Basic Energy Sciences

Program 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. 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.

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 the research effort that was 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 and is uniquely responsible for supporting fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences impacting energy resources, production, conversion, efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2002, the program funded research in more than 166 academic institutions located in 48 states and in 13 Department of Energy (DOE) laboratories located in 9 states. BES supports a large extramural research program, with approximately 35% of the program's research activities sited at academic institutions.

The BES program also supports world-class scientific user facilities, providing outstanding capabilities for imaging and characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples. The BES synchrotron radiation light sources, the neutron scattering facilities, and the electron beam characterization centers represent the largest and best collection of such facilities supported by a single organization in the world. Annually, 8,000 researchers from universities, national laboratories, and industrial laboratories perform experiments at these facilities. Spurred by results of past investments and by innovations in accelerator concepts, the BES program continues its pioneering role in the development of new generations of scientific research instruments and facilities.

The *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, 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 atomic-level understanding touches all of the disciplines supported by BES. Scientific endeavors that once were considered “observational” – endeavors as diverse as plant sciences or metal and alloy sciences – now are understood at the atomic level. This understanding that explains phenomena in these diverse disciplines also inextricably links them, providing the foundation for the remarkable nanoscale science revolution that is now upon us.

This new atomic-level understanding that allows us to see how the machinery of life functions, atom-by-atom, comes from the great synchrotron x-ray and neutron scattering sources, the electron microscopes, and other atomic probes as well as the terascale computers. The BES program has played a major role in enabling the coming 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 the world of complex nanostructures. Here, simple structures interact to create new phenomena and assemble themselves into devices. Here also, large complicated structures can be designed atom by atom for desired characteristics. We will be able to build atomic scale structures that interact with biological or inorganic systems and alter their functions. We will design new tiny objects "from scratch" that have unprecedented optical, mechanical, electrical, or chemical properties that address needs of human society.

New tools, new understanding, and a developing convergence of the disciplines of physics, chemistry, materials science, biology, computation, and engineering will enable us to build on our 20th century successes and begin to ask and solve questions that were, until the 21st century, the stuff of science fiction.

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 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 or biomolecular materials; and on the fundamental research challenges posed by the Department's energy missions. BESAC also led the Office of Science workshop on performance measurement. 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) a specially empanelled subcommittee of BESAC. During the past six 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 review committees, which made recommendations that helped guide 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., projects such as the Spallation Neutron Source or the Center for Nanophase Materials Sciences), it is reviewed with an external, independent committee 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 will review the major elements of the BES program using a Committee of Visitors (COVs). COVs are charged with (1) assessing the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document proposal actions and (2) assessing the breadth and depth of portfolio elements and the national and international standing of the elements. The first review, which was held in FY 2002, assessed the chemistry activities. The next two years will see similar reviews of the materials sciences and engineering activities and the x-ray and neutron scattering scientific user facilities. It is intended that this cycle be repeated every three years, 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.

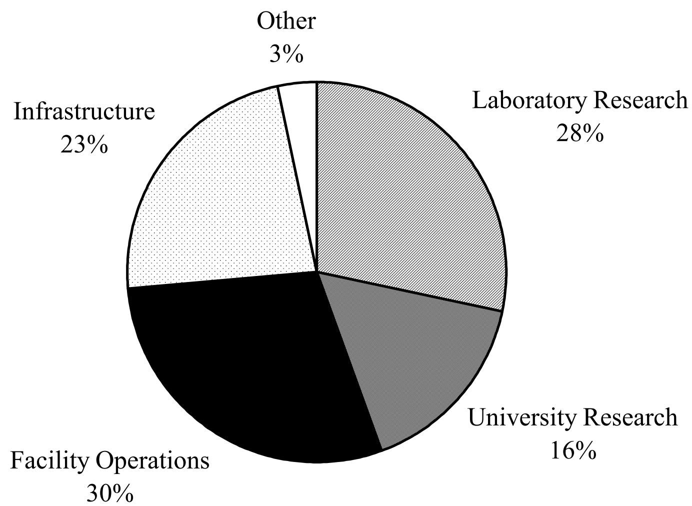
Inputs to our prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, these considerations have led to: increased investments in science at the nanoscale to take advantage of 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 2004 budget request continues priorities established in the past three 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 three Nanoscale Science Research Centers at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, and the combination of Sandia National Laboratories and Los Alamos National Laboratories. Project Engineering Design funding is requested for the Nanoscale Science Research Center at Brookhaven National Laboratory. Finally, 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 4th generation light source that will provide orders of magnitude higher intensities of x-ray light than do current synchrotron radiation light sources.

How We Spend Our Budget:

The BES program has three major program elements: research, facility operations, and construction and laboratory infrastructure support. Approximately 35% of the research funding goes to support work in universities with most of the remainder going to support work in DOE laboratories. This ratio has remained constant for more than a decade and is determined largely by peer review of proposals submitted to the BES program. 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. Construction remains a significant budget component in FY 2004 and includes the Spallation Neutron Source, various Nanoscale Science Research Centers, and the design of the Linac Coherent Light Source.

BASIC ENERGY SCIENCES
FY 2004



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 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 or large teams of closely collaborating researchers 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.

Program Strategic Performance Goals

SC4-1: Build leading research programs in the scientific disciplines encompassed by the BES mission areas and provide world-class, peer-reviewed research results cognizant of DOE needs as well as the needs of the broad scientific community (Materials Sciences and Engineering Subprogram; Chemical Sciences, Geosciences, and Energy Biosciences Subprogram).

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
BES used expert advisory committees and rigorous peer review to ascertain that the research performed by investigators in universities and DOE laboratories was focused and outstanding. (SC4-1) [Met Goal]	Competitively select and peer review at least 80 percent of all new research projects, and evaluate approximately 30 percent of ongoing projects using guidelines defined in 10 CFR 605 for the university projects and similar guidelines established by BES for the laboratory projects. (SC4-1)	Competitively select and peer review at least 80 percent of all new research projects, and evaluate approximately 30 percent of ongoing projects using guidelines defined in 10 CFR 605 for the university projects and similar guidelines established by BES for the laboratory projects. (SC4-1)
As part of the continuing, high-level review of the management processes and the quality, relevance, and national and international leadership of BES programs, the chemical sciences activities were reviewed using a BESAC-chartered Committee of Visitors. (SC4-1) [Met Goal]	As part of the continuing, high-level review of the management processes and the quality, relevance, and national and international leadership of BES programs, review the materials sciences and engineering activities using a BESAC-chartered Committee of Visitors. Implement recommendations from FY 2002 BESAC-chartered Committees of Visitors. (SC4-1)	Implement recommendations from FY 2003 BESAC-chartered Committees of Visitors. (SC4-1)
	Through a BESAC-chartered workshop on "Basic Research Needs to Assure a Secure Energy Future," evaluate future basic research directions appropriate for all activities of the BES program. (SC4-1)	Implement recommendations and new directions resulting from the BESAC-chartered workshop on "Basic Research Needs to Assure a Secure Energy Future." (SC4-1)
Selected aspects of the BES activities were evaluated using BES and BESAC workshops to direct activities toward international leadership and relevance to emerging technologies. (SC4-1) [Met Goal]	Evaluate the following ongoing efforts using BESAC and BES sponsored workshops, with the goal of directing the activities toward international leadership and relevance to emerging technologies: photovoltaics, radiation effects, materials synthesis and processing, and catalysis. Publish results and continue to structure BES programs in accordance with these results. (SC-4-1)	Evaluate aspects of the BES activities using workshops with the goal of directing the research activities toward international leadership and relevance to emerging technologies. Publish results and continue to structure BES programs per results. (SC4-1)

SC4-2: Enable U.S. leadership in nanoscale science, allowing the atom-by-atom design of materials and integrated systems of nanostructured components having new and improved properties for applications as diverse as high-efficiency solar cells and better catalysts for the production of fuels (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
PED was begun on three Nanoscale Science Research Centers. PED funding was obligated to LBNL (6% complete), ORNL (60% complete), and SNL (24% complete). (SC4-2). [Met Goal]	Begin construction of one Nanoscale Science Research Center (NSRC), meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheets for Project Number 03-R-312. Continue project engineering design (PED) activities to establish construction baselines on the two other NSRCs. (SC4-2)	Continue construction of one Nanoscale Science Research Center scheduled for completion in FY 2006 and begin construction on two others scheduled for completion in FY 2007, meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheet. Initiate PED activities to establish construction baselines on one additional Nanoscale Science Research Center. Begin MIE on the fifth and final Nanoscale Science Research Center. (SC4-2)
	Establish the instrument suites and identify fabrication capabilities for the new NSRC based upon user community input at national workshops held in late FY 2001 and FY 2002. (SC4-2)	Establish instrument suites and identify fabrication capabilities for the Nanoscale Science Research Centers based upon user community input at national workshops. (SC4-2)
In FY 2002, there were 46 new grants awarded to universities and 12 projects at DOE laboratories were initiated in selected areas of nanoscale science, engineering, and technology. (SC4-2) [Met Goal]		

SC4-3: Develop advanced research instruments for x-ray diffraction, scattering, and imaging to provide diverse communities of researchers with the tools necessary for exploration and discovery in materials sciences and engineering, chemistry, earth and geosciences, and biology. (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	Select and begin upgrade/fabrication of instruments at the BES synchrotron light sources, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis. (SC4-3)	Continue fabrication of instruments at the BES synchrotron light sources, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis. (SC4-3)

SC4-4: Restore U.S. preeminence in neutron scattering research, instrumentation, and facilities to provide researchers with the tools necessary for the exploration and discovery of advanced materials (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	Select and begin upgrade/fabrication of instruments at the BES neutron scattering facilities, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis. (SC4-3)	Continue fabrication of instruments at the BES neutron scattering facilities, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis. (SC4-3)

SC7-4: Manage BES facility operations and construction to the highest standards of overall performance using merit evaluation with independent peer review. (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
BES scientific user facilities were maintained and operated so that the unscheduled downtime on average was less than 10 percent of the total scheduled operating time. (SC7-4) [Met Goal]	Maintain and operate the BES scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-4)	Maintain and operate the BES scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-4)
The cost and schedule milestones for upgrades and construction of scientific user facilities were met. (SC7-4) [Met Goal]	Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4)	Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4)
Construction of the Spallation Neutron Source met the cost and schedule milestones within 10 percent of the baselines in the construction project data sheet, project number 99-E-334. At the end of FY 2002, construction was 47 percent complete. (SC7-4) [Met Goal]	Continue construction of the Spallation Neutron Source meeting the cost and schedule milestones within 10 percent of the construction project data sheet baselines. At the end of FY 2003, construction will be 61 percent complete. (SC7-4)	Continue construction of the Spallation Neutron Source, meeting the cost and schedule milestones within 10 percent of the construction project data sheet baselines. At the end of FY 2004, construction will be 80 percent complete. (SC7-4)
The upgrade of the SPEAR storage ring at the Stanford Synchrotron Radiation Laboratory met the cost and schedule milestones within 10 percent. At the end of FY 2002, the upgrade was 70% complete. (SC7-4) [Met Goal]	Complete the upgrade of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory), maintaining cost and schedule within 10 percent of baselines.	
	Begin PED of the Linac Coherent Light Source at the Stanford Linear Accelerator Facility. At the end of FY 2003, PED will be 18 percent complete. (SC7-4)	Continue PED of the Linac Coherent Light Source at the Stanford Linear Accelerator Facility. At the end of FY 2004, PED will be 40 percent complete. (SC7-4)

Program Assessment Rating Tool (PART) Assessment

The Office of Management and Budget's (OMB) PART assessment of the BES program rated the program highly for having a "well defined mission, merit-based reviews for awarding contracts and grants, and highly-regarded large project management practices." BES was rated lower for planning and results because of BES's "current lack of adequate long-term and annual performance measures" though OMB did acknowledge "the program has made significant strides toward developing such measures despite the problems inherent in measuring and predicting scientific progress."

The BES program was found to be focused, well managed, and was the first Office of Science program to institute a process whereby an ad hoc panel of outside experts favorably reviewed the program's research portfolio and processes. OMB also noted a recent GAO report validating the BES program's merit-based peer review process for awarding contracts and grants.

To address OMB's two concerns for the BES program: 1) The FY 2004 budget requests funds to operate the BES user facilities at 99 percent of maximum capacity, and to continue work on the design and construction of four new nanoscale science research facilities; and 2) the BES program will work with the DOE's Office of Science and Chief Financial Officer, and OMB to reform the BES performance measures and goals to more accurately predict future scientific progress in a scientifically justifiable and meaningful manner.

Significant Program Shifts

In FY 2004, construction will proceed on three Nanoscale Science Research Centers (NSRCs), project engineering design will be initiated on the fourth NSRC, and a Major Item of Equipment will be initiated for the fifth and final 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 and a wide variety of state-of-the-art instrumentation in a single building. 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 up to 450 researchers each.

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

Nanoscale Science Research Funding

	TEC	TPC	FY 2002 Enacted	FY 2003 Request	FY 2004 Request
Research					
Materials Sciences and Engineering			58,184	66,645	66,795
Chemical Sciences, Geosciences, and Biosciences			27,318	27,395	28,360
Capital Equipment					
Major Item of Equipment -- ANL, Center for Nanophase Materials			0	0	10,000
Nanoscale Science Research Centers					
PED – All sites	20,000		3,000	11,000	3,000
Construction					
BNL, Center for Functional Nanomaterials	70-85,000	TBD	0	0	0
LBNL, Molecular Foundry	83,700	85,000	0	0	35,000
ORNL, Center for Nanophase Materials Sciences	64,000	65,000	0	24,000	20,000
SNL/A and LANL, Center for Integrated Nanotechnologies	73,800	75,800	0	0	29,850
Total BES Nanoscale Science Funding			88,502	129,040	193,005

Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) activity is a set of coordinated investments across all Office of Science mission areas with the goal to achieve breakthrough scientific advances through computer simulation that were impossible using theoretical or laboratory studies alone. The power of computers and networks is increasing exponentially. By exploiting advances in computing and information technologies as tools for discovery, SciDAC encourages and enables a new model of multi-discipline collaboration among the scientific disciplines, computer scientists and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can fully exploit terascale computing and networking resources. The program will bring simulation to a parity level with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate prediction, plasma physics, particle physics, astrophysics and computational chemistry.

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 2003. 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 the cost and schedule variances for the construction projects and for large (>$20,000,000) Major

Items of Equipment. 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.

