift-tube linac and cavity-coupled linac portions of the warm linac commissioning will be completed. Other commissioning activities will continue in the linac. Cryogenic refrigerator installation and system cool down will be completed and cryogenic transfer line installation and testing will be completed. Cryogenic module fabrication and installation will continue. High-energy beam transport installation and testing will be completed. Ring fabrication and assembly activities will continue. Target fabrication and assembly activities will continue. Most SNS buildings will be 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 is requested to continue R&D, procurement, and installation of equipment for instrument systems. The extraction dump, high-energy beam transport, and accumulator ring will be commissioned; installation and testing for the ring-target beam transport system will be performed. Preparation for the ring-target beam transport system accelerator readiness review will begin. Installation and testing will be completed and preparation for the accelerator readiness review will start for target systems. Conventional facilities construction will be completed. Procurement, installation, and testing will continue for integrated control systems.

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.

▪ **Project Engineering and Design, Nanoscale Science Research Centers**	**11,850**	**2,982**	**2,012**

Funds appropriated in FY 2002, FY 2003 and FY 2004 will 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. Additional information follows later in PED data sheet 02-SC-002.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
▪ **Project Engineering and Design, Linac Coherent Light Source**	**5,925**	**7,456**	**20,075**

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

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

The proposed LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons; the light is coherent or "laser like" enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length to subfemtosecond levels) enabling studies of fast chemical and physical processes. The LCLS has considerable potential as a tool for groundbreaking research in the physical and life sciences. LCLS x-rays can be used to create and observe extreme conditions in matter, such as exotic excited states of atoms and warm dense plasmas, previously inaccessible to study. They can be used to directly observe changes in molecular and material structure on the natural time scales of atomic and molecular motions. LCLS x-rays offer an opportunity to image non-periodic molecular structures, such as single or small clusters of biomolecules or nanosctructured materials, at atomic or near-atomic resolution. These are only a few examples of breakthrough science that will be enabled by LCLS, planned to be the world's first "fourth generation" x-ray light source.

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

The proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

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. The preliminary Total Estimated Cost (TEC) is in the range of $220,000,000 to $260,000,000. FY 2005 Project Engineering Design (PED) funding of $20,075,000 and $4,000,000 of research and development budgeted in the Materials Sciences and Engineering subprogram are 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 2003	FY 2004	FY 2005
▪ **Linac Coherent Light Source**	**0**	**0**	**30,000**

In FY 2005, $30,000,000 is requested for the LCLS to initiate long-lead procurements. Early acquisition of selected critical path items will support 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. Early acquisition of the injector is required in order that first tests of the free-electron laser 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 2008.

	FY 2003	FY 2004	FY 2005
▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, Brookhaven National Laboratory**	**0**	**0**	**18,465**

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

FY 2005 funding is requested for the start of 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 2003	FY 2004	FY 2005
▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL**	**0**	**34,794**	**32,085**

The **Molecular Foundry**, a planned 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, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include clean rooms; controlled environmental rooms; scanning tunneling microscopes; atomic

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005

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 is appropriated for the start of construction of the Molecular Foundry at Lawrence Berkeley National Laboratory. FY 2005 funding is requested to continue construction and equipment procurement. 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 2003	FY 2004	FY 2005
▪ **Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL**	**23,701**	**19,882**	**17,811**

The **Center for Nanophase Materials Sciences (CNMS)**, a proposed 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, collaborated with 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 2003 and FY 2004 funding was appropriated for the start of construction of the Center for Nanophase Materials Science to be located at Oak Ridge National Laboratory. FY 2005 funding is requested to continue 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-312.

	FY 2003	FY 2004	FY 2005
▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, Sandia National Laboratories/Los Alamos National Laboratory**	**4,444**	**29,674**	**30,897**

The **Center for Integrated Nanotechnologies (CINT)**, a planned 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 Laboratory. 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.

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
FY 2003 and FY 2004 funding was appropriated for the construction for the Center for Integrated Nanotechnologies managed jointly by Sandia National Laboratories and Los Alamos National Laboratory. FY 2005 funding is requested to continue 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	**256,491**	**218,653**	**231,880**

Explanation of Funding Changes

	FY 2005 vs. FY 2004 ($000)
Construction	
▪ Decrease in funding for construction of the Spallation Neutron Source at ORNL, representing the scheduled ramp down of activities.	-43,330
▪ 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.	-970
▪ Increase in funding for Project Engineering Design (PED) related to design-only activities for the Linac Coherent Light Source (LCLS) at SLAC, representing the scheduled increase in activities.	+12,619
▪ Increase in funding to initiate long-lead procurements for the LCLS project.	+30,000
▪ Increase in funding for construction of the Center for Functional Nanomaterials at BNL, representing the start of construction.	+18,465
▪ Decrease in funding for construction of the Molecular Foundry at LBNL, representing the scheduled ramp down of activities.	-2,709
▪ Decrease in funding for construction of the Center for Nanophase Materials Sciences at ORNL, representing the scheduled ramp down of activities.	-2,071
▪ Increase in funding for construction of the Center for Integrated Nanotechnologies at SNL/LANL, representing the continuation of activities.	+1,223
Total Funding Change, Construction	+13,227

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 2003	FY 2004	FY 2005	$ Change	% Change
Major User Facilities					
Advanced Light Source	42,844	43,205	42,200	-1,005	-2.3%
Advanced Photon Source	90,894	93,410	97,400	+3,990	+4.3%
National Synchrotron Light Source	36,950	38,325	38,400	+75	+0.2%
Stanford Synchrotron Radiation Laboratory	25,903	30,305	28,100	-2,205	-7.3%
High Flux Isotope Reactor	36,838	37,805	39,832	+2,027	+5.4%
Radiochemical Engineering Development Center	6,515	6,305	6,300	-5	-0.1%
Intense Pulsed Neutron Source	16,714	16,655	17,222	+567	+3.4%
Manuel Lujan, Jr. Neutron Scattering Center	9,914	10,110	10,300	+190	+1.9%
Spallation Neutron Source	14,441	18,397	33,100	+14,703	+79.9%
Combustion Research Facility	5,935	5,967	6,169	+202	+3.4%
Total, Major User Facilities	286,948	300,484	319,023	+18,539	+6.2%

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.