Hours of Operation and Numbers of Users for the Synchrotron Light Sources and Neutron Scattering Facilities	FY 2000 Actual	FY 2001 Actual	FY 2002 Actual	FY 2003 Request Estimate	FY 2004 Request Estimate
ALL FACILITIES					
Maximum Hours.....................................	37,100	37,100	37,100	37,100	37,100
Scheduled Hours	30,937	27,563	31,215	37,100	37,100
Unscheduled Downtime	2%	4%	4%	<10%	<10%
Number of Users	6,533	6,982	7,608	7,380	8,280
ADVANCED LIGHT SOURCE					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	5,651	5,468	5,236	5,700	5,700
Unscheduled Downtime	5%	4%	7%	<10%	<10%
Number of Users	1,036	1,163	1,385	1,300	1,500
ADVANCED PHOTON SOURCE					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	5,047	5,000	4,856	5,700	5,700
Unscheduled Downtime	6%	4%	3%	<10%	<10%
Number of Users	1,527	1,989	2,299	1,800	2,400
NATIONAL SYNCHROTRON LIGHT SOURCE					
Maximum Hours	5,700	5,700	5,700	5,700	5,700
Scheduled Hours	4,980	5,556	5,818	5,700	5,700
Unscheduled Downtime	0%	0%	3%	<10%	<10%
Number of Users	2,551	2,523	2,413	2,500	2,500
STANFORD SYNCHROTRON RADIATION LABORATORY					
Maximum Hours	5,300	5,300	5,300	5,300	5,300
Scheduled Hours	4,280	4,781	4,706	5,300	5,300
Unscheduled Downtime	3%	5%	5%	<10%	<10%
Number of Users	895	907	800	900	1,000
HIGH FLUX ISOTOPE REACTOR					
Maximum Hours	6,100	6,100	6,100	6,100	6,100
Scheduled Hours	6,262	8	4,111	6,100	6,100
Unscheduled Downtime	7%	0%	3%	<10%	<10%
Number of Users.....................................	269	38	76	400	400

Hours of Operation and Numbers of Users for the Synchrotron Light Sources and Neutron Scattering Facilities	FY 2000 Actual	FY 2001 Actual	FY 2002 Actual	FY 2003 Request Estimate	FY 2004 Request Estimate
INTENSE PULSED NEUTRON SOURCE					
Maximum Hours	5,000	5,000	5,000	5,000	5,000
Scheduled Hours	3,783	3,868	4,308	5,000	5,000
Unscheduled Downtime	0%	0%	0%	<10%	<10%
Number of Users	230	240	243	280	280
MANUEL LUJAN, JR. NEUTRON SCATTERING CENTER					
Maximum Hours	3,600	3,600	3,600	3,600	3,600
Scheduled Hours	934	2,882	2,180	3,600	3,600
Unscheduled Downtime	21%	18%	12%	<10%	<10%
Number of Users	25	122	163	200	200

Cost and Schedule Variance	FY 2000 Actual	FY 2001 Actual	FY 2002 Actual	FY 2003 Request Estimate	FY 2004 Request
Spallation Neutron Source					
Cost Variance	-1.7%	+0.4%	-0.3%		
Schedule Variance	-6.2%	-6.7%	-1.8%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Critical Decision 3 – Start Construction Submit PSAR	None	Linac Design Complete	Front End Beam Available to Linac Target Design Complete Linac Tunnel Beneficial Occupancy Ring Tunnel Beneficial Occupancy	None
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 Mission Need	Approved Acquisition Execution Plan Approved Critical Decision 1 – Preliminary Baseline Range Approved Critical Decision 2 – Performance Baseline	Approve Critical Decision 3 – Start of Construction	None

Cost and Schedule Variance	FY 2000 Actual	FY 2001 Actual	FY 2002 Actual	FY 2003 Request Estimate	FY 2004 Request
SSRL SPEAR3 Upgrade					
Cost Variance	+8.3%	+0.3%	+2.0%		
Schedule Variance	-6.8%	-7.8%	-1.6%		
Major (Levels 0 and 1) Milestones Completed or Committed to	Main magnet designs completed Arc vacuum system design completed Start vacuum system production Test magnet prototypes Start magnet production	Preliminary Safety Assessment Document Approved	Complete RF System Production Complete Magnet Production	Approve Final Safety Assessment Document Complete Vacuum System Production Complete Raft Assemblies Start Major Installation	Complete Accelerator Readiness Review Start Commission-ing Approve Critical Decision 4 – Start Operations

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 2004 budget authority is requested to 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.

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 $200,000,000 to $240,000,000. FY 2004 Project Engineering Design (PED) funding of $7,500,000 requested for Title I and Title II design work and $2,000,000 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.

Nanoscale Science Research Centers (NSRCs)

Funds are requested for construction of NSRCs located at Oak Ridge National Laboratory, at Lawrence Berkeley National Laboratory, and at Sandia National Laboratories/Los Alamos National Laboratory. Funds are also requested for Project Engineering Design of an NSRC at Brookhaven National

Laboratory and for a 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, 04-R-313, and 04-R-314, 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 2000	FY 2001	FY 2002 Enacted	FY 2003 Request	FY 2004 Request
# University Grants	1,062	1,094	1,071	1,150	1,150
Ave. Size ($ thousands/yr)	116	134	140	140	140
# Permanent Ph.D.s	3,490	3,780	3,650	3,910	3,930
# Postdocs	1,005	1,090	1,050	1,140	1,130
# Grad Students	1,640	1,780	1,700	1,820	1,820

Funding Profile

	(dollars in thousands)				
	FY 2002 Comparable Appropriation	FY 2003 Request	FY 2004 Request	$ Change	% Change
Basic Energy Sciences					
Research					
Materials Sciences and Engineering	500,033	547,577	567,711	+20,134	+36.8%
Chemical Sciences, Geosciences, and Energy Biosciences	200,227	220,015	220,914	+899	+0.4%
Subtotal, Research	700,260	767,592	788,625	+21,033	+27.4%
Construction	279,300	251,571	219,950	-31,621	-12.6%
Total, Basic Energy Sciences	979,560 [abcd]	1,019,163	1,008,575	-10,588	-1.0%

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

[a] Excludes $15,672,000 which was transferred to the SBIR program and $940,000 which was transferred to the STTR program.

[b] Excludes $405,000 for the FY 2002 rescission contained in Section 1403 of P.L. 107-226, Supplemental Appropriations for further recovery from and response to terrorist attacks on the United States.

[c] Excludes $2,600,000 transferred to Safeguards and Security for a FY 2002 reprogramming.

[d] Excludes $428,000 and $437,000 in FY 2002 and FY 2003 respectively, transferred to Security Operations in FY 2004 for waste management activities at the New Brunswick Laboratory.

Funding by Site [a]

	FY 2002	FY 2003	FY 2004	$ Change	% Change
	(dollars in thousands)				
Albuquerque Operations Office					
Los Alamos National Laboratory	25,089	23,041	23,634	+593	+2.6%
National Renewable Energy Laboratory	5,412	4,562	4,562	0	--
Sandia National Laboratory	25,977	25,987	52,949	+26,962	+103.8%
Total, Albuquerque Operations Office	56,478	53,590	81,145	+27,555	+51.4%
Chicago Operations Office					
Ames Laboratory	18,377	16,507	16,502	-5	--
Argonne National Laboratory – East	156,916	152,734	166,066	+13,332	+8.7%
Brookhaven National Laboratory	59,158	57,398	61,755	+4,357	+7.6%
Chicago Operations Office	105,854	84,204	84,174	-30	--
Total, Chicago Operations Office	340,305	310,843	328,497	+17,654	+5.7%
Idaho Operations Office					
Idaho National Engineering and Environmental Laboratory	1,784	1,494	1,494	0	--
Oakland Operations Office					
Lawrence Berkeley National Laboratory	81,885	78,691	108,247	+29,556	+37.6%
Lawrence Livermore National Laboratory	5,481	4,676	4,676	0	--
Stanford Linear Accelerator Center (SSRL)	34,073	41,716	38,943	-2,773	-6.6%
Oakland Operations Office	44,352	34,497	34,497	0	--
Total, Oakland Operations Office	165,791	159,580	186,363	+26,783	+16.8%
Oak Ridge Operations Office					
Oak Ridge Institute For Science and Education	2,203	872	872	0	--
Oak Ridge National Laboratory	398,845	343,176	257,609	-85,567	-24.9%
Total, Oak Ridge Operations Office	401,048	344,048	258,481	-85,567	-24.9%
Richland Operations Office					
Pacific Northwest National Laboratory	13,128	11,648	11,648	0	--
Washington Headquarters	1,026	137,960	140,947	+2,987	+2.2%
Total, Basic Energy Sciences	979,560 [bcde]	1,019,163	1,008,575	-10,588	-1.0%

[a] On December 20, 2002, the National Nuclear Security Administration (NNSA) disestablished the Albuquerque, Oakland, and Nevada Operations Offices, renamed existing area offices as site offices, established a new Nevada Site Office, and established a single NNSA Service Center to be located in Albuquerque. Other aspects of the NNSA organizational changes will be phased in and consolidation of the Service Center in Albuquerque will be completed by September 30, 2004. For budget display purposes, DOE is displaying non-NNSA budgets by site in the traditional pre-NNSA organizational format.

[b] Excludes $15,672,000 which was transferred to the SBIR program and $940,000 which was transferred to the STTR program.

[c] Excludes $405,000 for the FY 2002 rescission contained in Section 1403 of P.L. 107-226, Supplemental Appropriations for further recovery from and response to terrorist attacks on the United States.

[d] Excludes $2,600,000 transferred to Safeguards and Security for a FY 2002 reprogramming.

[e] Excludes $428,000 and $437,000 in FY 2002 and FY 2003 respectively, transferred to Security Operations in FY 2004 for waste management activities at the New Brunswick Laboratory.

Site Description

Ames Laboratory

Ames Laboratory is a Multiprogram Laboratory located on 10 acres in Ames, Iowa. The laboratory was built on the campus of Iowa State University during World War II to emphasize the purification and science of rare earth materials. This emphasis continues today. The BES Materials Sciences and Engineering subprogram supports experimental and theoretical research on rare earth elements in novel mechanical, magnetic, and superconducting materials. Ames scientists are experts on magnets, superconductors, and quasicrystals that incorporate rare earth elements. The BES Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports theoretical studies for the prediction of molecular energetics and chemical reaction rates. Ames Laboratory provides leadership in analytical and separations chemistry.

Ames Laboratory is home to the **Materials Preparation Center** (MPC), which is dedicated to the preparation, purification, and characterization of rare-earth, alkaline-earth, and refractory metal and oxide materials. Established in 1981, the MPC is a one-of-a-kind resource that provides scientists at university, industrial, and government laboratories with research and developmental quantities of high-purity materials and unique analytical and characterization services that are not available from commercial suppliers. The MPC is renowned for its technical expertise in alloy design and for creating materials that exhibit ultrafine microstructures, high strength, magnetism, and high conductivity. The MPC also operates the Materials Referral System and Hotline, where users may obtain free information from a database of over 2,500 expert sources for the preparation and characterization of a wide variety of commercial materials and research samples.

Argonne National Laboratory

Argonne National Laboratory (ANL) in Argonne, Illinois, is a Multiprogram Laboratory located on 1,700 acres in suburban Chicago. ANL has a satellite site located in Idaho Falls, Idaho. ANL is home to research activities in broad areas of materials and chemical sciences. It is also the site of three BES supported user facilities -- the Advanced Photon Source (APS), the Intense Pulsed Neutron Source (IPNS), and the Electron Microscopy Center for Materials Research (EMC).

The Materials Sciences and Engineering subprogram supports research in high-temperature superconductivity; polymeric superconductors; thin-film magnetism; surface science; the synthesis, advanced electron beam microcharacterization, and atomistic computer simulation of interfaces in advanced ceramic thin-films; defects and disordered materials; and synthesis and electronic and structural characterization of oxide ceramic materials, including high-temperature superconductors. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in actinide separations; physical and chemical properties of actinide compounds; structural aspects fundamental to advanced electrochemical energy storage; the chemistry of complex hydrocarbons; experimental and theoretical studies of metal clusters of catalytically active transition metals; molecular dynamics of gas-phase chemical reactions of small molecules and radicals; photosynthesis mechanisms; atomic, molecular, and optical physics; organic geochemistry related to hydrocarbon formation, and computational microtomography of porous earth materials. ANL has one of three pulsed radiolysis activities that together form a national research program in this area. The other two are at Brookhaven National Laboratory and the University of Notre Dame.

The **Advanced Photon Source** is one of only three third-generation, hard x-ray synchrotron radiation light sources in the world. Dedicated in 1996, the construction project was completed five months ahead of schedule and for less than the budget. The 7 GeV hard x-ray light source has since met or exceeded all technical specifications. For example, the APS is 10 times more brilliant than its original specifications and the vertical stability of the particle beam is three times better than its design goal. The 1,104-meter circumference facility -- large enough to house a baseball park in its center -- includes 34 bending magnets and 34 insertion devices, which generate a capacity of 68 beamlines for experimental research. Instruments on these beamlines attract researchers to study the structure and properties of materials in a variety of disciplines, including condensed matter physics, materials sciences, chemistry, geosciences, structural biology, medical imaging, and environmental sciences. The high-quality, reliable x-ray beams at the APS have already brought about new discoveries in materials structure.

The **Intense Pulsed Neutron Source** is a 30 Hz short-pulsed spallation neutron source that first operated all instruments in the user mode in 1981. Twelve neutron beam lines serve 14 instruments, one of which is a test station for instrument development. Distinguishing characteristics of IPNS include its innovative instrumentation and source technology and its dedication to serving the users. The first generation of virtually every pulsed source neutron scattering instrument was developed at IPNS. In addition, the source and moderator technologies developed at IPNS, including uranium targets, liquid hydrogen and methane moderators, solid methane moderators, and decoupled reflectors, have impacted spallation sources worldwide. A recent BESAC review of this facility described it as a "reservoir of expertise with a track record of seminal developments in source and pulsed source instruments second to none" and noted that ANL is "fully committed from top to bottom to supporting the user program." This is reflected by a large group of loyal, devoted users. Research at IPNS is conducted on the structure of high-temperature superconductors, alloys, composites, polymers, catalysts, liquids and non-crystalline materials, materials for advanced energy technologies, and biological materials. The staff of the IPNS is taking a leadership role in the design and construction of instrumentation for the Spallation Neutron Source at Oak Ridge National Laboratory.

The **Electron Microscopy Center for Materials Research** provides in-situ, high-voltage and intermediate voltage, high-spatial resolution electron microscope capabilities for direct observation of ion-solid interactions during irradiation of samples with high-energy ion beams. The EMC employs both a tandem accelerator and an ion implanter in conjunction with a transmission electron microscope for simultaneous ion irradiation and electron beam microcharacterization. It is the only instrumentation of its type in the Western Hemisphere. The unique combination of two ion accelerators and an electron microscope permits direct, real-time, in-situ observation of the effects of ion bombardment of materials and consequently attracts users from around the world.

The **Center for Nanoscale Materials**, a planned BES Nanoscale Science Research Center, will have as its focus research in advanced magnetic materials, complex oxides, nanophotonics, and bio-inorganic hybrids. An x-ray nanoprobe beam line at the Advanced Photon Source will be fabricated and run by the Center for use by its users. The facility will use existing facilities such as the Advanced Photon Source, the Intense Pulsed Neutron Source, and the Electron Microscopy Center. The State of Illinois is providing in FY 2003 and FY 2004 a total of $36,000,000 for construction of the building, which is appended to the Advanced Photon Source. BES will provide funding for clean rooms and specialized equipment as well as the operations following commissioning.

Brookhaven National Laboratory

Brookhaven National Laboratory (BNL) is a Multiprogram Laboratory located on 5,200 acres in Upton, New York. BNL is home to BES major research efforts in materials and chemical sciences as well as to efforts in geosciences and biosciences. BNL is also the site of the National Synchrotron Light Source (NSLS).

The Materials Sciences and Engineering subprogram emphasizes experiments that make use of the NSLS. BNL scientists are among the world leaders in neutron and x-ray scattering applied to a wide variety of research problems such as high-temperature superconductivity, magnetism, structural and phase transformations in solids, and polymeric conductors. BNL has strong research programs in nanoscale structure and defects, the structure and composition of grain boundaries and interfaces, high temperature superconductors, and aqueous and galvanic corrosion.

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports one of three national activities for pulsed radiolysis research at BNL. The innovative short-pulse radiation chemistry facility contributes to radiation sciences research across broad areas of chemistry. There is also research on the spectroscopy of reactive combustion intermediates and studies of the mechanisms of electron transfer related to artificial photosynthesis. Other chemistry research at BNL is focused around the unique capabilities of the NSLS in obtaining time dependant structural data of reacting systems, the structural changes accompanying catalytic and electrochemical reactions, the formation of atmospheric aerosols and their reactivity, and the interactions of rock-fluid systems. Biosciences research activities include mechanistic and molecular-based studies on photosynthesis, lipid metabolism, and genetic systems.

The **National Synchrotron Light Source** (NSLS) is among the largest and most diverse scientific user facilities in the world. The NSLS, commissioned in 1982, has consistently operated at >95% reliability 24 hours a day, seven days a week, with scheduled periods for maintenance and machine studies. Adding to its breadth is the fact that the NSLS consists of two distinct electron storage rings. The x-ray storage ring is 170 meters in circumference and can accommodate 60 beamlines or experimental stations, and the vacuum-ultraviolet (VUV) storage ring can provide 25 additional beamlines around its circumference of 51 meters. Synchrotron light from the x-ray ring is used to determine the atomic structure of materials using diffraction, absorption, and imaging techniques. Experiments at the VUV ring help solve the atomic and electronic structure as well as the magnetic properties of a wide array of materials. These data are fundamentally important to virtually all of the physical and life sciences as well as providing immensely useful information for practical applications. The petroleum industry, for example, uses the NSLS to develop new catalysts for refining crude oil and making by-products like plastics.

The **Center for Functional Nanomaterials**, 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.

Idaho National Engineering and Environmental Laboratory

Idaho National Environmental and Engineering Laboratory (INEEL) is a Multiprogram Laboratory located on 572,000 acres in Idaho Falls, Idaho. The Materials Sciences and Engineering subprogram supports studies to establish controls of biologically based engineering systems, to understand and improve the life expectancy of material systems used in engineering such as welded systems, and to develop new diagnostic techniques for engineering systems. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram focuses on fundamental understanding of negative ion mass spectrometry, studies of secondary ion mass spectrometry, and computer simulation of ion motion and configuration of electromagnetic fields crucial to the design of ion optics.

Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory (LBNL) is a Multiprogram Laboratory located in Berkeley, California, on a 200-acre site adjacent to the Berkeley campus of the University of California. LBNL is home to BES major research efforts in materials and chemical sciences as well as to efforts in geosciences, engineering, and biosciences. Collocated with the University of California at Berkeley, the Laboratory benefits from regular collaborations and joint appointments with numerous outstanding faculty members. The Laboratory is the home to the research of many students and postdoctoral appointees. LBNL is also the site of two BES supported user facilities -- the Advanced Light Source (ALS) and the National Center for Electron Microscopy (NCEM).

The Materials Sciences and Engineering subprogram supports research in laser spectroscopy, superconductivity, thin films, femtosecond processes, x-ray optics, biopolymers, polymers and composites, surface science, theory, and nonlinear dynamics. Research is carried out on new aluminum-based alloys containing germanium and silicon; the structures of magnetic, optical, and electrical thin films and coatings; processing, mechanical fatigue, and high-temperature corrosion of structural ceramics and ceramic coatings; mechanical behavior of metals; and the synthesis, structure, and properties of advanced semiconductor and semiconductor-metal systems. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports fundamental, chemical dynamics research using molecular-beam techniques. Femtosecond spectroscopy studies of energy transfer on surfaces has also been developed. LBNL is recognized for its work in radiochemistry, the chemistry of the actinides, inorganic chemistry, and both homogeneous and heterogeneous chemical catalysis. Experimental and computational geosciences research is supported on coupled reactive fluid flow and transport properties and processes in the subsurface, and how to track and image them. In particular, geochemical studies focus on experimental and modeling studies on critical shallow earth mineral systems, improving analytical precision in synchrotron x-ray studies, and improving our understanding of how isotopic distributions act as tracers for geologic processes and their rates. Biosciences research focuses on the physics of the photosynthetic apparatus and on the formation of subcellular organelles.

The **Advanced Light Source** (ALS) began operations in October 1993 and now serves over 1,000 users as one of the world's brightest sources of high-quality, reliable vacuum-ultraviolet (VUV) light and long-wavelength (soft) x-rays. Soft x-rays and VUV light are used by the researchers at the ALS as high-resolution tools for probing the electronic and magnetic structure of atoms, molecules, and solids, such as those for high-temperature superconductors. The high brightness and coherence of the ALS light are particularly suited for soft x-ray imaging of biological structures, environmental samples, polymers, magnetic nanostructures, and other inhomogeneous materials. Other uses of the ALS include holography, interferometry and the study of molecules adsorbed on solid surfaces. The pulsed nature of the ALS light offers special opportunities for time resolved research, such as the dynamics of chemical reactions. Shorter wavelength (intermediate-energy) x-rays are also used at structural biology experimental stations for x-ray crystallography and x-ray spectroscopy of proteins and other important biological macromolecules. The ALS is a growing facility with a lengthening portfolio of beamlines that have already been applied to make important discoveries in a wide variety of scientific disciplines.

The **National Center for Electron Microscopy** (NCEM) provides instrumentation for high-resolution, electron-optical microcharacterization of atomic structure and composition of metals, ceramics, semiconductors, superconductors, and magnetic materials. This facility contains one of the highest resolution electron microscopes in the U.S.

The **Molecular Foundry**, a planned BES Nanoscale Science Research Center, will have as its focus the interface between soft materials such as are found in living systems and hard materials such as carbon nanotubes. The Molecular Foundry will use existing facilities such as the ALS, the NCEM, and the National Energy Research Scientific Computing Center. The facility will provide laboratories for materials science, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include clean rooms, controlled environmental rooms, scanning tunneling microscopes, atomic force microscopes, transmission electron microscope, fluorescence microscopes, mass spectrometers, DNA synthesizer and sequencer, nuclear magnetic resonance spectrometer, ultrahigh vacuum scanning-probe microscopes, photo, uv, and e-beam lithography equipment, peptide synthesizer, advanced preparative and analytical chromatographic equipment, and cell culture facilities.

Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory (LLNL) is a Multiprogram Laboratory located on 821 acres in Livermore, California. This laboratory was built in Livermore as a weapons laboratory 42 miles from the campus of the University of California at Berkeley to take advantage of the expertise of the university in the physical sciences. The Materials Sciences and Engineering subprogram supports research in positron materials science, superplasticity in alloys, adhesion and bonding at interfaces, kinetics of phase transformations in welds. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports plasma assisted catalysis for environmental control of pollutants, geosciences research on the source(s) of electromagnetic responses in crustal rocks, seismology theory and modeling, the mechanisms and kinetics of low-temperature geochemical processes and the relationships among reactive fluid flow, geochemical transport and fracture permeability.

Los Alamos National Laboratory

Los Alamos National Laboratory (LANL) is a Multiprogram Laboratory located on 27,000 acres in Los Alamos, New Mexico. LANL is home to BES major research efforts in materials sciences with other efforts in chemical sciences, geosciences, and engineering. LANL is also the site of the Manuel Lujan Jr., Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE).

The Materials Sciences and Engineering subprogram supports research on strongly correlated electronic materials, high-magnetic fields, microstructures, deformation, alloys, bulk ferromagnetic glasses, mechanical properties, ion enhanced synthesis of materials, metastable phases and microstructures, and mixtures of particles in liquids. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research to understand the electronic structure and reactivity of actinides through the study of organometallic compounds. Also supported is work to understand the chemistry of plutonium and other light actinides in both near-neutral pH conditions and under strongly alkaline conditions relevant to radioactive wastes and research in physical electrochemistry fundamental to energy storage systems. In the areas of geosciences, experimental and theoretical research is supported on rock physics, seismic imaging, the physics of the earth's magnetic field, fundamental geochemical studies of isotopic equilibrium/disequilibrium, and mineral-fluid-microbial interactions.

The **Los Alamos Neutron Science Center** provides an intense pulsed source of neutrons for both national security research and civilian research. LANSCE is comprised of a high-power 800-MeV proton linear accelerator, a proton storage ring, production targets to the Manuel Lujan Jr. Neutron Scattering Center and the Weapons Neutron Research facility, and a variety of associated experiment areas and spectrometers. The Lujan Center features instruments for measurement of high-pressure and high-temperature samples, strain measurement, liquid studies, and texture measurement. The facility has a long history and extensive experience in handling actinide samples. A new 30 Tesla magnet is available for use with neutron scattering to study samples in high-magnetic fields.

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.

National Renewable Energy Laboratory

National Renewable Energy Laboratory (NREL) is a program-dedicated laboratory (Solar) located on 300 acres in Golden, Colorado. NREL was built to emphasize renewable energy technologies such as photovoltaics and other means of exploiting solar energy. The Materials Sciences and Engineering subprogram supports basic research efforts that underpin this technological emphasis at the Laboratory, for example on overcoming semiconductor doping limits, novel and ordered semiconductor alloys, theoretical and experimental studies of properties of advanced semiconductor alloys for prototype solar cells. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research addressing the fundamental understanding of solid-state, artificial photosynthetic systems. This research includes the preparation and study of novel dye-sensitized semiconductor electrodes, characterization of the photophysical and chemical properties of quantum dots, and study of charge carrier dynamics in semiconductors.

Oak Ridge Institute for Science and Education

Oak Ridge Institute for Science and Education (ORISE) is located on 150 acres in Oak Ridge, Tennessee. The BES program provides funding to ORISE for support of a consortium of university and industry scientists to share the ORNL research station at NSLS to study the atomic and molecular structure of matter (known as ORSOAR, the Oak Ridge Synchrotron Organization for Advanced Research). The BES program also funds ORISE to provide administrative support for panel reviews and site reviews commissioned and led by the BES program staff. ORISE also assists with the administration of topical scientific workshops and provides administrative support for other activities such as for the reviews of BES construction projects. ORISE manages the **Shared Research Equipment (SHaRE)** program at ORNL. The SHaRE program makes available state-of-the-art electron beam microcharacterization facilities for collaboration with researchers from universities, industry and other government laboratories.

Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) is a Multiprogram Laboratory located on 24,000 acres in Oak Ridge, Tennessee. ORNL is home to major research efforts in materials and chemical sciences with additional programs in engineering and geosciences. It is the site of the High Flux Isotope Reactor (HFIR) and the Radiochemical Engineering Development Center (REDC). ORNL also leads the six-laboratory collaboration that is designing and constructing the Spallation Neutron Source (SNS).

ORNL has perhaps the most comprehensive materials research program in the country. The Materials Sciences and Engineering subprogram supports basic research that underpins technological efforts such as those supported by the energy efficiency program. Research is conducted in microscopy and microanalysis, atomistic mechanisms in interface science, theoretical studies of metals, alloys, and ceramics, theory and design of dual phase alloys, radiation effects, domain structure in epitaxial ferroelectrics, semiconductor nanocrystals for carbon dioxide fixation, high temperature alloy design, welding science, microstructural design of advanced ceramics, acoustic harmonic generation, non-equilibrium processes. Research is also conducted in superconductivity, magnetic materials, neutron scattering and x-ray scattering, electron microscopy, pulsed laser ablation, thin films, lithium battery materials, thermoelectric materials, surfaces, polymers, structural ceramics, alloys; and intermetallics. The subprogram emphasizes experiments at HFIR and other specialized research facilities that include the High Temperature Materials Laboratory and the Shared Research Equipment (SHaRE) program.

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in analytical chemistry, particularly in the area of mass spectrometry, separation chemistry, and thermo-physical properties. Examples of the science include solvation in supercritical fluids, electric field-assisted separations, speciation of actinide elements, ion-imprinted sol-gels for actinide separations, ligand design, stability of macromolecules and ion fragmentation, imaging of organic and biological materials with secondary ion mass spectrometry, and the physics of highly charged species. The subprogram also supports research on the collision physics of highly charged ions and their interactions with surfaces. In the area of geosciences, work is supported to study low-temperature geochemical processes and rates in mineral-fluid systems.

The **High Flux Isotope Reactor** is a light-water cooled and moderated reactor that began full-power operations in 1966. HFIR operates at 85 megawatts to provide state-of-the-art facilities for neutron scattering, materials irradiation, and neutron activation analysis and is the world's leading source of elements heavier than plutonium for research, medicine, and industrial applications. The neutron-scattering experiments at HFIR reveal the structure and dynamics of a very wide range of materials. The neutron-scattering instruments installed on the four horizontal beam tubes are used in fundamental studies of materials of interest to solid-state physicists, chemists, biologists, polymer scientists, metallurgists, and colloid scientists. Recently, a number of improvements at HFIR have increased its neutron scattering capabilities to 14 state-of-the-art neutron scattering instruments on the world's brightest beams of steady-state neutrons. These upgrades include the installation of larger beam tubes and shutters, a high-performance liquid hydrogen cold source, and neutron scattering instrumentation. The new installation of the cold source provides beams of cold neutrons for scattering research that are as bright as any in the world. Use of these forefront instruments by researchers from universities, industries, and government laboratories are granted on the basis of scientific merit.

The **Radiochemical Engineering Development Center**, located adjacent to HFIR, provides unique capabilities for the processing, separation, and purification of transplutonium elements.

The **Center for Nanophase Materials Sciences (CNMS)**, a proposed BES Nanoscale Science Research Center, will establish 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, wet and dry laboratories for sample preparation, fabrication and analysis. Included will be equipment to synthesize, manipulate, and characterize nanoscale materials and structures. The facility, which will be collocated with the Spallation Neutron Source complex, will house over 100 research scientists and an additional 100 students and postdoctoral fellows. 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 capabilities in neutron scattering.

Pacific Northwest National Laboratory

Pacific Northwest National Laboratory (PNNL) is a Multiprogram Laboratory located on 640 acres at the Department's Hanford site in Richland, Washington. The BES Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in interfacial chemistry of water-oxide systems, near-field optical microscopy of single molecules on surfaces, inorganic molecular clusters, and direct photon and/or electron excitation of surfaces and surface species. Programs in analytical chemistry and in applications of theoretical chemistry to understanding surface catalysis are also supported. Included among these studies are high-resolution laser spectroscopy for analysis of trace metals on ultra small samples; understanding of the fundamental inter- and intra-molecular effects unique to solvation in supercritical fluids; and interfacing theoretical chemistry with experimental methods to address complex questions in catalysis. Geosciences research includes theoretical and experimental studies to improve our understanding of phase change phenomena in microchannels. The Materials Sciences and Engineering subprogram supports research on molecularly tailored nanostructured materials, stress corrosion and corrosion fatigue, interfacial dynamics during heterogeneous deformation, irradiation assisted stress corrosion cracking, bulk defect and defect processing in ceramics, chemistry and physics of ceramic surfaces and interfacial deformation mechanisms in aluminum alloys.

Sandia National Laboratory

Sandia National Laboratory (SNL) is a Multiprogram Laboratory located on 3,700 acres in Albuquerque, New Mexico (SNL/NM), with sites in Livermore, California (SNL/CA), and Tonopah, Nevada. SNL is home to significant research efforts in materials and chemical sciences with additional programs in engineering and geosciences. SNL/CA is also the site of the Combustion Research Facility (CRF). SNL has a historic emphasis on electronic components needed for Defense Programs. The laboratory has very modern facilities in which unusual microcircuits and structures can be fabricated out of various semiconductors. The Materials Sciences and Engineering subprogram supports projects on the physics and chemistry of ceramics, adhesion and interfacial wetting, localized corrosion initiation, long range particle interactions and collections phenomena in plasma and colloidal crystals, advanced epitaxial growth techniques, energetic particle synthesis, artificially structured semiconductors, field structured anisotropic composites, surface interface and bulk properties of advanced ceramics, transitions in the strongly collective behavior of dislocations, and mixtures of particles in liquids. The Chemical

Sciences, Geosciences, and Energy Biosciences subprogram supports geosciences research on mineral-fluid reactivity, rock mechanics, reactive fluid flow and particulate flow through fractured and porous media, and seismic and electromagnetic imaging and inversion studies.

The **Combustion Research Facility** at SNL/CA is an internationally recognized facility for the study of combustion science and technology. In-house 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 combustion intermediates. Basic research supported by the Chemical Sciences, Geosciences, and Energy Biosciences subprogram is often done in close collaboration with applied problems. A principal effort in turbulent combustion is coordinated among the BES chemical physics program, and programs in Fossil Energy and Energy Efficiency and Renewable Energy.