Detailed Justification

	(dollars in thousands)		
	FY 2003	FY 2004	FY 2005
Major User Facilities	**286,948**	**300,484**	**319,023**
▪ Advanced Light Source at Lawrence Berkeley National Laboratory	42,844	43,205	42,200
▪ Advanced Photon Source at Argonne National Laboratory	90,894	93,410	97,400
▪ National Synchrotron Light Source at Brookhaven National Laboratory.	36,950	38,325	38,400
▪ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.	25,903	30,305	28,100
▪ High Flux Isotope Reactor at Oak Ridge National Laboratory	36,838	37,805	39,832
▪ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	6,515	6,305	6,300
▪ Intense Pulsed Neutron Source at Argonne National Laboratory	16,714	16,655	17,222
▪ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	9,914	10,110	10,300
▪ Spallation Neutron Source at Oak Ridge National Laboratory	14,441	18,397	33,100
▪ Combustion Research Facility at Sandia National Laboratories/California.	5,935	5,967	6,169
Total, Major User Facilities	286,948	300,484	319,023

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

	(dollars in thousands)				
	FY 2003	FY 2004	FY 2005	$ Change	% Change
General Plant Projects	12,461	12,108	13,572	+1,464	+12.1%
Accelerator Improvement Projects	8,957	9,900	9,759	-141	-1.4%
Capital Equipment	82,846	80,681	81,838	+1,157	+1.4%
Total, Capital Operating Expenses	104,264	102,689	105,169	+2,480	+2.4%

Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2003	FY 2004	FY 2005	Unapprop-riated Balances
99-E-334, ORNL, Spallation Neutron Source	1,192,700	736,629	210,571	123,865	80,535	41,100
02-SC-002 PED, Nanoscale Science Research Centers	19,844 [a]	3,000	11,850	2,982	2,012	0
03-SC-002, PED, SLAC, Linac Coherent Light Source	36,000 [b]	0	5,925	7,456	20,075	2,544
03-R-312, ORNL, Center for Nanophase Material Sciences	63,882 [c]	0	23,701	19,882	17,811	0
03-R-313, SNL, Center for Integrated Nanotechnologies	73,800[d]	0	4,444	29,674	30,897	4,626
04-R-313, LBNL, The Molecular Foundry	83,700[e]	0	0	34,794	32,085	9,606
05-R-320, SLAC, Linac Coherent Light Source	260,000[b]	0	0	0	30,000	194,000
05-R-321, BNL, Center for Functional Nanomaterials	79,700[f]	0	0	0	18,465	55,253
Total, Construction		739,629	256,491	218,653	231,880	343,129

[a] The full Total Estimated Cost (design and construction) ranges between $266,500,000 and $286,500,000. This estimate is based on conceptual data and should not be construed as a project baseline.

[b] The full TEC Projection (design and construction) ranges between $220,000,000 and $260,000,000. This estimate is based on conceptual design and should not be construed as a project baseline.

[c] Includes $2,488,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

[d] Includes $4,159,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

[e] Includes $7,215,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

[f] Includes $5,982,000 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 Estimated Cost (TEC)	Prior Year Approp-riations	FY 2003	FY 2004	FY 2005	Accept-ance Date
SPEAR3 Upgrade	29,000[a]	19,000	10,000	0	0	FY 2004
ANL Center for Nanophase Materials	36,000	0	0	10,000	12,000	FY 2006
SNS Instrumentation[b]	50,000-75,000	0	5,635	7,387	7,643	FY 2007-FY 2011 est.
Total, Major Items of Equipment		19,000	15,635	17,387	19,643	

[a] DOE portion only; total estimated Federal cost, including NIH funding (beginning in FY 1999), is $58,000,000.

[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.

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

(Changes from FY 2004 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 Budget Request (*Amended*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2002 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2003 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2004 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2005 Budget Request (*Current Estimate*)	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]	207,139
2005	80,535[b]	80,535[b]	96,081
2006	41,100	41,100	46,398

[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 establlsh 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; and
9. Engineering Diffractometer – the Canada Foundation for Innovation.

The final 10 SNS instruments will be selected under this process and identified when they are approved and funded.

[b] Construction funding was reduced by $735,140 as a result of the FY 2004 rescission. The reduction is restored in FY 2005 to maintain the TEC and project scope.

3. Project Description, Justification and Scope [a]

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 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

[a] 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) will be located 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 will be adjacent to the SNS Laboratory – Office Building and will be connected to it by a walkway. See construction project datasheet 03-R-312 for further information on the CNMS.

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 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 has reduced the number of instruments provided within the project TEC. Although this translates 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; the other two will be completed, with installation occurring during initial low power operations. 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 2003 were used to continue R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The ion source was commissioned, and the drift tube linac installation and commissioning were begun. Installation of other linac components proceeded and installation of ring components began. Target building construction and equipment installation continued in concert with each other. Numerous conventional facilities, including the klystron, central utilities, and ring service buildings as well as the linac and ring tunnels, were completed. All site utilities were made available to support linac commissioning activities.

FY 2004 budget authority will continue instrument R&D, design, and procurement. The drift tube linac and coupled cavity linac subsystems will be installed and commissioned. Other commissioning activities will continue in the linac. Cryogenic refrigerator installation and system cool down will be completed, and cryogenic transfer line installation and testing will be completed. Cryogenic module fabrication and installation will continue. The high-energy beam transport installation and testing will be completed. Ring fabrication and assembly activities will continue. Target fabrication and assembly activities will continue. Most buildings will be completed with the exception of ongoing construction work in the target building and the central laboratory and office building.

FY 2005 budget authority is requested to continue R&D, procurement, and installation of equipment for instrument systems. The extraction dump, high-energy beam transport, and accumulator ring will be commissioned; installation and testing for the ring-target beam transport system will be performed. Preparation for the ring-target beam transport system accelerator readiness review will begin. Installation and testing will be completed and preparation for the accelerator readiness review will start for target systems. Conventional facilities construction will be completed. Procurement, installation, and testing will continue for integrated control systems.