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Stanford Linear Accelerator Center

Stanford Linear Accelerator Center (SLAC) is a program-dedicated laboratory (High Energy Physics) located on 426 acres in Menlo Park, California. It is the home of the **Stanford Synchrotron Radiation Laboratory** (SSRL) and peer-reviewed research projects associated with SSRL. The Stanford Synchrotron Radiation Laboratory was built in 1974 to take and use for synchrotron studies the intense x-ray beams from the SPEAR storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third-generation synchrotron sources. In FY 2000, the facility was comprised of 32 experimental stations and was used by nearly 900 researchers from industry, government laboratories and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. The Materials Sciences and Engineering subprogram supports a research program at SSRL with emphasis in both the x-ray and ultraviolet regions of the spectrum. SSRL scientists are experts in photoemission studies of high-temperature superconductors and in x-ray scattering. The SPEAR 3 upgrade at SSRL will provide major improvements that will increase the brightness of the ring for all experimental stations.

The **Linac Coherent Light Source (LCLS)** will 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. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. A newly constructed long undulator will bunch the electrons, leading 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.

All Other Sites

The BES program funds research at 168 colleges/universities located in 48 states. Also included are funds for research awaiting distribution pending completion of peer review results.

Materials Sciences and Engineering

Mission Supporting Goals and Measures

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.

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. 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.

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.

Selected FY 2002 Research Accomplishments:

- *Giant Magnetoresistance (GMR).* GMR is revolutionizing the magnetic recording and data storage industry by enabling major increases in data density and ease of read/write processes. GMR is the term applied to layered magnetic systems that undergo very large changes in resistance in the presence of a magnetic field. The origin of GMR and its relationship to layered structure is unknown. New experiments in which the GMR is measured with current flowing perpendicular to the layer interfaces have yielded insight into the factors underlying the effect. Measurements of the GMR in samples with quantitatively determined interfacial structure, characterized by microscopy and x-ray scattering, have shown a direct relationship between the GMR and the interfacial roughness. Since most GMR-based devices rely on the magnitude of the effect, these results provide guidance for their optimization by interfacial roughness tailoring.

- *Multifunctional Materials.* For the first time, organic materials that exhibit bistability simultaneously in three channels – magnetic, optical, and electrical – have been produced. The new materials have many interesting properties. In one state, they are paramagnetic (attracted to a magnetic field), infrared transparent, and electrically insulating; in the other state, they are diamagnetic (repelled by both poles of a magnet), infrared opaque, and electrically conducting. The switching between the two states is thermally driven, and a switching temperature just above technologically useful room temperature has been achieved. These multifunctional materials have the potential for use in new types of devices for electronics, computers, and data storage where multiple channels are used for reading, writing, and transferring information.

- *Transparent Electronic Devices.* Rather than ordinary glass, imagine that your window panes at home are a multi-functional wide band-gap semiconductor device that might serve as: an energy generator, a microprocessor, a detector, and a light modulator. The potential of wide-gap semiconductors is enormous, ranging from highly efficient solid-state light sources and high-density data storage to invisible monitoring devices for national security. The key in making this dream a reality is to be able to dope these materials with impurities to achieve both the n- and p-type mechanisms of electrical conduction. Achieving p-type doping had been an insurmountable problem. The root cause was found to be twofold: the spontaneous formation of native defects and the low-dopant solubility. Suppression of the defect formation was achieved by chemical design of the band structure of the semiconductor oxides. This approach has led to a family of new p-type transparent conducting materials. These studies have facilitated the experimental exploration of transparent electronic device materials.

- *World's Smallest Ultraviolet Nanolasers.* The world's smallest ultraviolet-emitting lasers, based on "nanowires" of zinc oxide, have a broad range of potential applications in fields ranging from photonics – the use of light for superfast data processing and transmission – to the so-called "lab on a chip" technology in which a microchip equipped with nano-sized light sources and sensors performs instant and detailed analyses for chemistry, biology, and medical studies. The nanolasers were fabricated using a new processing method that can grow arrays of zinc oxide nanowires between 70 and 100 nm in diameter with adjustable lengths between 2 and 10 microns. This development continues the progress in semiconductor laser research, providing new materials that extend the availability of these versatile and inexpensive light sources from the near infrared and red regions of the spectrum into the green-blue and near ultraviolet.

- *Nanotubes Increase Heat Conduction in Fluids.* Fluids containing 1 percent carbon nanotubes in oil exhibit a 250 percent increase in heat conduction. This addition of nanotubes resulted in the highest thermal conductivity enhancement ever achieved in a liquid – ten times higher than predicted by existing theories. This has required the development of new heat conduction models for solid/liquid suspensions. This research could lead to a major breakthrough in solid/liquid composites for numerous engineering applications, such as coolants for automobiles, air conditioning, and supercomputers.

- *Molecular Based Spintronic Material.* For years scientists have dreamed of separately controlling the spin and charge of the electron to create "spin electronics" or spintronics for next generation electronic devices. We have advanced one step closer to this goal with the fabrication of a new molecular solid integrating alternate layers of spin networks with organic metal networks through crystal engineering. The close proximity of the spin to the metal – less than one nanometer apart –

promises strong communication of spin and charge while allowing each to be manipulated separately. The new material is made by relatively inexpensively using bottom-up self-assembly as opposed to the elaborate and expensive top-down lithography for other semiconductor materials.

- *Deformation at the Nanoscale.* Large-scale atomic-level simulations reveal how and why conventional dislocation deformation processes in materials break down at the nanoscale. Nanostructures can experience very high internal stress levels; thus, mechanical stability and compliance represent major obstacles in the development of nanodevices. The computer simulations demonstrated that, as the grain size becomes ever smaller, a material becomes harder to deform. However, at a critical size, dislocations no longer can exist because they are comparable to that of the grains themselves, and the material suddenly softens again due to the onset of novel deformation mechanisms mediated by the grain boundaries that contain the grains. This "strongest size" was shown to be a function of not only the material itself but also the stress level to which it is subjected. These insights will enable the design of nanodevices with tailored mechanical performance capable of withstanding the very high stresses under which they often operate.

- *Nano-onions.* Carbon "nano-onions," generated by carbon-arc discharge in deionized water, are the latest entry in the fullerene family. Their structures resemble onions, with a fullerene at the core, surrounded by multiple layers of fullerene-like carbon. The arc method produces "nano-onions" with diameters from about 10 to 150 nm. These "Buckyonions" are easily fractionated on the basis of diameter by using flow field-flow fractionation, with small particles eluting before larger ones. Characterization of these "nano-onions" using electron microscopy and light scattering methods could lead to new and novel applications for these materials.

- *A Trillion Elements per Square Inch.* Magnetic storage arrays with more than a trillion elements per square inch, ultrahigh resolution field emission displays, and high resolution, on-chip macromolecular separations devices have been constructed using a new, patented technique of self-assembly of polymers. By means of routine chemical etching processes, large area arrays of nanopores (4-50 nm in diameter) with very high aspect ratios are produced in a simple, robust manner. These serve as templates for pattern transfer to substrates and as scaffolds to direct surface chemistry or electrochemical deposition of metals for the generation of ultrahigh density, multilayered nanowire arrays. The simplicity of this technique has a broad impact across many disciplines ranging from bioactivity to semiconductor devices.

- *Molecules of Gases and Water Swim Upstream.* A theoretical analysis has shown that molecules of hydrogen, oxygen, and even water can travel across conducting membranes in opposite directions from what would normally be expected. An understanding of these membranes is important in the development of advanced materials systems for energy storage such as fuel cells. The analysis pertains to a class of materials called perovskites that can, under some circumstances, conduct charge via both individual electrons and ionized atoms of hydrogen and oxygen. Individual chemical species can move in the "wrong" direction from areas where they are at a lower concentration to areas of higher concentration. This is normally explained by other driving forces that are taken into account in a quantity referred to as the chemical potential. In mixed-conducting membranes, however, the new analysis shows that neutral (uncharged) molecules can even move contrary to the gradient in the chemical potential as a result of the simultaneous, coupled transport of multiple species.

- *Ultra-Sensitive Sensors.* A new principle for chemical sensors with ultra-high sensitivity has been developed and successfully demonstrated based on computer simulations of the structure and properties of particle composites. These sensors are fabricated by dispersing electrically conducting magnetic particles into an insulating liquid, then organizing the particles into chains with a magnetic field while the liquid solidifies by polymerization. These materials are referred to as Field-Structured Composites. The particle chains conduct electricity quite well. When exposed to certain chemical vapors, the polymer absorbs the chemicals and swells. The chains are stretched ever so slightly to create gaps between the particles, resulting in conductivity decreases of ten billion or more. The unprecedented magnitude of this effect makes these materials sensitive to even trace amounts of vapors. Inexpensive, portable devices for chemical identification can be achieved by making an array of sensors, each of which is fabricated with a polymer having unique chemical affinities, so that any single vapor leaves an identifying signature on the array.

- *New Analysis Method Enables Prediction of Dendritic Pattern Formation.* Just as water freezes into the elaborate patterns of snowflakes, so do metals form highly branched patterns called dendrites. These dendrites control many aspects of the processing and microstructure that determine alloy properties and hence our ability to use materials. Dendrite patterns are controlled by minute variations of the interface between the material and its melt. While simulations have modeled the atomic processes that occur during solidification, they have proven inadequate to extract the more subtle information about the anisotropy. An entirely new method to extract the anisotropy of energy and mobility from supercomputer simulations has been devised. The critical step was the identification of a related quantity that can be calculated with sufficient precision and then used to simulate dendritic growth. Additional supercomputer simulations have exploited this new information to predict the precise nature of dendritic pattern formation in a range of materials from silicon to nickel.

- *Superconductors Show Their Stripes.* Like tigers and zebras, superconductors are distinguished by their stripes. Some physicists believe that electricity runs without resistance along "stripes" of electric charge in these materials. Stripes have now been observed for the first time in the most widely studied of the cuprate high-temperature superconductors. The material consists of planes of copper and oxygen atoms located in a square pattern. Some of the electrons are missing in these planes leaving positively charged holes that pair together to produce superconductivity. In a standard superconductor, these pairs travel through the material without hindrance producing the perfect conductivity inherent to a superconductor. However, in the cuprate materials, the copper atoms have a magnetic moment that makes conductivity in the planes difficult. Recent neutron scattering measurements made at the High Flux Isotope Reactor show that the holes form lines or stripes in the superconductor in which there are no magnetic moments. The holes can thus move along the stripe in an unimpeded manner.

- *Neutron Instrumentation for Nanoscience.* Nanoscience requires the study of structures ranging from a few nanometers to a few microns. A new neutron scattering technique for study of materials in this size range has been developed. The method uses the fact that the spin of the neutron has unique behavior in a magnetic field -- the spin precesses like a top in a magnetic field so that the total rotation angle of the spin depends on the time the neutron spends in the magnetic field. By appropriately designing the magnetic fields, the rotation angle can be made to depend on the direction of travel of the neutron with respect to some fixed spatial direction, effectively "coding" the trajectory angle into the value of the neutrons spin. This technique can easily be implemented and could be perfected in time to impact early measurements at the Spallation Neutron Source.

Selected FY 2002 Facility Accomplishments:

- The Advanced Light Source
  - ► *Superbend Magnets Extend Synchrotron Spectral Range.* Originally designed for highest brightness at longer x-ray wavelengths (soft x rays), the ALS has been retrofitted with superconducting bend magnets (superbends) that dramatically boost the synchrotron radiation intensity at shorter x-ray wavelengths (hard x rays) without disrupting the soft x-ray performance of the existing beamlines, thereby allowing the ALS to service a broader user community.
  - ► *Higher-Order-Mode Dampers Increase Storage Ring Stability.* The beam in the ALS storage ring comprises more than 300 discrete "bunches" of electrons spaced more or less equally around the ring, but interactions between the bunches can cause the beam to become unstable. Addition of antennae to the radio-frequency (RF) cavities that power the storage ring has substantially improved the reliability of the feedback system that combats beam instabilities.
  - ► *A New Radio-Frequency (RF) Feedback Loop Saves Electrical Power and Money.* Driven by the soaring costs that came with the California energy crisis, staff at the ALS found a way to reduce the electricity bill an estimated 11% by implementing a feedback loop that reduced power consumption by a klystron power amplifier without interfering with other RF-cavity controls.
  - ► *Beamline for Ultrahigh-Resolution Chemical Crystallography Commissioned.* Based on a novel miniaturized design that is low-cost yet robust and high-performance, the ALS has put into operation a new beamline that meets the demands of chemists for a tool to rapidly determine the atomic structure of molecules with sub-angstrom resolution from solid samples (crystals) as small as a few micrometers on a side.
  - ► *An Experimental Station Has Been Designed to Study Magnetic Nanostructures.* Consisting of multiple layers of magnetic and nonmagnetic materials, each only a few atoms thick, magnetic nanostructures are the foundation for advanced magnetic devices. The new station at the ALS will allow complete magnetic characterization of each layer separately with x rays that are polarized in any desired orientation.
- The Advanced Photon Source
  - ► *Operating in Top-up Mode.* One of the principal operational goals has been to run the storage ring in the "constant current" or top-up mode. Top-up mode consists of injecting a small amount of charge into the storage ring at regular intervals in order to maintain a 100 mA current. The major benefit of top-up operation is the virtual elimination of the beam lifetime (the decay of beam current over time) as a factor in further improvements or enhancements of the storage ring performance. As an example, the APS can now operate efficiently with a lower horizontal emittance, which reduces the source size by a factor of two. This reduction in size provides a smaller beam spot that can be used to illuminate smaller samples. Normally, the decrease in beam lifetime would severely reduce the average current available to the users, but with top-up, the reduction is non-existent. Top-up operation is now the standard and comprises 75 percent of the total operating time of the APS. The APS is the first synchrotron facility to have conceived and implemented top-up operation.

- ► *Canted Undulators for Increased Beamline Capacity.* New technologies devised to offset the ever-increasing demand for beamline access include the "canted undulator" configuration that produces two beamlines originating from one point on the ring.
- ► *New Information on High-Pressure Fuel Sprays.* An x-ray imaging technique devised at the Basic Energy Sciences-funded Synchrotron Radiation Instrumentation Collaborative Access Team (SRI-CAT) has produced unprecedented details of the structure of diesel fuel sprays, including the first evidence of supersonic shockwaves in sprays as they leave high-pressure fuel injectors. This information may lead to improvements in fuel injector-engine emissions and efficiency, and earned a 2002 National Laboratory Combustion & Emissions Control R&D Award from the Department of Energy.
- ► *Nanotomography of Integrated Circuit Interconnects.* A high-resolution scanning transmission x-ray microscope is providing superior 3-D images of the tiny wire interconnects and other embedded structures in computer chips without damage to the chips. This unique capability makes it possible to more easily identify and correct manufacturing problems, and ultimately to build faster, smaller, more-efficient, and more-reliable computers.
- ► *New Lens for Imaging.* An offshoot of APS expertise in x-ray beamline instrumentation is the first full-scale crystal-diffraction medical-imaging lens. Resolution with this lens is a factor of three better than with most current imaging systems. It can be applied to small test animals used by the pharmaceutical industry and to imaging small parts of the human body. There are also many possibilities for nonmedical applications, including examination of nuclear fuel elements and location of radioactive material within a larger mass.

- The National Synchrotron Light Source
  - ► *Source Development Laboratory Laser at 400 nm.* The Deep Ultra-Violet Free Electron Laser (DUV-FEL) facility marked an important milestone, generating laser light at 400 nm by the process of Self Amplified Spontaneous Emission (SASE). Achieving intensity 20,000 times higher than the spontaneous emission, the result showed that the electron beam and the undulator system can support lasing down to 88 nm, which has strong user interest in the chemical physics community.
  - ► *Soft X-ray Undulator Beamline Monochromator Upgrade.* A new water-cooled, 6-position interferometrically controlled grating chamber was installed at beamline X1B. At present, four new gratings (300, 600,1200, and 1600 lines/mm) covering the soft x-ray photon energy range from 100eV to 1600eV were outfitted. Resolving power of more than 10,000 was achieved. The high energy resolution and extended energy range provided by the new monochromator will benefit greatly all the experimental programs using the beamline, including soft x-ray resonant scattering, emission, and imaging.
  - ► *Ultra-high Vacuum Compatible Soft X-ray Scattering End Station.* A novel resonant soft x-ray scattering instrument has become operational at the X1B undulator beamline. The instrument combines the element and electronic state specificity of soft x-ray spectroscopy with x-ray diffraction, which enables the direct probing of intrinsic inhomogeneities in strongly correlated electron systems and nanoscale magnetic systems. For example, the spatial distribution of the doped holes in an epitaxial film of oxygen-doped $La_2CuO_{4+\delta}$ was determined recently using this instrument for the first time.