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	159,500
Construction management at approximately 2% of construction costs	15,900	14,000
Project management at approximately 13% of construction costs	104,700	104,700
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	31,500	31,500
Buildings	239,800	196,300
Utilities (electrical, water, steam, and sewer lines)	20,900	20,900
Technical Components	520,600	507,200
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	1,147,900	1,088,100
Contingencies at approximately 4% of above costs [b]	44,800	104,600
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 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 procurement, testing and

[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%.

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 2003	FY 2004	FY 2005	Outyears	Total
Project Cost						
Facility Cost [a]						
Line Item TEC....................................	566,195	276,887	207,139	96,081	46,398	1,192,700
Other project costs						
R&D necessary to complete project [b]	78,784	3,062	1,442	799	359	84,446
Conceptual design cost [c]...................	14,397	0	0	0	0	14,397
NEPA Documentation costs [d].............	1,958	-30	0	0	0	1,928
Other project-related costs [e]..............	20,696	11,505	18,493	32,158	34,274	117,126
Capital equipment not related construction [f]	846	65	107	85	0	1,103
Total, Other project costs...........................	116,681	14,602	20,042	33,042	34,633	219,000
Total project cost (TPC).............................	682,876	291,489	227,181	129,123	81,031	1,411,700

[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 $84,446,000 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 $117,126,000 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.

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	40,000
Capital equipment not related to construction but related to the programmatic effort in the facility	14,100	11,800
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	150,000

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. By the time SNS is fully instrumented and the facility is upgraded to reach its full scientific potential, the annual funding requirements will increase by an additional 10-15 percent.

02-SC-002, Project Engineering Design (PED), Various Locations

(Changes from the FY 2004 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 2002 Budget Request *(Preliminary Estimate)*	2Q 2002	3Q 2004	N/A	N/A	14,000
FY 2003 Budget Request	2Q 2002	3Q 2003	N/A	N/A	15,000
FY 2004 Budget Request	2Q 2002	3Q 2003	N/A	N/A	20,000
FY 2005 Budget Request *(Current Estimate)*	2Q 2002	4Q 2004	N/A	N/A	19,844

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	3,000	3,000	1,547
2003	11,850	11,850	10,436
2004	2,982	2,982	4,905
2005	2,012	2,012	2,956

3. Project Description, Justification and Scope

This PED request provides for Title I and Title II Architect-Engineering (A-E) services for projects related to the establishment of user centers for nanoscale science, engineering, and technology research. These funds allow designated projects 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 and 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 procured in the fiscal year in which Title III construction activities are funded.

[a] . . . Based on the results of peer review, the total design cost is $19,844,769, reduced from the FY 2004 President's Request of $20,000,000 due to the general reduction and rescission in FY 2003 and the rescission in FY 2004. The full Total Estimated Cost for each of the four currently proposed NSRC construction projects is identified in the FY 2005 construction datasheets.

Updated PED design projects are described below. Some changes may occur due to continuing conceptual design studies or developments prior to enactment of an appropriation. These changes will be reflected in subsequent years.

Nanoscale Science Research Centers (NSRCs)

To support research in nanoscale science, engineering, and technology, the U.S. has constructed outstanding facilities for *characterization and analysis* of materials at the nanoscale. Most of these world-class facilities are owned and operated by BES. They include, for example, the synchrotron radiation light source facilities, the neutron scattering facilities, and the electron beam microscope centers. However, world-class facilities that are widely available to the scientific research community for nanoscale *synthesis, processing, and fabrication* do not exist. NSRCs are intended to fill that need. NSRCs will serve the Nation's researchers and complement university and industrial capabilities in the tradition of the BES user facilities and collaborative research centers. Through the establishment of NSRCs affiliated with existing major user facilities, BES will provide state-of-the-art equipment for materials synthesis, processing, and fabrication at the nanoscale in the same location as facilities for characterization and analysis. NSRCs will build on the existing research and facility strengths of the host institutions in materials science and chemistry research and in x-ray and neutron scattering. This powerful combination of colocated fabrication and characterization tools will provide an invaluable resource for the Nation's researchers.

In summary, the purposes of NSRCs are to:

- provide state-of-the-art nanofabrication and characterization equipment to in-house and visiting researchers,
- advance the fundamental understanding and control of materials at the nanoscale,
- provide an environment to support research of a scope, complexity, and disciplinary breadth not possible under traditional individual investigator or small group efforts,
- provide a formal mechanism for both short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers,
- provide training for graduate students and postdoctoral associates in interdisciplinary nanoscale science, engineering, and technology research,
- provide the foundation for the development of nanotechnologies important to the Department.

Centers have been proposed by: Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL), Oak Ridge National Laboratory (ORNL), and a consortium of Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL). Based on peer review of the Center proposals, PED funding has been provided for BNL, LBNL, ORNL, and LANL/SNL. Funding for the ANL Center is included as a Major Item of Equipment beginning in FY 2004. Construction funding is also requested for BNL, LBNL, ORNL, and LANL/SNL in FY 2005.

FY 2002 Proposed Design Projects

02-01: Center for Nanoscale Materials – Argonne National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
N/A	N/A	N/A	N/A	0 [a]	0 [a]

Fiscal Year	Appropriations	Obligations	Costs
2002	0 [a]	0[a]	0[a]
2003	0 [a]	0[a]	0[a]

The Center for Nanoscale Materials (CNM) at ANL will consist of conventional facilities, fabrication facilities, characterization instruments, computational capabilities, and a beamline at the Advanced Photon Source (APS). The CNM will be attached to the APS at a location not occupied by one of the standard Laboratory-Office Modules that serve the majority of the APS sectors. The CNM is being coordinated with a State of Illinois effort. The State of Illinois is providing design and construction funding in FY 2002-2004 for the building. For this reason, PED funding is not planned or requested for this effort.

02-02: The Molecular Foundry – Lawrence Berkeley National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
3Q 2002	1Q 2004	2Q 2004	1Q 2007	7,215 [b]	83,700

Fiscal Year	Appropriations	Obligations	Costs
2002	500 [b]	500 [b]	38
2003	6,715 [b]	6,715 [b]	5,263
2004	0	0	1,258
2005	0	0	656

[a] The FY 2002 Request included funding of $1,000,000 in FY 2002 and FY 2003 for this project. Based on results of peer review, funding was not planned for FY 2002 or in the FY 2003 Request. The building portion of the project is being funded by the State of Illinois while DOE plans to fund capital equipment for the Center as one or more MIEs. The CNM is funded at $10,000,000 in FY 2004 President's Request with a MIE TEC of $36,000,000. Funding for the CNM MIE is continued in the FY 2005 Request at $12,000,000.

[b] The FY 2004 Request identified $500,000 for FY 2002 and $6,800,000 for FY 2003. The FY 2003 funding was reduced by $84,531 as a result of the general reduction and rescission. The project received construction funds in FY 2004.

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 special equipment to support nanoscale scientific research. The research building will be an advanced facility 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 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. New and existing beamlines at the ALS, not part of this PED activity, will support efforts at the Molecular Foundry. Construction funding for this project was initiated in FY 2004.

02-03: Center for Functional Nanomaterials – Brookhaven National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
4Q 2003	4Q 2004	3Q 2005	2Q 2008	5,982[a]	79,700

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	0 [a]	0 [a]	0
2003	988 [a]	988 [a]	733
2004	2,982 [a]	2,982 [a]	2,949
2005	2,012 [a]	2,012 [a]	2,300

The Center for Functional Nanomaterials will be housed in a laboratory/office building of approximately 85,000 square feet that includes class 10 clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. There will be an initial set of equipment necessary to explore, manipulate, and fabricate nanoscale materials and structures. Also included are individual offices, seminar area, transient user space for visiting collaborators with access to computer terminals, conference areas, vending/lounge areas, and other support spaces. Equipment procurement for the project will include equipment needed for laboratory and fabrication facilities for e-beam lithography, transmission electron microscopy, scanning probes and surface characterization, material synthesis and fabrication, and spectroscopy. The building will incorporate human factors into its design to encourage peer interactions and collaborative interchange by BNL staff and research teams from collaborating institutions. In addition to flexible office and laboratory space it will provide

[a] The FY 2002 Request included $1,000,000 in FY 2002 and $2,000,000 in FY 2003 for this project. Based on results of peer review, funding was not planned for FY 2002 or in the FY 2003 Request. Based on the merits of a revised proposal, $988,000 of PED funding was provided in FY 2003, $2,982,000 was provided in FY 2004, and $2,012,000 is requested in FY 2005. PED funding was reduced by $12,000 as a result of the FY 2003 general reduction and rescission and by $17,700 as a result of the FY 2004 rescission.

"interaction areas" 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. Based on the results of the FY 2001 peer review of the Center for Functional Nanomaterials, PED funding was not planned for FY 2002. Based on the review of a revised proposal, PED funding was provided in FY 2003 and FY 2004 and is requested in FY 2005.

02-04: Center for Nanophase Materials Sciences – Oak Ridge National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	1Q 2003	3Q 2003	4Q 2006	2,488 [a]	64,000

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	1,500 [a]	1,500 [a]	1,342
2003	988 [a]	988 [a]	1,121
2004	0	0	25

A major focus of the Center for Nanophase Materials Sciences (CNMS) will be the application of neutron scattering for characterization of nanophase materials. In this area, CNMS will be a world leader. With the construction of the new Spallation Neutron Source (SNS) and the upgraded High Flux Isotope Reactor (HFIR), it is essential that the U.S.-based neutron science R&D community grow to the levels found elsewhere in the world and assume a scientific leadership role. Neutron scattering provides unique information about both atomic-scale structure and the dynamics of a wide variety of condensed matter systems including polymers, macromolecular systems, magnetic and superconducting materials, and chemically complex materials, particularly oxides and hydrogen-containing structures. Consequently, the intense neutron beams at HFIR and SNS will make, for the first time, broad classes of related nanoscale phenomena accessible to fundamental study.

The CNMS building (approximately 80,000 gross square feet) will contain wet and dry materials synthesis and characterization laboratories; clean rooms and materials imaging, manipulation, and integration facilities in a nanofabrication research laboratory; computer-access laboratories for nanomaterials theory and modeling; and office space for staff and visitors. The CNMS facility will consist of a multi-story building for materials synthesis and characterization contiguous with a single-story structure for nanofabrication having Class 100, Class 1,000, and Class 10,000 clean areas. The latter portion of the facility will be built using a construction approach that will meet low electromagnetic field, vibration, and acoustic noise requirements for special nanofabrication and characterization equipment. Construction funding for this project was initiated in FY 2003.

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[a] Funding of $1,000,000 in FY 2003 and $2,000,000 in FY 2004 was identified in the FY 2003 Request for this project. Based on the results of peer review, this project was funded at $1,500,000 in FY 2002 and $988,000 in FY 2003. PED funding was reduced $12,000 as a result of the FY 2003 general reduction and rescission.

02-06: The Center for Integrated Nanotechnologies (CINT) – Sandia National Laboratories/Los Alamos National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
4Q 2002	2Q 2004	1Q 2004	3Q 2007	4,159 [a]	73,800

Fiscal Year	Appropriations	Obligations	Costs
2002	1,000 [a]	1,000 [a]	167
2003	3,159 [a]	3,159 [a]	3,319
2004	0	0	673

The Center for Integrated Nanotechnologies (CINT), jointly managed by the Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL), has as its primary objective the development of the scientific principles that govern the performance and integration of nanoscale materials, thereby building the foundations for future nanotechnologies. CINT will consist of a core research facility of approximately 95,000 square feet to be located in an unrestricted area just outside the restricted area at SNL and two smaller "gateway" facilities located on the campuses of SNL and LANL. These gateways will provide office space and, in the case of the LANL gateway limited amounts of laboratory space, for researchers who need access to specialized facilities located on these campuses. The SNL gateway will use existing space in SNL's Integrated Materials Research Laboratory; the LANL gateway will require construction of a small building of approximately 34,000 square feet. The CINT gateway to SNL will focus on specialized microfabrication and nanomaterials capabilities and expertise. The CINT gateway to LANL will focus on connecting CINT researchers to the extensive biosciences and nanomaterials capabilities at LANL. The core research facility and the gateways will be managed as one integrated facility by a single management structure led by SNL. The CINT will focus on nanophotonics, nanoelectronics, nanomechnics, and functional nanomaterials. The 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, and the Microelectronics Development Laboratory and the Compound Semiconductor Research Laboratory at SNL. Construction funding for this project was initiated in FY 2003.