- *New End Station for Soft X-ray Coherent Scattering and Imaging.* To facilitate nanoscience research, imaging techniques with nanometer spatial resolution are needed. A new end station for soft x-ray coherent scattering and imaging was designed and constructed. It will be used to develop two and three dimensional diffraction imaging and tomography with tens of nanometer spatial resolution for nano-magnetic, organic, and biological systems

- The Stanford Synchrotron Radiation Laboratory
  - *Accelerator Modeling Toolbox Developed.* An interactive accelerator modeling software tool called Accelerator Toolbox has been developed that greatly increases productivity and flexibility in interactive computer modeling. By making the Accelerator Toolbox available to other laboratories via the web, a community of users has grown who share code and experience in solving similar accelerator modeling problems.
  - *High Power X-ray Monochromators Deployed.* X-ray monochromators with high-efficiency crystal cooling utilizing liquid nitrogen have been designed, fabricated and successfully installed on four high-power wiggler beam lines. Their enhanced performance under high heat loads has already resulted in significant improvements in the stability and throughput of these beam lines. These monochromators and others to be implemented will be critical elements in obtaining the ultimate performance available from the SPEAR3 accelerator when it becomes operational in 2004.
  - *Improved Microfocusing System for X-ray Microspectroscopy.* Improved tapered metal capillary focusing optics with a 5 micrometer focal spot have been successfully integrated into a new system for performing microspectroscopy measurements. These developments, which included sample scanning capabilities and software for mapping the chemical states of the elemental distributions, will ultimately be propagated to a number of beam lines to enable microspectroscopy research in biology, materials sciences, and environmental sciences.
  - *Major Progress in SSRL Beamline Upgrade Program.* A beam line upgrade program is underway whose goal is to bring all SSRL beam lines to optimal performance with SPEAR3 running at 500 mA. Improvements to date include high-stability mirror systems for the insertion device-based beam lines, new permanent magnet wigglers, a high-resolution soft x-ray monochromator, and new liquid nitrogen-cooled two-crystal x-ray monochromators. Some upgrades have been completed during the current SPEAR2 operations phase, bringing higher performance to the ongoing user research programs.

- The Intense Pulsed Neutron Source
  - *Upgrades of IPNS Instruments.* 1) A project was initiated for the development of a large-aperture, magnetic bearings-suspension, high-resolution chopper system for the HRMECS and LRMECS chopper spectrometers at IPNS. 2) A new scattering chamber for the Small Angle Diffractometer is being installed. It will improve the data quality and collection rates. 3) Through an IPNS/RIKEN collaboration a neutron compound refractive lens based on an assembly of MgF_2 single-crystal prism elements was tested on the POSY II beamline for focusing cold neutrons.
  - *Outstanding Operations at IPNS Continues.* For the fifth consecutive year, IPNS has exceeded its goal of offering at least 95% reliable operations. This includes delivering the 7 billionth pulse to the target. This accomplishment constitutes more pulses delivered to target than any other

pulsed neutron source in the US. In May of 2002, IPNS was designated a Nuclear Historic Landmark by the American Nuclear Society.

- *IPNS Hosts the National Neutron and X-Ray Scattering School.* During the two-week period of August 12-23, 2002, Argonne National Laboratory once again hosted the National School on Neutron and X-Ray Scattering. The school continues to attract outstanding graduate students and post-doctoral appointees with 160 applications for the 60 positions available in 2001.

- The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center
  - *Four Instruments Commissioned.* Four world-class neutron scattering instruments completed commissioning and entered the user program. These are HIPPO, SMARTS, Protein Crystallography Station, and Asterix. New data acquisition systems were completed and installed on the new instruments.
  - *Pharos Rebuilt.* Inelastic chopper spectrometer Pharos enjoyed substantial upgrades, including detectors on the wide-angle bank, commissioning of the new vacuum system, new data acquisition electronics and computer system, and a new chopper control system. Pharos took its first data and accepted its first users since 1997.
  - *Designed and Installed New Robust Target System, Mark II.* Using a simplified Monte Carlo model, the new target improves cooling in Mark I moderator and upper target. A beryllium reflector replaced the lead reflector, cooling was simplified, and cadmium decoupling in the reflector was removed for more robust operation. The target received first beam on July 8, 2002, as scheduled.
  - *Completed Basis for Interim Operation for actinide experiments.* The new authorization basis enabled over a dozen plutonium and uranium studies to be completed and restores an important capability to the DOE science complex.
  - *New Shutters and Interlocks.* Greater safety, reliability and performance were achieved by replacement of Personnel Access Control Systems interlocks on all flight paths, replacement of all mercury reservoirs and plumbing, and installation of a new fire detection system. Two new mechanical shutters and over 300 tons of shielding were installed to enable two new flight paths for new instruments.
  - *Proton Storage Ring Instability Tamed.* A series of successful Proton Storage Ring development tests confirmed that the "e-p instability" could be controlled at accumulated charge levels approaching 10 μC, well above the goal of 6.7μC.

- The High Flux Isotope Reactor
  - *Major Refurbishment of Reactor Vessel Completed.* The refurbishment of the pressure vessel's internal components included replacing the permanent and semipermanent beryllium reflectors and their support structures. This required maintenance was accomplished without incident and will support the substantial upgrade in neutron scattering research capabilities at HFIR.
  - *HFIR Cooling Tower Replaced.* The original 36-year-old wooden cooling tower had significant structural degradation, required excessive maintenance, and could no longer reliably support reactor operations. The more efficient replacement tower will cost less to operate and should last for the remaining life of HFIR.

- *New Thermal Neutron Beam Tubes Installed at HFIR.* The new beam tubes, which replaced existing tubes that had reached their end of life, are capable of providing more neutrons to a greater number of scientific instruments.
- *Operational Readiness Review (ORR).* The ORR at HFIR was the first to be conducted at any Category 1 DOE facility since the current ORR guidance was issued. The ORR included a comprehensive restart plan, independent-contractor and DOE reviews, and close coordination with DOE headquarters and the site office. Reactor operations were resumed on December 18, 2001
- *Facility Improvements Support Neutron Scattering Instrument Upgrades.* New monochromator drums were fabricated for the triple-axis spectrometers at HB-1, 2, and 3. A shielding tunnel and neutron guide were fabricated for HB-2, where a 20-cm-diameter beam tube was installed with beryllium inserts to support four beam lines. The resulting beam intensity is expected to be three times that of the original design for some of the instruments.

Subprogram Goals

Build leading research programs in materials sciences and engineering and provide world-class, peer-reviewed research results cognizant of DOE needs as well as the needs of the broad scientific community.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	As part of the continuing, high-level review of the management processes and the quality, relevance, and national and international leadership of BES programs, review the materials sciences and engineering activities using a BESAC-chartered Committee of Visitors.	Implement recommendations of the BESAC-chartered Committee of Visitors for the materials sciences and engineering activities.
The ongoing BES superconductivity area was evaluated using a research workshop entitled "High Temperature Superconductivity" on April 6-8, 2002, in San Diego, CA with the goal of directing the activities toward international leadership and relevance to emerging technologies. [Met Goal]	Evaluate the following ongoing efforts using Basic Energy Sciences research workshops with the goal of directing the activities toward international leadership and relevance to emerging technologies: photovoltaics, radiation effects, and materials synthesis and processing. Publish results and continue to structure BES programs per results.	Evaluate energy storage efforts using Basic Energy Sciences research workshops with the goal of directing the activities toward international leadership and relevance to emerging technologies. Publish results and continue to structure BES programs per results.

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
A BESAC-chartered workshop on "Biomolecular Materials" held January 13-15, 2002 in San Diego, CA examined future research directions in biomolecular or biomimetic materials designed for nonmedical applications whose structure or synthesis is derived from or is inspired by biology. [Met Goal]		Implement recommendations and new program directions in materials sciences and engineering that resulted from the BESAC-chartered workshop on "Basic Research Needs to Assure a Secure Energy Future."
	Initiate R&D for the Transmission Electron Achromatic Microscope (TEAM).	Complete R&D for TEAM.

Enable U.S. leadership in nanoscale science, allowing the atom-by-atom design of materials and integrated systems of nanostructured components having new and improved properties for applications as diverse as high-efficiency solar cells and better catalysts for the production of fuels.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
PED was begun on three Nanoscale Science Research Centers. PED funding was obligated to LBNL (6% complete), ORNL (60% complete), and SNL (24% complete). [Met Goal]	Begin construction of one Nanoscale Science Research Center scheduled for completion in FY 2006, meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheet. Continue PED on two other Nanoscale Science Research Centers.	Continue construction of one Nanoscale Science Research Center scheduled for completion in FY 2006 and begin construction on two others scheduled for completion in FY 2007, meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheet. Initiate PED activities to establish construction baselines on one additional Nanoscale Science Research Center. Begin MIE on the fifth and final Nanoscale Science Research Center.
	Establish instrument suites and identify fabrication capabilities for the Center for Nanophase Materials Sciences at ORNL and the Center for Nanophase Materials at ANL based upon user community input at national workshops.	Establish instrument suites and identify fabrication capabilities for the Molecular Foundry at LBNL and the Center for Integrated Nanotechnologies at SNL/LANL based upon user community input at national workshops.

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
		Establish user programs for the Nanoscale Science Research Centers prior to the commissioning of the new facilities.
Conducted a joint BESAC- and ASCAC-sponsored Workshop on Theory and Modeling in Nanoscience (May 10-11, 2002) to identify opportunities and challenges in theory, modeling and simulation that can accelerate discovery and understanding at the nanoscale. [Met Goal]		
In FY 2002, there were 27 new grants awarded to universities and 6 projects at DOE laboratories were initiated in selected materials sciences and engineering areas of nanoscale science, engineering, and technology. [Met Goal]		

Develop advanced research instruments for x-ray diffraction, scattering, and imaging to provide diverse communities of researchers with the tools necessary for exploration and discovery in materials sciences and engineering, chemistry, earth and geosciences, and biology.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	Select and begin upgrade/fabrication of at least two instruments at the BES synchrotron light sources, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis.	Continue fabrication of instruments at the BES synchrotron light sources, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis.
	Establish laboratory to laboratory agreement between SLAC and DESY (Germany) for joint R&D on 1 angstrom free-electron lasers.	

Restore U.S. preeminence in neutron scattering research, instrumentation, and facilities to provide researchers with the tools necessary for the exploration and discovery of advanced materials.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	Select and begin upgrade/fabrication of two to four instruments at the BES neutron scattering facilities, based on peer review of submitted proposals, to keep the facilities at the forefront of science. At least $5,000,000 will be awarded for fabrication of new instruments for the Spallation Neutron Source.	Continue fabrication of instruments at the BES neutron scattering facilities, based on peer review of submitted proposals, to keep the facilities at the forefront of science. At least $5,000,000 of continued funding will be made available for fabrication of new instruments for the Spallation Neutron Source.

Manage facility operations and construction to the highest standards of overall performance using merit evaluation with independent peer review.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
Construction of the Spallation Neutron Source (SNS) met the cost and schedule milestones within 10 percent of the baselines in the construction project data sheet, project number 99-E-334. At the end of FY 2002, construction of the SNS was 47 percent complete. [Met Goal]	Continue construction of the Spallation Neutron Source (SNS) meeting the cost and schedule milestones within 10 percent of the construction project data sheet baselines. At the end of FY 2003, construction of the SNS will be 61 percent complete.	Continue construction of the Spallation Neutron Source (SNS) meeting the cost and schedule milestones within 10 percent of the construction project data sheet baselines. At the end of FY 2004, construction of the Spallation Neutron Source will be 80 percent complete.
The upgrade of the SPEAR storage ring at the Stanford Synchrotron Radiation Laboratory met the cost and schedule milestones within 10 percent. At the end of FY 2002, the upgrade was 70% complete. [Met Goal]	Complete the upgrade of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory), maintaining cost and schedule within 10 percent of baselines.	

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
	Begin PED of the Linac Coherent Light Source at the Stanford Linear Accelerator Facility. At the end of FY 2003, PED will be 18 percent complete.	Continue PED of the Linac Coherent Light Source at the Stanford Linear Accelerator Facility. At the end of FY 2004, PED will be 40 percent complete.
		Implement recommendations from FY 2003 BESAC-chartered subpanel on future directions in next-generation light sources.
		As part of the continuing, high-level review of the management processes and the quality, the relevance, and the national and international leadership of BES programs, review the BES management of the operations of the major x-ray and neutron scattering facilities using a BESAC-chartered Committee of Visitors.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Materials Sciences and Engineering Research	232,001	260,722	263,759	+3,037	+1.2%
Facilities Operations	268,032	274,118	290,004	+15,886	+5.8%
SBIR/STTR	0	12,737	13,948	+1,211	+9.5%
Total, Materials Sciences and Engineering	500,033	547,577	567,711	+20,134	+3.7%

Detailed Program Justification

(dollars in thousands)

	FY 2002	FY 2003	FY 2004
Materials Sciences and Engineering Research	**232,001**	**260,722**	**263,759**
▪ **Structure and Composition of Materials**	**35,168**	**36,391**	**36,646**

This activity supports basic research in the structure and characterization of materials, the relationship of structure to the behavior and performance of materials, predictive theory and modeling, and new materials such as bulk metallic glasses and nanophase materials. 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 network-interfaced centers contain a variety of highly specialized instruments to characterize localized atomic positions and configurations, chemical gradients, interatomic bonding forces, etc.

The properties and performance of materials used in all areas of energy technology depend upon their

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the structural characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g. dislocations, grain boundaries, magnetic domain walls and precipitates, etc.) 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, etc.

In FY 2004, major activities will be responsive to the need for 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.

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

	FY 2002	FY 2003	FY 2004
▪ **Mechanical Behavior and Radiation Effects**............................	**14,530**	**14,530**	**14,510**

This activity supports basic research to understand the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties. The objective is to understand at the atomic level the relationship between mechanical properties and defects in materials, including defect formation, growth, migration, and propagation. In the area of mechanical behavior, the research aims to build on this atomic level understanding in order to develop predictive models for the design of materials having prescribed mechanical behavior, with some emphasis on very high temperatures. In the areas of radiation effects, the research aims to advance atomic level understanding of amorphization mechanisms (transition from crystalline to a non-crystalline phase) to predict and suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by such techniques 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 2004, major activities will include continued development of experimental techniques and methods for the characterization of mechanical behavior, the development of a universal model for mechanical behavior that includes all length scales from atomic to nanoscale to bulk dimensions, and advancement of computer simulations for modeling behavior and radiation induced degradation.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

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

▪ **Physical Behavior of Materials**...	**15,735**	**15,735**	**15,713**

This activity supports basic research at the atomic and molecular level to understand, predict, and control physical behavior of materials by developing rigorous 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; diffusion and the transport of ions in ceramic electrolytes for improved performance 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 2004, major activities will continue fundamental studies of corrosion resistance and surface degradation; semiconductor performance; high-temperature superconductors; and the interactions, and transport of defects in crystalline matter.

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**	**14,497**	**18,595**	**18,570**

This activity supports basic research on understanding and developing innovative ways to make materials with desired structure, properties, or behavior. Examples include materials synthesis and processing to achieve new or improved behavior, for minimization of waste, and for hard and wear resistant surfaces; high-rate, superplastic forming of light-weight metallic alloys for fuel efficient vehicles; high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel efficient and low-pollutant engines; non-destructive analysis for early warning of impending failure and flaw detection during production; response of magnetic materials to applied static and cyclical stress; plasma, laser, charged particle beam surface modification to increase corrosion resistance; and processing of high-temperature, intermetallic alloys.