The CINT core facility in Albuquerque will provide an open environment readily accessible by students and visitors, including foreign nationals. This structure will house state-of-the-art clean rooms and an initial set of 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 complex will require class 1,000 clean room space for nanofabrication and characterization equipment and an additional class 100 clean room space for lithography activities. This facility will also

[a] The FY 2002 Request included a total of $1,000,000 in FY 2002 and $2,000,000 in FY 2003 for the LANL and SNL components of this combined project. Based on results of peer review, current PED funding plan for the combined project is $1,000,000 for FY 2002 and $3,159,000 in FY 2003. PED funding of $41,000 and construction funding of $56,074 were reduced as a result of the FY 2003 general reduction and rescission.

require general purpose chemistry/biology laboratories and electronic and physical measurement laboratories. To house the Center staff, collaborators, Center-sponsored post docs, visiting students and faculty, and industry collaborators, offices and meeting rooms will be provided.

4. Details of Cost Estimate [a]

(dollars in thousands)	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	14,844	15,000
Design Management costs (15.1% of TEC)	3,000	3,000
Project Management costs (10.1% of TEC)	2,000	2,000
Total Design Costs (100% of TEC)	19,844	20,000
Total, Line Item Costs (TEC)	19,844	20,000

5. Method of Performance

Design services are obtained through competitively awarded fixed price contracts. M&O contractor staff may be utilized in areas involving security, production, proliferation, etc. concerns.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2003	FY 2004	FY 2005	Total
Facility Cost					
PED	1,547	10,436	4,905	2,956	19,844
Other project costs					
Conceptual design cost[b]	1,490	0	0	0	1,490
Total, Project Costs	3,037	10,436	4,905	2,956	21,334

[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 when available. The cost estimate includes design phase activities only. Construction activities will be requested as individual line items on completion of Title I design.

[b] Only Conceptual Design Costs associated with the NSRCs are included. Other project costs are identified for individual NSRCs on the individual construction project data sheets for Project 03-R-312, Center for Nanophase Materials Sciences; Project 04-R-313, Molecular Foundry; Project 03-R-313, Center for Integrated Nanotechnologies; and 05-R-321, Center for Functional Nanomaterials.

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

(Changes from the FY 2004 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 Project 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 *(Current Estimate)*......	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	3,644
2004	7,456 [b]	7,456	9,000
2005	20,075 [b]	20,075	17,756
2006	2,544 [b]	2,544	5,600

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 procured in the fiscal year in which Title III construction activities are funded.

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[a] The full TEC Projection (design and construction) ranges between $220,000,000 and $260,000,000. This is a preliminary estimate; the baseline TEC will be established at Critical Decision 2 (Approve Performance Baseline).

[b] PED funding was reduced as a result of the FY 2003 general reduction and rescission by $74,765 and as a result of the FY 2004 rescission by $44,250. This total reduction is restored in FY 2005 and FY 2006 to maintain the TEC and project scope.

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. 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 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 proposed 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 experimental buildings, the Near Hall and the Far 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)	26,000	26,000
Design Management costs (13.9% of TEC)	5,000	5,000
Project Management costs (13.9% of TEC)	5,000	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 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 the risk of the project and accelerate 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).

[a] This cost estimate includes design phase activities only. Construction funding is requested as an individual line item on completion of Title I design.

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) will be contracted to an experienced Architect/Engineering (A/E) firm to perform Title I and II design in FY 2004. The A/E contract will be awarded under full and open competition to pre-qualified offerors using fixed-priced contracts.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2003	FY 2004	FY 2005	Outyears	Total
Facility Cost						
PED	0	3,644	9,000	17,756	5,600	36,000
Other project costs						
Conceptual design cost	1,470	0	0	0	0	1,470
Research and development costs	0	0	2,000	4,000	0	6,000
NEPA documentation costs	30	0	0	0	0	30
Total, Other Project Costs	1,500	0	2,000	4,000	0	7,500
Total Project Cost (TPC)	1,500	3,644	11,000	21,756	5,600	43,500

03-R-312, Center For Nanophase Materials Sciences
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Changes from FY 2004 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 2003 Budget Request *(Preliminary Estimate)*...........................	2Q2002	1Q2003	3Q2003	4Q2006	64,000	65,000
FY 2004 Budget Request.......................	2Q2002	1Q2003	3Q2003	4Q2006	64,000	65,000
FY 2005 Budget Request *(Current Estimate)*................................	2Q2002	1Q2003	3Q2003	4Q2006	63,882[a]	64,882[a]

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering & Design (PED)			
2002	1,500	1,500	1,342
2003	988[b]	988[b]	1,121
2004	0	0	25
Construction			
2003	23,701[b]	23,701[b]	1,160
2004	19,882[b]	19,882 [b]	18,267
2005	17,811	17,811	19,215
2006	0	0	22,752

[a] The TEC and TPC are reduced by $118,000 due to the FY 2004 Rescission.

[b] PED and construction funding were reduced by $12,000 and $299,062, respectively, as a result of the FY 2003 general reduction and rescission and by $118,000 as result of the FY 2004 rescission.

3. Project Description, Justification and Scope

This proposed Center for Nanophase Materials Sciences (CNMS) will establish a nanoscale science research center at Oak Ridge National Laboratory (ORNL) that will integrate nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation of nanophase materials. The total gross area of the new building will be approximately 80,000 square feet, providing state-of-the-art clean rooms, and general laboratories for sample preparation, fabrication and analysis. Included will be initial equipment for nanoscale materials research such as surface analysis equipment, nanofabrication facilities, etc. The facility, co-located with the Spallation Neutron Source complex, will house ORNL staff members and visiting scientists from academia and industry. There are no existing buildings at ORNL that could serve these needs.

The CNMS's major scientific thrusts will be in 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 to determine the structure of nanomaterials, to develop a detailed understanding of synthesis and self-assembly processes in "soft" materials, and to study and understand collective (cooperative) phenomena that emerge on the nanoscale. Neutron scattering provides unique information (complementary to that provided by other methods) about both the atomic-scale structure and the dynamics of a wide variety of condensed matter systems including polymers, macromolecular systems, magnetic and superconducting materials, and chemically complex materials, particularly oxides and hydrogen-containing structures. The intense neutron beams available at the upgraded High Flux Isotope Reactor and the new Spallation Neutron Source will make broad classes of related nanoscale phenomena accessible to fundamental study.

Since the late 1980s, there has been a recognized need to enhance U.S. capabilities in the synthesis of materials. These concerns are exacerbated by the challenges of controlled synthesis of nanophase materials. There is currently a critical, unmet national need for the synthesis of high quality nanophase research materials. It is also recognized that the existence of capabilities for science-driven synthesis of novel materials has played a central role in some of the most spectacular recent discoveries of new phenomena, including high-temperature superconductivity, the quantum and fractional quantum Hall effects, conducting polymers, and colossal magnetoresistance. Therefore, synthesis and characterization of nanophase materials (including copolymers and macromolecular systems, multilayered nanostructures, ceramics, composites, and alloys with nanoscale spatial charge and/or magnetic ordering) will be an essential component of the CNMS. With these capabilities the CNMS will become a national resource for nanophase materials for use by researchers across the nation.

The CNMS project scope includes preliminary and final design, as well as procurement of an initial set of experimental capital equipment and construction of facilities. PED funding was allocated in FY 2002 and FY 2003 to complete design of the CNMS. FY 2003 construction funding was used to initiate construction and equipment procurement. FY 2004 and FY 2005 funding will be used to continue funding the conventional construction and equipment procurement.

4. Details of Cost Estimate[a]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design Costs	2,067	1,700
Design Management Costs (0.6% of TEC)	366	200
Project Management Costs (0.1% of TEC)	55	100
Total, Design Costs	2,488	2,000
Construction Phase		
Improvements to Land	125	500
Buildings	27,269	19,700
Special Equipment[b]	21,149	26,000
Utilities	500	500
Inspection, design and project liaison, testing, checkout and Acceptance	1,638	1,800
Construction Management (2.8% of TEC)	1,800	900
Project Management (1.7% of TEC)	1,100	800
Total, Construction Costs	53,581	50,200
Contingencies		
Design Phase (0% of TEC)	0	500
Construction Phase (12.2% of TEC)	7,813	11,300
Total, Contingencies (12.2% of TEC)	7,813	11,800
Total, Line Item Costs (TEC)	63,882	64,000

5. Method of Performance

Design will be performed by an architect-engineer utilizing a fixed price subcontract. Construction will be performed by a fixed-price construction contractor administered by the ORNL operating contractor. Procurement of research capital equipment will be performed by the ORNL operating contractor. Project and construction management, inspection, coordination, utility tie-ins, testing and checkout witnessing, and acceptance will be performed by the ORNL operating contractor.

[a] The annual escalation rates are: FY 2002 – 2.6%, FY 2003 – 2.8%, FY 2004 – 2.8%, FY 2005 – 2.9% and FY 2006 – 2.9% as directed by DOE.

[b] Initial research equipment, including testing and acceptance.

6. Schedule of Project Funding

	(dollars in thousands)					
	Prior Years	FY 2003	FY 2004	FY 2005	Outyears	Total
Project Cost						
Facility Cost						
Design	1,342	1,121	25	0	0	2,488
Construction	0	1,160	18,267	19,215	22,752	61,394
Total, Line item TEC	1,342	2,281	18,292	19,215	22,752	63,882
Other project costs						
Conceptual design costs	150	0	0	0	0	150
NEPA documentation Costs	5	0	0	0	0	5
Other project related Costs [a]	320	100	250	100	75	845
Total, Other Project Costs	475	100	250	100	75	1,000
Total, Project Cost (TPC)	1,817	2,381	18,542	19,315	22,827	64,882

7. Related Annual Funding Requirements

	(FY 2006 dollars in thousands)	
	Current Estimate	Previous Estimate
Annual facility operating costs	18,000	18,000
Total related annual funding	18,000	18,000

[a] 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 BES.

03-R-313, 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 2004 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

The revisions in the approximate square footages of both the Core Facility (95,000 GSF) and the Gateway to Los Alamos Facility (34,000 GSF) from those presented in the FY 2004 CINT Project Data Sheet are the result of the completion of Title I design.

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 *(Current Estimate)*	4Q 2002	2Q 2004	1Q 2004	3Q 2007	73,800	75,800

2. Financial Schedule [a]

(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	673
Construction			
2003	4,444 [c]	4,444 [c]	0
2004	29,674 [d]	29,674 [d]	11,747
2005	30,897 [c]	30,897	40,908
2006	4,626 [d]	4,626	15,667
2007	0	0	1,319

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. 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

[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 is restored in the FY 2005 request to maintain the TEC and project scope.

[c] Construction funding was reduced by $56,074 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission is restored in the FY 2005 request to maintain the TEC and project scope.

[d] Construction funding was reduced by $176,115 as a result of the FY 2004 rescission. This rescission is restored in FY 2006 to maintain the TEC and project scope.

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 making those resources available to the user community. In order to provide a strong central focus for the user community while also providing extraordinary leveraging 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 will be constructed on DOE property outside of the Kirtland Air Force Base.