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 unique, research-grade materials that are not otherwise available to academic, governmental, and industrial research communities.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

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 2004, major activities will include continued support for research on nanoscale synthesis and processing. The mechanical properties of materials change dramatically as the grain size in polycrystalline materials approaches the nanometer scale. At conventional grain sizes, a gain in strength of a material typically results in a loss in both ductility and fracture toughness resulting in a brittle material; however, by using nanocomposites and understanding deformation physics, it should be possible to make materials that are strong, tough (resistant to impact fracture) and ductile. There is also great need for nanoparticles of uniform size, composition, and surface stability because experiments have shown that fracture toughness may undergo a profound increase as the grain size falls below 10 to 50 nm in high-temperature structural ceramics. These materials might be used in advanced fuel efficient engines, turbines, and machine cutting tools.

Capital equipment includes furnaces, lasers, processing equipment, plasma and ion sources, and deposition equipment.

▪ **Engineering Research**	**16,464**	**16,480**	**16,457**

This activity focuses on nanotechnology and microsystems; multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. In the area of nanoscience, work focuses on nanomechanics and nano to micro assembly, networks of nano sensors, hybrid microdevices, energy transport and conversion, nanobioengineering, nucleation and nanoparticle engineering issues.

In FY 2004, efforts will continue in select topics of nano-engineering; predictive non-destructive evaluation of structures coupled with micromechanics and nano/microtechnology; multi-phase flow and heat transfer; system sciences, control, and instrumentation; and data and engineering analysis.

▪ **Neutron and X-ray Scattering**	**35,032**	**54,277**	**54,277**

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. Neutron and x-ray scattering, together with the electron scattering probes supported under Structure and Composition of Materials, are the primary tools for characterizing the atomic, electronic and magnetic structures of materials.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

Of these funds, $5,000,000 is provided in FY 2003 and in FY 2004 for the development of instrumentation to exploit the scientific potential of the SNS facility. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories and the SNS based on scientific merit and importance to users from universities, industries, and government laboratories.

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

- **Experimental Condensed Matter Physics** **33,667** **38,020** **37,968**

This activity supports condensed matter and materials 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. 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 will be made under extreme conditions of temperature, pressure, and magnetic field - especially with the availability of the 100 Tesla pulsed field magnet at LANL.

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 in National Nuclear Security Administration (NNSA) (photoemission, positron research, and electronic and optical materials). In addition, it supports, more fundamentally, several DOE technologies and the strategically important information technology and electronics industries through its results in the fields of semiconductor physics, ion implantation and electronics research; the petroleum recovery efforts of Fossil Energy and the clean-up efforts of Environmental Management (EM) programs through research on granular materials and on fluids; through EE research on advanced materials and magnets; energy conservation efforts through research on ion implantation, ultra-hard materials, superconductivity, thermoelectrics, and power source component materials; and NNSA through research on advanced laser crystals and weapons-related materials.

In FY 2004, 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 become possible. Also thermodynamic properties, including collective phenomena and phase transitions such as ferromagnetism, ferroelectricity, and superconductivity can change when structures contain a small 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.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

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

▪ **Condensed Matter Theory**...	**18,007**	**18,007**	**17,982**

This activity supports basic research in theory, modeling, and simulations, and it complements the experimental work. The 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, which may be described by bulk properties plus the effects of interfaces and lattice defects.

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 2004, this activity will provide support for theory, modeling and large-scale computer simulation to explore new nanoscale phenomena and the nanoscale regime. Also supported is the Computational Materials Sciences Network for studies of such topics as polymers at interfaces; fracture mechanics - understanding ductile and brittle behavior; microstructural evolution and microstructural effects on mechanics of materials; magnetic materials; modeling oxidation processes at surfaces and interfaces; and excited state electronic structure and response functions.

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

▪ **Materials Chemistry**..	**27,287**	**29,602**	**29,563**

This activity supports basic research on the chemical properties of materials to understand the effect of chemical reactivity on the behavior of materials and to synthesize new chemical compounds and structures from which better materials can be made. Research topics supported include solid state chemistry, surface chemistry, polymer chemistry, crystallography, synthetic chemistry, and colloid chemistry. Also supported are investigations of novel materials such as low-dimensional, self-assembled monolayers; polymeric conductors; organic superconductors and magnets; complex fluids; and biomolecular materials. The research employs a wide variety of experimental techniques to characterize these materials, including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance, and x-ray and neutron reflectometry. The activity also supports the development of new experimental techniques, such as high-resolution magnetic resonance imaging without magnets, neutron reflectometry, and atomic force microscopy of liquids.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

The research underpins many technological areas, such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics, and environmental chemistry. New techniques for fabrication of nanocrystals, such as a unique inverse micellar process, make possible the efficient elimination of dangerous chlorinated organic and phenolic pollutants (e.g., PCPs). Research on solid electrolytes has led to very thin rechargeable batteries that can be recharged many more times than existing commercial cells. Research on chemical vapor deposition (CVD) continues to impact the electronics industry. The development of synthetic membranes using biological synthesis may yield materials for separations and energy storage, and research on polymers may lead to light-weight structural materials which can be used in automobiles and thereby providing substantial savings in energy efficiency.

In FY 2004, work will continue on the systematic and parallel patterning of matter on the nanometer scale. There are many powerful approaches to patterning on the nanoscale that are fundamentally serial in nature, for instance, atom manipulation using scanning probe tips or electron beam lithography. The research in this activity will focus on methods to prepare macroscopic quantities of nanoscale components in complex, designed patterns, using techniques of self assembly.

Capital equipment is provided for such items as chambers to synthesize and grow new materials, nuclear magnetic resonance and electron spin resonance spectrometers, lasers, neutron reflectometers, x-ray beamlines, and atomic force microscopes.

	FY 2002	FY 2003	FY 2004
▪ **Experimental Program to Stimulate Competitive Research**	**7,679**	**7,685**	**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 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 2002	FY 2003 Estimate	FY 2004 Estimate
Alabama	814	375	815
Alaska[a]	0	0	0
Arkansas	205	65	140
Hawaii[b]	0	0	0
Idaho	0	60	0
Kansas	802	615	560
Kentucky	611	471	355
Louisiana	130	130	0
Maine	0	0	0
Mississippi	589	535	535
Montana	580	465	515
Nebraska	475	300	300
Nevada	543	325	250
New Mexico[b]	0	0	0
North Dakota	0	55	0
Oklahoma	204	65	140
Puerto Rico	435	435	375
South Carolina	558	120	140
South Dakota	0	0	0
Vermont	857	585	857
West Virginia	794	525	360
Wyoming	31	65	0
Technical Support	51	400	100
Other	0	2,094 [c]	2,231 [c]
Total	7,679	7,685	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 2003 and FY 2004 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**	**2,000**	**2,000**	**2,000**

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

▪ **Linac Coherent Light Source (LCLS)**	**1,500**	**0**	**2,000**

Research and development (R&D) funds are provided to support the physics design of several key LCLS components: the radiofrequency 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**	**1,160**	**100**	**400**

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 (TMF) located at LBNL, and the Center for Integrated Nanotechnologies (CINT) located at Sandia National Laboratories.

▪ **SPEAR3 Upgrade**	**8,300**	**9,300**	**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.

▪ **Advanced Light Source Beamline**	**975**	**0**	**0**

This beamline is a major item of equipment with a total estimated cost of $6,000,000 that will provide capabilities for surface and interfacial science important to geosciences, environmental science, and aqueous corrosion science. It was funded jointly by the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

	FY 2002	FY 2003	FY 2004
	(dollars in thousands)		
▪ **The Center for Nanophase Materials**	**0**	**0**	**10,000**

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 Nanophase Materials at Argonne National Laboratory. The instrumentation will be contained in a new building, which is being constructed by the State of Illinois for the Center at a cost of $36,000,000 and which will be dedicated to the Center operations. The building will be appended to the Advanced Photon Source. Included within the Center's instrument suite will be an x-ray nanoprobe beamline at the Advanced Photon Source. This beamline will be the highest spatial resolution instrument of its kind in the world, which will permit nondestructive examination of magnetic, electronic, and photonic materials important both for basic science and as foundations for future nanotechnologies. The Center will build on ANL's recognized strengths in magnetism, superconductivity, and novel materials with "spintronic" functionality.

	FY 2002	FY 2003	FY 2004
Facilities Operations	**268,032**	**274,118**	**290,004**
▪ **Operation of National User Facilities**	**268,032**	**274,118**	**290,004**

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.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Facilities			
Advanced Light Source	37,674	39,561	40,917
Advanced Photon Source	88,880	91,291	94,500
National Synchrotron Light Source	34,611	35,893	37,250
Stanford Synchrotron Radiation Laboratory	21,594	22,673	26,400
High Flux Isotope Reactor	38,697	36,854	38,357
Radiochemical Engineering Development Center	6,606	6,712	6,712
Intense Pulsed Neutron Source	15,826	17,015	17,200
Manuel Lujan, Jr. Neutron Scattering Center	9,044	9,678	10,271
Spallation Neutron Source	15,100	14,441	18,397
Total, Facilities	268,032	274,118	290,004

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**12,737**	**13,948**

In FY 2002, $14,363,000 and $862,000 were transferred to the SBIR and STTR programs, respectively. The FY 2003 and FY 2004 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

	FY 2002	FY 2003	FY 2004
Total, Materials Sciences and Engineering	**500,033**	**547,577**	**567,711**

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Materials Sciences and Engineering Research	
▪ Increase for structure and composition of materials research for the design of components for an aberration corrected transmission electron microscope	+255
▪ Decrease in mechanical behavior and radiation effects research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-20
▪ Decrease in physical behavior of materials research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%	-22
▪ Decrease in synthesis and processing science research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-25

	FY 2004 vs. FY 2003 ($000)
▪ Decrease in engineering research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-23
▪ Decrease in condensed matter physics research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%	-52
▪ Decrease in condensed matter theory research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%	-25
▪ Decrease in materials chemistry research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-39
▪ Decrease in experimental program to stimulate competitive research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-12
▪ Increase for research and development for the Linac Coherent Light Source.	+2,000
▪ Increase for MIE for the ANL Center for Nanophase Materials	+10,000
▪ Increase for other project costs per schedule associated with the Nanoscale Science Research Centers	+300
▪ Decrease due to completion of the SPEAR3 Upgrade	-9,300
Total, Materials Sciences and Engineering Research	+3,037
Facilities Operations	
▪ Increase for operations for the Advanced Light Source.	+1,356
▪ Increase for operations for the Advanced Photon Source.	+3,209
▪ Increase for operations for the National Synchrotron Light Source	+1,357
▪ Increase for operations for the Stanford Synchrotron Radiation Laboratory.	+3,727
▪ Increase for operations for the High-Flux Isotope Reactor	+1,503
▪ Increase for operations for the Intense Pulsed Neutron Source.	+185
▪ Increase for operations for the Manuel Lujan, Jr. Neutron Scattering Center	+593
▪ Increase in the Spallation Neutron Source Other Project Costs per FY 2004 project datasheet	+3,956
Total, Materials Sciences and Engineering Facilities Operations.	+15,886
SBIR/STTR	
▪ Increase in SBIR/STTR funding because of an increase in operating expenses and an increase in STTR percentage from .15% to .3%	+1,211
Total Funding Change, Materials Sciences and Engineering	+20,134

Chemical Sciences, Geosciences, and Energy Biosciences

Mission Supporting Goals and Measures

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. 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. Ultimately, this research 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.

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. This work 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.

In the area of bioscience, 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 Nation's primary support for homogeneous and heterogeneous catalysis, photochemistry, radiation chemistry, separations and analysis, and gas-phase chemical dynamics.

Selected FY 2002 Research Accomplishments:

- *Catalytic Chemistry of Gold Nanoparticles.* Gold spheres of 2.7 nm diameter supported on titanium oxide are able to oxidize carbon monoxide, and spheres of 2.4 nm diameter are able to activate oxygen from air and insert it into propene readily and very selectively. Yet bulk gold metal is inert, and particles of slightly smaller or larger diameter than those cited are also unreactive or unselective. Using a variety of spectroscopic and chemisorption techniques, atomic-resolution microscopy, and theoretical electronic structure calculations, it was shown that decreasing metal particle size provokes changes in the electronic structures of gold and titanium oxide such that the particles are able to acquire a partial charge. Those variations are shown to decrease the binding energy of gold on titanium oxide (and thus alter the morphology of the clusters), as well as increase the binding energy of reactants such as oxygen, carbon monoxide, and propene to gold. The results explain why gold clusters are active and selective oxidation catalysts and provide a semiquantitative framework to predict catalytic reactivity on the basis of electronic structure of metal clusters.

- *New Nanoporous Catalysts Developed.* Nanocrystalline materials possess unique properties and offer great promise for promoting selected physical and chemical processes. Crystalline films of magnesium oxide that consist of tilted arrays of filaments attached to a flat substrate have been synthesized by impinging a magnesium atom beam in an oxygen background toward a surface off-normal by 70° to 85°. The individual filaments are thermally stable, highly ordered and porous, and contain enormous numbers of binding sites in comparison to a magnesium oxide flat surface deposited on a substrate. The high surface area (~1,000 m^2/g) and high density of binding sites potentially render these nanoporous materials extraordinary catalysts.
- *Multidimensional Catalyst Arrays.* Studies of the affects of particle spacing on the reactivity of catalysts has been hampered by the inability to produce uniform nanoparticles that are regularly distributed in a supporting matrix. Recent work shows that two- and three-dimensional arrays of platinum nanoparticles are achievable. Two-dimensional arrays of platinum supported on 4-inch silicon wafers were produced using electron beam lithography and spacer photolithography. The latter technique permits variation of particle size from 600 nm to 10 nm. More recently, three-dimensional arrays of 2-5 nm platinum nanoparticles of vary narrow size distribution were prepared, and the resulting x-ray and electron diffraction patterns are typical of crystallinity, hence regularity. The results significantly enhance enable the production of designer catalysts and will answer fundamental questions in catalysis.
- *Nanostructured Anodes.* There is considerable interest in tin/lithium anodes for high-energy electrochemical storage systems because, in principle, they can deliver substantially more storage capacity than carbon based lithium ion batteries. However, the tin-based anode functions by reversibly alloying lithium into the tin, and a very large volume expansion occurs when lithium is alloyed (as much as 300 percent). As a result, the tin based anode system typically has poor cycle life because the volume expansion and contraction during cycling causes the anode to self-destruct. New research has shown that nanostructured tin/lithium anodes prepared via a membrane template method do not suffer from this loss of cycle life, even after 1,400 charge discharge cycles. The nanostructured electrode gives good cycle life because the absolute volume change for a nanofiber is correspondingly small and because the brush like configuration of nanofibers provides room to accommodate the volume expansion.
- *Nanometer-Scale Faceting of Metals, a Means to Control Reactivity.* Bimetallic catalysts are providing new insights into chemical reactivity. Upon annealing at elevated temperatures, the atomically rough, "unstable" surfaces were observed to undergo massive reconstruction at the nanometer scale, in some instances leading to the formation of surface alloys. These structural rearrangements were accompanied by corresponding changes in electronic structure, morphology, and catalytic activity. Time-dependent, atomically resolved images allowed the measurement of the rate of facet growth and of their reconstruction in the presence of adsorbates such as sulfur and oxygen. Catalytic activity was found to dramatically depend on the composition, structure, size, and shape of the facets exposed under reaction conditions.

- *Organic Semiconductors.* Molecular and polymeric semiconductors are very important organic compounds that have the potential to replace inorganic semiconductors for applications in photoelectrochemical and photovoltaic cells for solar energy conversion of sunlight to electricity and solar fuels (hydrogen, methane, and alcohols). Photoconversion devices based on organic semiconductors could be much less expensive and easier to produce and process because of the present vast technology available for polymer and molecular processing into continuous thin films and sheets. Doping the molecular semiconductors to produce the required n-type and p-type electrical conductivity to create p-n junctions has been problematic as the dopant has not become part of the molecular or atomic structure of the compound. Recently, scientists successfully doped molecular semiconductors and increased the conductivity by five orders of magnitude.
- *Long-Lived Charge Separation in a Novel Artificial Photosynthetic Reaction Center.* Fullerenes and porphyrins have molecular architectures that are ideally suited for photochemical conversion and storage of solar energy. Their use as three-dimensional electron acceptors holds great promise because of their small reorganization energy in electron transfer reactions that can significantly improve light-induced charge-separation processes. Recent research indicated a 24 percent efficient charge-separation within a molecular tetrad. In this linear array, a light harvesting antenna assembly composed of two porphyrins and a fullerene-ferrocene photosynthetic reaction-center mimic were integrated into a single molecule. The 380 millisecond lifetime of the spatially-separated and high energy radical pair, a product of sequential short-range energy and electron transfer reactions, enters a time domain that has never been achieved in an artificial reaction center.
- *New Technique for Detection of Impact Ionization in Semiconductors.* The thermodynamic conversion efficiency with which solar radiant energy can be converted to electricity or to stored chemical energy in solar-derived fuels is limited by the energy loss of high energy electrons and positive holes created by the absorption of high energy solar photons in the photoconversion device. The thermodynamic efficiency limit can be more than doubled if the high energy photons can be used to create additional photogenerated current through a process called impact ionization. For the first time, scientists have demonstrated a contactless, optical method to detect impact ionization in semiconductors useful for solar photoconversion. The method is based on femtosecond time-resolved visible pump-infrared probe spectroscopy, and can be used to study impact ionization in colloidal semiconductor quantum dots where electrical contact to the colloidal particles is not possible. Impact ionization in semiconductor quantum dots is expected to be greatly enhanced.
- *Gas-Phase Chemistry of Actinide Ions.* The studies of gas-phase reactions of ions provide important insights into fundamental chemistry. Such studies have previously been limited to transition metal ions and to thorium and uranium in the actinide series; however, recent work has expanded this approach to the radioactive actinides, which cannot easily be studied by conventional techniques. One type of reaction that has been particularly enlightening involves the metal- or metal-oxide-catalyzed removal of hydrogen from alkene hydrocarbons. In these alkene dehydrogenation reactions, the neptunium ion is highly reactive, the plutonium ion is significantly less reactive, and the americium ion is essentially unreactive. This provides clear evidence that the 5f electrons of the actinides beyond neptunium are inert in these organometallic reactions. Results for the actinide oxide ions have also been illuminating, revealing a decrease in reactivity between uranium oxide ions and heavier actinide-oxide ions. The role of 5f electrons in bonding is central issue in contemporary actinide science, and these results provide experimental evidence for a change in the bonding nature

of the actinide 5f electrons in molecular compounds, ranging from being chemically active for the early members of the series to being inert for the actinides beyond neptunium.

- *Lattice Disorder and f-electrons: Evidence For a New State of Matter.* An important question is the nature of the non-superconducting high-temperature superconducting (HTSC) ground state from which superconductivity arises. Intermetallic alloys containing *f*-electron elements, in which superconductivity is absent or is easily suppressed, allow one to explore this question. Like HTSCs, *f*-electron intermetallic alloys often behave as "non-Fermi liquids" (NFL), so named because they are not consistent with Fermi liquid theory, which, until recently, has been the basis for explaining the properties of metals. Of specific interest is how the atoms surrounding an *f*-electron atom, and how disorder in their arrangement, affect magnetic and conducting properties. A recent study of these arrangements in the NFL compound UCu_4Pd showed that significant lattice disorder exists. Although such disorder can produce NFL behavior within a Fermi liquid model, the study showed that there is insufficient disorder for the model to match the measured magnetic and conductivity data. That is, the system acts as though it is more disordered than it actually is. These results strongly imply that lattice disorder precipitates NFL behavior in this material, perhaps by amplifying the effect of the disorder, and thereby the possibility of a new type of metallic ground state.
- *Cellulose Biosynthesis.* The detection and isolation of cellulose synthase genes is driving new efforts to understand how cellulose acquires its structural characteristics in hopes of eventually devising methods of tailoring these characteristics to facilitate its use as a renewable resource. Scientists have provided a key piece of information in the biochemical dissection of the three steps of cellulose synthesis: 1) initiation of the sugar chain; 2) adding sugars to the growing chain; and 3) stopping the process at a predetermined length. A single copy of a cellulose synthase gene was introduced into yeast cells that do not normally make cellulose. The result was the formation of a specific lipid-sugar compound that serves as a primer for subsequent chain growth. Understanding the critical steps in the synthesis of cellulose, the most abundant biomolecule, will lead to understanding the function of plant cell walls and to engineering modified renewable resources.
- *Boron in Plant Cell Walls.* Research has confirmed the role of the element boron in the growth and development of plant cell walls. Over 90 percent of a plant's boron is associated with the cell wall, and boron deficiency leads to stunted plants with malformed and brittle leaves. Arabidopsis thaliana mutants with a small change in the structure of a major type of cell wall carbohydrate show the same characteristics but can be rescued by feeding with excess borate. This defect was shown to reduce the plant's ability to bind the borate that is needed to form and stabilize the cross-linked cell wall. Future mechanistic studies relating borate-carbohydrate crosslinking to physiological growth could lead to improved strategies for the development and production of renewable biomass resources.
- *Naturally Occurring Organochlorine Compounds.* Organochlorine molecules are commonly observed in natural soils and have been attributed to pollution from manmade sources. Natural organic matter, such as humic and fulvic acid, in the shallow subsurface is both universal and little understood. It has no fixed stoichiometry or structure, cannot be crystallized, and is famously difficult to characterize reproducibly. Synchrotron x-ray spectroscopy has been used to document changes in the chemical state of chlorine in humic materials. This research confirmed the startling conclusion that natural organochlorine compounds are common in soil and that there is a net transfer of chlorine from inorganic to organic forms with common weathering. Abundant catalytic

peroxidase facilitates the chlorination of natural aromatic organics. These results add strong support to the hypothesis that chlorination of organic compounds in humic materials is widespread, and may explain the puzzling organochlorine concentrations found in otherwise unpolluted environments. Accurately understanding natural conditions is critical in identifying and taking action to correct man-made problems.

- *Quantum Degenerate Fermi Gases.* A new theoretical formulation predicts an unusually high critical temperature for the onset of superfluidity in a gas of fermionic potassium atoms. This new form of quantum matter, which lies between high-temperature superconductors and systems that undergo Bose-Einstein condensation should soon be achievable experimentally using optical traps. The ultimate goal of these experiments is to achieve Cooper pairing, in which pairs of fermionic atoms "condense" and occupy the lowest quantum states available to the ensemble of trapped atoms. Such an accomplishment would permit studies of the underlying mechanism of superconductivity.

Selected FY 2002 Facility Accomplishments:

- The Combustion Research Facility
  - *Stagnation-flow Reactor Designed to Probe High-temperature Chemistry.* Chemically reacting flows at interfaces are an important class of processes occurring in combustion, catalysis, thin film formation, and materials synthesis. An innovative stagnation-flow reactor with access for optical diagnostics and mass spectrometry is nearing completion and will provide a valuable tool for probing high-temperature chemistry for a broad range of industrially relevant processes.
  - *Fiber-based Laser Systems Developed.* Fiber lasers and amplifiers are unique optical sources that provide many advantages for detection of chemical and biological compounds. The CRF has established the capability to fabricate them in-house. The facility will allow the pursuit of new research in optical diagnostics and will help DOE remain at the forefront of this field.
  - *New Reactor Allows Investigation of Gasification Processes.* The design and facility modifications have been completed for a new reactor that will allow unprecedented optical access to pressurized combustion and gasification processes. This reactor will give the CRF the capability to investigate gas-phase kinetics, materials behavior, advanced diagnostic development, and solid and liquid fuel combustion chemistry and physics under pressurized conditions.

Subprogram Goals

Build leading research programs in chemical sciences, geosciences, and energy biosciences and provide world-class, peer-reviewed research results cognizant of DOE needs as well as the needs of the broad scientific community.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
As part of the continuing, high-level review of the management processes and the quality, the relevance, and the national and international leadership of BES programs, the chemical sciences activities in BES were reviewed using a Basic Energy Sciences Advisory Committee - chartered Committee of Visitors. [Met Goal]		
Conducted workshop on research opportunities and needs related to electron initiated chemistry in aqueous media. [Met Goal]		
	Sponsor a workshop on plant systems science to identify opportunities and challenges associated with the molecular level understanding of plant processes. Specifically identify opportunities at the interfaces among the biological, physical, mathematical, and computational sciences.	Implement workshop recommendations in the area of plant systems science.
		Evaluate the following ongoing efforts using Basic Energy Sciences research workshops with the goal of directing the activities toward international leadership and relevance to emerging technologies: chemical physics and fundamental chemical interactions. Publish results and continue to structure BES programs per results.
		Implement recommendations and new program directions in chemical sciences, geosciences, and biosciences that resulted from the BESAC-chartered workshop on "Basic Research Needs to Assure a Secure Energy Future."

Enable U.S. leadership in nanoscale science, allowing the atom-by-atom design of materials and integrated systems of nanostructured components having new and improved properties for applications as diverse as high-efficiency solar cells and better catalysts for the production of fuels.

Performance Indicators

Validation of results by merit review with external peer evaluation.

Validation of program directions by Basic Energy Sciences Advisory Committee.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Updated Targets	FY 2004 Targets
Conducted a joint BESAC- and ASCAC-sponsored Workshop on Theory and Modeling in Nanoscience (May 10-11, 2002) to identify opportunities and challenges in theory, modeling and simulation that can accelerate discovery and understanding at the nanoscale. [Met Goal]		
Conducted a BESAC-chartered workshop on Catalysis (May 14-16, 2002) [Met Goal]	Implement the recommendations of the Catalysis workshop by initiating multi-disciplinary, multi-institution research efforts in catalysis enabled by emerging nanoscience technologies including biosciences.	Continue implementation of the recommendations of the Catalysis workshop with continuing emphasis on multi-disciplinary approaches.
In FY 2002, there were 19 new grants awarded to universities and 6 projects at DOE laboratories were initiated in selected chemical sciences, geosciences, and energy biosciences areas of nanoscale science, engineering, and technology. [Met Goal]		

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Chemical Sciences, Geosciences, and Energy Biosciences Research	194,850	209,188	209,597	+409	+0.2%
Facilities Operations	5,377	5,805	5,967	+162	+2.8%
SBIR/STTR	0	5,022	5,350	+328	+6.5%
Total, Chemical Sciences, Geosciences, and Energy Biosciences	200,227	220,015	220,914	+899	+0.4%

Detailed Program Justification

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Chemical Sciences, Geosciences, and Energy Biosciences Research	**194,850**	**209,188**	**209,597**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**11,815**	**11,815**	**12,275**

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. This activity also supports the James R. MacDonald Laboratory at Kansas State University, a multi-investigator program and BES collaborative research center devoted to studies of collision processes involving highly charged ions.

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 2004, 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, which provides strong linkages between atomic and condensed matter physics at the nanoscale.

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

▪ **Chemical Physics Research**	**33,285**	**33,285**	**33,239**

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.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

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 and 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.

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

- **Photochemistry and Radiation Research** **26,096** **29,032** **28,973**

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 Molecular 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 2004, 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.

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 2002	FY 2003	FY 2004
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	**12,060**	**12,150**	**12,133**

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.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Metabolic Regulation of Energy Production**	**19,130**	**19,224**	**19,195**

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, 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, nutrient availability).

In FY 2004, 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 and catalytic and enzyme-substrate recognition and how these molecules transfer within and 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**..................................	**24,779**	**31,333**	**32,333**

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.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

In FY 2004, 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. Recommendations of the workshop include the use of multidisciplinary approaches involving the establishment of competitively selected centers of excellence that provide access to special research facilities especially state-of-the-art microscopes, light sources, neutron sources, terascale computers, and/or nanoscience centers in order to capitalize on their unique capabilities.

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.

	FY 2002	FY 2003	FY 2004
▪ **Separations and Analyses**	**12,967**	**14,407**	**14,387**

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 5 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 2004, major activities will include studies in 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

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

of how molecules interact with pore walls, with one another, and with other molecules to effect separation between molecules.

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

▪ **Heavy Element Chemistry**	**7,637**	**8,637**	**8,625**

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 2004, 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.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

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.

	FY 2002	FY 2003	FY 2004
▪ **Geosciences Research**	**21,252**	**21,262**	**21,232**

The Geosciences activity supports long-term basic research in geochemistry and geophysics. Geochemical research focuses on subsurface solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand physical properties of fluids, rocks and minerals. It seeks fundamental understanding of the physics of wave propagation in complex media 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.

	FY 2002	FY 2003	FY 2004
▪ **Chemical Energy and Chemical Engineering**	**10,953**	**10,953**	**10,937**

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.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

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 2004, 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.

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

	FY 2002	FY 2003	FY 2004
▪ **General Plant Projects (GPP)**..	**10,265**	**12,210**	**12,210**

GPP funding is 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 2002	FY 2003	FY 2004
▪ **General Purpose Equipment (GPE)**	**2,936**	**4,180**	**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 ORNL, ANL, and Ames site and facilities to correct deficiencies due to aging, changing technology, and inadequate past investments.

	FY 2002	FY 2003	FY 2004
▪ **SPEAR3 Upgrade**	**700**	**700**	**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

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

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.

▪ **Advanced Light Source Beamline**	**975**	**0**	**0**

This beamline is a major item of equipment with a total estimated cost of $6,000,000 that will provide capabilities for surface and interfacial science important to geosciences, environmental science, and aqueous corrosion science. It is being funded jointly by the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

Facility Operations	**5,377**	**5,805**	**5,967**

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 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. The x-ray and neutron scattering facility operations, formerly funded in Chemical Sciences, are now funded in the Materials Sciences and Engineering subprogram.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Facilities			
Combustion Research Facility	5,377	5,805	5,967
Total, Facilities	5,377	5,805	5,967

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**5,022**	**5,350**

In FY 2002 $1,309,000 and $78,000 were transferred to the SBIR and STTR programs, respectively. The FY 2003 and FY 2004 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**200,227**	**220,015**	**220,914**

Explanation of Funding Changes from FY 2003 to FY 2004

	FY 2004 vs. FY 2003 ($000)
Chemical Sciences, Geosciences, and Energy Biosciences Research	
▪ Increase in atomic, molecular, and optical science to advance ultrafast science through the application of new x-ray sources, including short wave length high power light sources.	+460
▪ Decrease in chemical physics research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-46
▪ Decrease in photochemistry and radiation research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-59
▪ Decrease in molecular mechanisms of natural solar energy conversion research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-17
▪ Decrease in metabolic regulation of energy production research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-29
▪ Increase in catalysis research to understand the role nanoscale properties play in altering and controlling catalytic transformations.	+1,000
▪ Decrease in separations and analyses research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-20
▪ Decrease in heavy element chemistry research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-12
▪ Decrease in geosciences research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-30
▪ Decrease in chemical energy and chemical engineering research due to increase in FY 2004 for STTR. The percentage increases from .15% to .3%.	-16
▪ Decrease in general purpose equipment.	-122
▪ Decrease due to completion of SPEAR3 Upgrade	-700
Total, Chemical Sciences, Geosciences, and Energy Biosciences Research	+409
Facilities Operations	
▪ Increase for operations of the Combustion Research Facility.	+162
Total, Chemical Sciences, Geosciences, and Energy Biosciences Facilities Operations	+162

	FY 2004 vs. FY 2003 ($000)
SBIR/STTR	
▪ Increase SBIR/STTR funding because of an increase in operating expenses and an increase in STTR percentage from .15% to .3%.	+328
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	+899

Construction

Mission Supporting Goals and Measures

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.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
SNS	276,300	210,571	124,600	-85,971	-40.8%
Project Engineering Design, NSRCs	3,000	11,000	3,000	-8,000	-72.7%
Project Engineering Design, LCLS	0	6,000	7,500	+1,500	+25.0%
Center for Nanophase Materials Science (ORNL)	0	24,000	20,000	-4,000	-16.7%
The Molecular Foundry (LBNL)	0	0	35,000	+35,000	--
Center for Integrated Nanotechnologies (SNL/LANL)	0	0	29,850	+29,850	--
Total, Construction	279,300	251,571	219,950	-31,621	-12.6%

Detailed Program Justification

(dollars in thousands)

	FY 2002	FY 2003	FY 2004
Construction	**279,300**	**251,571**	**219,950**
Spallation Neutron Source	**276,300**	**210,571**	**124,600**

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.