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 the 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 the Los Alamos Facility will be located in the center of the Los Alamos materials science complex which is in the 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 construction funding was used to initiate construction and equipment procurement. Obligations for FY 2004 and FY 2005 will be used to continue funding the conventional construction and equipment procurement.

4. Details of Cost Estimate [a]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs	2,507	2,640
Design Management Costs (1.1% of TEC)	806	540
Project Management Costs (1.0% of TEC)	710	400
Total, Design Costs (5.5% of TEC)	4,023	3,580
Construction Phase		
Buildings	34,415	35,990
Improvements to Land[b]	1,430	0
Utilities[b]	1,777	0
Special Equipment[c]	16,645	15,760
Standard Equipment	2,178	1,540
Inspection, Design and Project Liaison, Testing, Checkout and Acceptance	3,151	2,900
Construction and Project Management (1.6% of TEC)	1,212	1,030
Total, Construction Costs	60,808	57,220
Contingencies		
Design Phase (0.2% of TEC)	136	620
Construction Phase (12.0% of TEC)	8,833	12,380
Total, Contingencies (12.2% of TEC)	8,969	13,000
Total, Line Item Costs (TEC)	73,800	73,800

[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] This cost was previously included in the cost estimate for the element "Buildings." The current cost estimate is based on a completed Title II design, vendor bids, and independent project review of site utilities conducted September 2003.

[c] Initial research equipment including testing and acceptance.

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. The outcome of this phase of the project was all necessary information to acquire CD-1 approval. Title I and II design for the Core Facility is being provided by contracted A-E support. The construction contractor shall be selected using a competitive best value process. The process will consider the contractors' qualifications and experience and the quoted price. The resultant contract will likely be fixed price (incentive) type.

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

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

6. Schedule of Project Funding

(dollars in thousands)

	Prior Years	FY 2003	FY 2004	FY 2005	Outyears	Total
Project Cost						
Facility Cost						
Design	167	3,319	673	0	0	4,159
Construction	0	0	11,747	40,908	16,986	69,641
Total, Line item TEC	167	3,319	12,420	40,908	16,986	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	0	150	500	550	1,471
Total, Other Project Costs	800	0	150	500	550	2,000
Total, Project Costs (TPC)	967	3,319	12,570	41,408	17,536	75,800

[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.

7. Related Annual Funding Requirements [a]

	(FY 2006 dollars in thousands)	
	Current Estimate	Previous Estimate
Annual facility operating costs	18,500	18,500
Total related annual funding	18,500	18,500

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

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

(Changes from the FY 2004 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 *(PreliminaryEstimate)*	3Q 2002	1Q 2004	2Q 2004	2Q 2006	83,700	85,000
FY 2005 Budget Request *(Current Estimate)*	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	1,258
2005	0	0	656
Construction			
2004	34,794 [b]	34,794 [b]	15,813
2005	32,085 [a]	32,085 [a]	43,263
2006	9,606 [b]	9,606 [b]	17,204
2007	0	0	205

[a] PED funding was reduced by $84,531 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission is restored in the FY 2005 request to maintain the TEC and project scope.

[b] Construction funding was reduced by $206,500 as a result of the FY 2004 rescission. This reduction is restored in FY 2006 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 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	4,877	4,300
Design Management costs (1.9% of TEC)	1,570	1,650
Total, Design Costs (7.7% of TEC)	6,447	5,950
Construction Phase		
Building & Improvements to land	47,450	43,300
Special Equipment[b]	15,000	15,300
Inspection, design and project liaison, check out	2,446	1,700
Construction Management & Project Management (2.5% of TEC)	2,106	2,150
Total, Construction Costs	67,002	62,450
Contingencies		
Design Phase (0.3% of TEC)	768	1,330
Construction Phase (12.0% of TEC)	9,483	13,970
Total, Contingencies (12.2% of TEC)	10,251	15,300
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 will provide technical oversight during Title III construction. A Construction Management (CM) contractor will perform 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 will bid out the design to subcontractors. The University will have the option to proceed with the CM contractor or bid the project to a separate subcontractor. Construction subcontract(s) will be awarded on a competitive basis using best value source selection criteria that will include price, safety, and other considerations.

[a] This cost estimate is based on Title I 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 2003	FY 2004	FY 2005	Outyears	Total
Facility Cost						
PED	38	5,263	1,258	656	0	7,215
Construction	0	0	15,813	43,263	17,409	76,485
Total, Line Item TEC	38	5,263	17,071	43,919	17,409	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]	150	12	0	0	368	530
Total, Other Project Costs	920	12	0	0	368	1,300
Total, Project Costs (TPC)	958	5,275	17,071	43,919	17,777	85,000

7. Related Annual Funding Requirements

	(FY 2006 dollars in thousands)	
	Current Estimate	Previous Estimate
Annual facility operating costs	18,000	18,000
Total related annual funding	18,000	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.

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

A Performance Baseline has been established for long-lead procurements in order to request funds to initiate these procurements in FY 2005. Thus, the funds requested for FY 2005 will ensure that selected critical path items can be procured in that year. The overall cost and schedule for the LCLS Project are only preliminary estimates. Plans call for a cost and schedule Performance Baseline to be developed during FY 2004 and approved by the Acquisition Executive at the completion of preliminary design (Critical Decision 2 – Approve Performance Baseline). The outyear funding projections (FY 2006-FY 2008) will support the completion of the LCLS at the Stanford Linear Accelerator Center and will be adjusted as necessary at Critical Decision 2 to support the Performance Baseline.

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 *(Current Estimate)*	2Q 2003	4Q 2006	1Q2006	4Q2008	260,000	315,000

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]	9,000
2005	20,075 [b]	20,075	17,756
2006	2,544 [b]	2,544	5,600
Construction			
2005	30,000 [c]	30,000	24,000
2006	83,000	83,000	76,000
2007	83,000	83,000	80,500
2008	28,000	28,000	43,500

[a] The TEC and TPC are currently projections based on ranges of $220,000,000 to $260,000,000 for the TEC and $265,000,000 to $315,000,000 for the TPC. The baseline TEC and TPC will be established at Critical Decision 2 (Approve Performance Baseline).

[b] PED funding was reduced by $74,765 as a result of the FY 2003 general reduction and rescission and by $44,250 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.

[c] FY 2005 funding is for long lead procurements. Project construction begins in FY 2006.

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), final design (Title II), and construction. 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 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. 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 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 230 femtoseconds or less. These characteristics of the LCLS will open new realms of scientific application in the chemical, material, and biological sciences.

The proposed 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 experimental buildings, the Near Hall and the Far Hall, will be constructed and connected by the beam line tunnel. A Central Laboratory

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 will be executed 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 in FY 2005 is for long-lead procurements. 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 free-electron laser (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 2008. The main linac magnets and radiofrequency systems must be ready for operation shortly after the linac has reached its performance goals.

4. Details of Cost Estimate [a]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	18,500	N/A
Design Management costs (2.0% of TEC)	5,000	N/A
Project Management costs (2.0% of TEC)	5,000	N/A
Total Design Costs	28,500	N/A
Construction Phase		
Improvements to Land	8,000	N/A
Buildings	36,300	N/A
Other Structures	1,800	N/A
Special Equipment	98,000	N/A
Inspection, design and project liaison, testing, checkout and acceptance	4,500	N/A
Construction Management (2.3% of TEC)	6,000	N/A
Project Management	11,700	N/A
Total, Construction Costs	166,300	N/A
Contingencies		
Design Phase (2.9% of TEC)	7,500	N/A
Long Lead Procurements (2.3% of TEC)	6,000	N/A
Construction Phase (20.0% of TEC)	51,700	N/A
Total, Contingencies (25.1% of TEC)	65,200	N/A
Total, Line Item Costs (TEC)	260,000	N/A

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 the risk of the project and accelerate 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) will be contracted to an experienced Architect/Engineering (A/E) firm

[a] Long-lead procurements are scheduled for FY 2005. The outyear (FY 2006-FY 2008) construction costs are estimates only. A baseline for outyear construction costs will be established when Critical Decision 2 for the LCLS Project is approved.

to perform Title I and II design in FY 2004. The A/E contract will be awarded under full and open competition to pre-qualified offerors using fixed-priced contracts.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2003	FY 2004	FY 2005	Outyears[a]	Totals
Facility Cost						
PED	0	3,644	9,000	17,756	5,600	36,000
Long-Lead Procurements	0	0	0	24,000	6,000	30,000
Construction	0	0	0	0	194,000	194,000
Total, Line Item TEC	0	3,644	9,000	41,756	205,600	260,000
Other project costs						
Research & Development	0	0	2,000	4,000	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	0	39,500	39,500
Spares	0	0	0	0	8,000	8,000
Total, Other Project Costs	1,500	0	2,000	4,000	47,500	55,000
Total Project Cost (TPC)	1,500	3,644	11,000	45,756	253,100	315,000

7. Related Annual Funding Requirements

(FY 2009 dollars in thousands)

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

FY 2009 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.

[a] The outyear (FY 2006-FY 2008) construction costs are estimates only. A baseline for outyear construction costs will be established when Critical Decision 2 for the LCLS Project is approved.

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

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 *(Current Estimate)*	4Q 2003	4Q 2004	3Q 2005	2Q 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]	2,949
2005	2,012	2,012	2,300
Construction			
2005	18,465 [a]	18,465	12,000
2006	36,553 [a]	36,553	30,000
2007	18,700	18,700	27,200
2008	0	0	4,518

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).

[a] PED funding was reduced by $12,000 as a result of the FY 2003 general reduction and rescission and by $17,700 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.

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 clusters established to provide the necessary primary user service. Cluster 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 85,000 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 laboratory equipment for the CFN laboratory clusters Nanopatterning, Ultrafast Optical Sources, Electron Microscopy, Materials Synthesis, Proximal Probes, and Theory and Computing as well as for the cluster designated CFN Endstations at the NSLS.

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”: 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[a]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications at $2,340K)	3,105	N/A
Project Management costs (2.3% of TEC)	1,820	N/A
Design Management Costs (0.5% of TEC)	415	N/A
Total, Design Costs (6.7% of TEC)	5,340	N/A
Construction Phase		
Technical Facilities		
Equipment	29,480	N/A
Inspection, design & project liaison, testing, checkout and acceptance	330	N/A
Project Management (0.2% of TEC)	135	N/A
Total, Technical Costs	29,945	N/A
Conventional Facilities		
Improvements to Land	945	N/A
Building Construction	23,465	N/A
Site Utilities	4,420	N/A
Standard Equipment	920	N/A
Removal less salvage	0	N/A
Inspection, design & project liaison, testing, checkout and acceptance	875	N/A
Project Management (2.2% of TEC)	1,725	N/A
Total, Construction Costs	32,350	N/A
Contingencies		
Design Phase (0.8% of TEC)	642	N/A
Construction Phase (14.3% of TEC)	11,423	N/A
Total Contingencies	12,065	N/A
Total, Line Item Costs (TEC)	79,700	N/A

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.

[a] The annual escalation rates assumed for FY 2004 through FY 2007 are 2.5 2.9, 2.8, and 2.6 percent, respectively, using DOE FY 2004 Guidance, January 2002 Update.

6. Schedule of Project Funding

	(dollars in thousands)					
	Prior Years	FY 2003	FY 2004	FY 2005	Outyears	Total
Project Cost						
Facility Cost						
Design	0	733	2,949	2,300	0	5,982
Construction	0	0	0	12,000	61,718	73,718
Total, Line Item TEC	0	733	2,949	14,300	61,718	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	0	1,300
Total, Project Costs	300	733	2,949	14,300	62,718	81,000
Total, Project Cost (TPC)	300	733	2,949	14,300	62,718	81,000

7. Related Annual Funding Requirements

	(FY 2008 dollars in thousands)	
	Current Estimate	Previous Estimate
Annual facility operating costs	18,500	N/A
Total annual operating funding	18,500	N/A

[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.