(dollars in thousands)		
FY 2002	FY 2003	FY 2004

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 addition to these two instruments, in FY 2003 and FY 2004, the BES program will provide $5,000,000 of Materials Sciences and Engineering subprogram funding for continuing the development of instruments to exploit the scientific potential of the SNS facility. 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 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.

FY 2003 budget authority is requested to continue 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.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

FY 2004 budget authority is requested to 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.

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.

Performance will be measured by continued construction of the SNS, meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Once completed in mid-2006, the SNS will provide beams of neutrons used to probe and understand the physical, chemical, and biological properties of materials at an atomic level, leading to improvements in high technology industries. Additional information follows later in construction project data sheet 99-E-334.

	FY 2002	FY 2003	FY 2004
Project Engineering and Design, Nanoscale Science Research Centers	**3,000**	**11,000**	**3,000**

FY 2002 and FY 2003 budget authority is requested to provide Title I and Title II design-only funding for Nanoscale Science Research Centers (NSRCs) at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, and Sandia National Laboratories (Albuquerque). *FY 2004 budget authority is requested for a NSRC at 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.

	FY 2002	FY 2003	FY 2004
Project Engineering and Design, Linac Coherent Light Source..	**0**	**6,000**	**7,500**

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.

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) enabling studies of fast chemical and physical processes. These characteristics 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 proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment. The preliminary Total Estimated Cost (TEC) is in the range of $200,000,000 to $240,000,000. FY 2004 Project Engineering Design (PED) funding of $7,500,000 and $2,000,000 of research and development 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 2002	FY 2003	FY 2004
Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL	**0**	**24,000**	**20,000**

FY 2003 funding is requested for the start of construction of the Center for Nanophase Materials Science to be located at Oak Ridge National Laboratory. FY 2004 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 2002	FY 2003	FY 2004
Nanoscale Science Research Center – The Molecular Foundry, LBNL	**0**	**0**	**35,000**

FY 2004 funding is requested for the start of construction of the Molecular Foundry at Lawrence Berkeley 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 04-R-313.

	FY 2002	FY 2003	FY 2004
Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, Sandia National Laboratories/Los Alamos National Laboratory	**0**	**0**	**29,850**

FY 2004 funding is requested for the start of construction of the Center for Integrated Nanotechnologies managed jointly by Sandia National Laboratories and Los Alamos National Laboratory. **Performance will be measured** by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information follows later in construction project data sheet 04-R-314.

	FY 2002	FY 2003	FY 2004
Total, Construction	**279,300**	**251,571**	**219,950**

(dollars in thousands)

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Construction	
▪ Decrease in funding for the Spallation Neutron Source, representing the scheduled ramp down of activities.	-85,971
▪ Decrease in Project Engineering and Design for Nanoscale Science Research Centers at ORNL, LBNL, SNL, and BNL.	-8,000

	FY 2004 vs. FY 2003 ($000)
▪ Increase in funding for Project Engineering Design related to design-only activities for the Linac Coherent Light Source (LCLS) to be located at the Stanford Linear Accelerator Center (SLAC).	+1,500
▪ Decrease in funding for construction of the Center for Nanophase Materials Sciences to be located at ORNL, representing the scheduled ramp down of activities	-4,000
▪ Increase in funding for construction of the Molecular Foundry to be located at LBNL, representing the start of construction.	+35,000
▪ Increase in funding for construction of the Center for Integrated Nanotechnologies, to be located at SNL, representing the start of construction.	+29,850
Total Funding Change, Construction	-31,621

Major User Facilities

Mission Supporting Goals and Objectives

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. A description of each facility is provided in the "Site Descriptions" section. Any unusual or nonrecurring aspects of funding are described in the following section "Detailed Program Justification."

The facilities are planned in collaboration with the scientific community and are constructed and operated by BES for support of forefront research in areas important to BES activities and also in areas that extend beyond the scope of BES activities such as structural biology, medical imaging, and micro machining. These facilities are used by researchers in materials sciences, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, and medical research and technology development. The facilities are open to all qualified scientists from academia, industry, and the federal laboratory system whose intention is to publish in the open literature. The funding schedule includes only those facilities that have operating budgets for personnel, utilities, and maintenance.

Funding Schedule

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 2002	FY 2003	FY 2004	$ Change	% Change
Advanced Light Source	37,674	39,561	40,917	+1,356	+3.4%
Advanced Photon Source	88,880	91,291	94,500	+3,209	+3.5%
National Synchrotron Light Source	34,611	35,893	37,250	+1,357	+3.8%
Stanford Synchrotron Radiation Laboratory	21,594	22,673	26,400	+3,727	+16.4%
High Flux Isotope Reactor	38,697	36,854	38,357	+1,503	+4.1%
Radiochemical Engineering Development Center	6,606	6,712	6,712	0	--
Intense Pulsed Neutron Source	15,826	17,015	17,200	+185	+1.1%
Manuel Lujan, Jr. Neutron Scattering Center	9,044	9,678	10,271	+593	+6.1%
Spallation Neutron Source	15,100	14,441	18,397	+3,956	+27.4%
Combustion Research Facility	5,377	5,805	5,967	+162	+2.8%
Total, Major User Facilities	273,409	279,923	295,971	+16,048	+5.7%

Detailed Program Justification

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Major User Facilities	**273,409**	**279,923**	**295,971**
▪ Advanced Light Source at Lawrence Berkeley National Laboratory	37,674	39,561	40,917
▪ Advanced Photon Source at Argonne National Laboratory.	88,880	91,291	94,500
▪ National Synchrotron Light Source at Brookhaven National Laboratory	34,611	35,893	37,250
▪ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.	21,594	22,673	26,400
▪ High Flux Isotope Reactor at Oak Ridge National Laboratory.	38,697	36,854	38,357
▪ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	6,606	6,712	6,712
▪ Intense Pulsed Neutron Source at Argonne National Laboratory.	15,826	17,015	17,200
▪ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	9,044	9,678	10,271
▪ Spallation Neutron Source at Oak Ridge National Laboratory.	15,100	14,441	18,397
▪ Combustion Research Facility at Sandia National Laboratories/California.	5,377	5,805	5,967
Total, Major User Facilities	273,409	279,923	295,971

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

	(dollars in thousands)				
	FY 2002	FY 2003	FY 2004	$ Change	% Change
General Plant Projects	10,613	12,570	12,618	+48	+0.4%
Accelerator Improvement Projects	11,292	9,067	9,440	+373	+4.1%
Capital Equipment	62,437	76,249	77,328	+1,079	+1.4%
Total, Capital Operating Expenses	84,342	97,886	99,386	+1,500	+1.5%

Construction Projects

	(dollars in thousands)					
	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2002	FY 2003	FY 2004	Unapprop-riated Balances
99-E-334, ORNL, Spallation Neutron Source	1,192,700	460,329	276,300	210,571	124,600	120,900
02-SC-002 PED, Nanoscale Science Research Centers	20,000 [a]	0	3,000	11,000	3,000	3,000
03-SC-002, PED, SLAC, Linac Coherent Light Source	36,000 [b]	0	0	6,000	7,500	22,500
03-R-312, ORNL, Center for Nanophase Material Sciences	64,000 [c]	0	0	24,000	20,000	17,500
04-R-313, LBNL, The Molecular Foundry	83,700[d]	0	0	0	35,000	41,400
04-R-314, SNL, Center for Integrated Nanotechnologies	73,800[e]	0	0	0	29,850	39,750
Total, Construction		460,329	279,300	251,571	219,950	

[a] The full Total Estimated Cost (design and construction) ranges between $286,500,000,000 and $306,500,000. 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 $200,000,000 and $240,000,000. This is a preliminary estimate based on conceptual design and should not be construed as a project baseline.

[c] Includes $2,500,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

[d] Includes $7,300,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

[e] Includes $4,200,000 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 2002	FY 2003	FY 2004	Accept-ance Date
SPEAR3 Upgrade	29,000[a]	10,000	9,000	10,000	0	FY 2004
ALS Beamline	6,000	4,050	1,950	0	0	FY 2003
ANL Center for Nanophase Materials	36,000	0	0	0	10,000	FY 2006
Total, Major Items of Equipment		14,050	10,950	10,000	10,000	

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

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

(Changes from FY 2003 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 (*Current Estimate*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700

2. Financial Schedule [1]

(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	170,453
2002	276,300	276,300	253,059
2003	210,571	210,571	322,277
2004	124,600	124,600	176,690
2005	79,800	79,800	73,065
2006	41,100	41,100	54,474

[1] In FY 2001, two grants were awarded to universities for research covering the design, fabrication and installation of instruments for neutron scattering. Both awards were made based on competitive peer review under 10CFR Part 605, Financial Assistance Program. Both instruments will be located at the SNS. These awards follow the advice of the Basic Energy Sciences Advisory Committee, that the Department should "expand the university base for neutron scattering. The only way to build the user base required to be internationally competitive is to enhance the participation from academic institutions. An immediate injection of funds to support the exploitation of pulsed neutron sources for science by the U.S. academic community is needed." Several universities participate in these grants, including MIT, University of California, University of Delaware, University of Colorado, University of Utah, Johns Hopkins, University of New Mexico, and Syracuse University. Pennsylvania State University submitted an application on April 12, 2001. After peer review the award to Pennsylvania State University was made for 5 years, starting August 15, 2001, and ending August 14, 2006, for a total of $12,824,168 of operating funds for an instrument for research in inelastic neutron scattering, quantum liquids, magnetism, environmental chemistry, polymer dynamics, and lubrication. This instrument will be owned by Pennsylvania State University. In order to efficiently fund certain work related to this instrument that must uniquely be performed by the SNS project (e.g., design and procurement of target interfacing components, technical coordination, instrument installation), DOE will be providing about 20 percent of the above grant amount directly to Oak Ridge National Laboratory and the grant will be reduced accordingly.

The California Institute of Technology submitted an application on June 11, 2001. After peer review, the award to California Institute of Technology was made for 5 years, starting September 15, 2001, and ending September 14, 2006, for a total of $11,579,000 of operating funds for an instrument for research in lattice dynamics, magnetic dynamics, chemical physics, and characterization of novel materials. This instrument will be owned by California Institute of Technology. As with the above instrument grant and for the same reasons, DOE will be providing about 20 percent of the grant amount directly to Oak Ridge National Laboratory and the grant will be reduced accordingly.

In addition to the two above identified instruments, the Basic Energy Sciences program will provide $5,000,000 of Materials Sciences and Engineering subprogram funding in FY 2003 and FY 2004 to continue the development of instrumentation to exploit the scientific potential of the SNS facility. 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. The instruments will be operated for users by the SNS based on applications for experiments selected competitively by the peer review procedures established for access to the SNS. See further discussion in Materials Sciences and Engineering subprogram under X-ray and Neutron Scattering.

3. Project Description, Justification and Scope [1]

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 operation, will be used by 1,000-2,000 scientists and engineers each year and that it will meet the national need for neutron science capabilities well into the 21st Century.

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

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

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

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[1] 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.

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 the 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 2002 continue 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 continued on the ring, target, and instrument systems. The completed ion source and portions of the drift tube linac were delivered to the site and their installation was begun. Other system components for the accelerator, ring, target, and instruments continued to be manufactured. Work on conventional facilities continued, with some reaching completion and being turned over for equipment installation, such as the front end building, and portions of the klystron building and linac tunnel. Construction work began on the ring tunnel.

FY 2003 budget authority is requested to continue 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 is requested to continue instrument R&D, design, and procurement. The drift tube linac and coupled cavity linac subsystems will be 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.

4. Details of Cost Estimate [1]

	(dollars in thousands) Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 21% of construction costs	159,500	159,500
Construction management at approximately 2% of construction costs	14,000	14,000
Project management at approximately 14% of construction costs	104,700	104,700
Land and land rights	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	31,500	31,500
Buildings	196,300	181,600
Utilities (electrical, water, steam, and sewer lines)	20,900	20,900
Technical Components	507,200	505,500
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	1,088,100	1,071,700
Contingencies at approximately 10% of above costs [2]	104,600	121,000
Total Line Item Cost	1,192,700	1,192,700
Less: Non-Agency Contribution	0	0
Total, Line Item Costs (TEC)	1,192,700	1,192,700

[1] 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.

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

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, Los Alamos National Laboratories and Thomas Jefferson National Accelerator Facility. Each laboratory is assigned responsibility for accomplishing a well defined portion of the project's scope that takes advantage of their technical strengths: Argonne – Instruments; Brookhaven – Accumulator Ring; Lawrence Berkeley – Ion Source; Los Alamos – Normal conducting linac and RF power systems; TJNAF – Superconducting Linac; Oak Ridge - Target. Project execution is the responsibility of the SNS Project 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 Project 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 commissioning support. Procurements by all six laboratories will be 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 2002	FY 2003	FY 2004	Outyears	Total
Project Cost						
Facility Cost [1]						
Line Item TEC	313,135	253,059	322,277	176,690	127,539	1,192,700
Plant Engineering & Design	0	0	0	0	0	0
Expense-funded equipment	0	0	0	0	0	0
Inventories	0	0	0	0	0	0
Total direct cost	313,135	253,059	322,277	176,690	127,539	1,192,700
Other project costs						
R&D necessary to complete project [2]	73,374	5,409	2,122	1,663	1,156	83,724
Conceptual design cost [3]	14,397	0	0	0	0	14,397
Decontamination & Decommissioning (D&D)	0	0	0	0	0	0
NEPA Documentation costs [4]	1,948	10	0	0	0	1,958
Other project-related costs [5]	10,531	10,165	13,048	17,376	66,698	117,818
Capital equipment not related construction [6]	847	-1	150	107	0	1,103
Total, Other project costs	101,097	15,583	15,320	19,146	67,854	219,000
Total project cost (TPC)	414,232	268,642	337,597	195,836	195,393	1,411,700

[1] 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.

[2] A research and development program at an estimated cost of $83,724,000 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.

[3] 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.

[4] Costs of $1,958,000 are included for completion of the Environmental Impact Statement.

[5] Estimated costs of $117,818,000 are included to cover pre-operations costs.

[6] 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	40,000	40,000
Capital equipment not related to construction but related to the programmatic effort in the facility	11,800	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)	150,000	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.

8. Design and Construction of Federal Facilities

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088, “Federal Compliance with Pollution Control Standards”; section 19 of the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, and the related Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); and the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. This project includes the construction of new buildings and/or building additions; therefore, a review of the GSA Inventory of Federal Scientific Laboratories is required. The project will be located in an area not subject to flooding determined in accordance with the Executive Order 11988.

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

(Changes from the FY 2003 Congressional Budget Request are denoted with a vertical line in the left margin.)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($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 (Current Estimate)	2Q 2002	3Q 2003	N/A	N/A	20,000[a]

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	3,000	3,000	1,547
2003	11,000	11,000	11,163
2004	3,000	3,000	4,290
2005	3,000	3,000	3,000

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] The full Total Estimated Cost (design and construction) ranges between $286,500,000 - $306,500,000. This estimate was based on conceptual data and should not be construed as a project baseline. Based on the results of peer review, the total design cost is increased to $20,000,000. The full Total Estimated Cost for each of the three currently proposed NSRC construction projects is identified in the FY 2004 construction datasheets.

Updated FY 2002 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. Construction funding for three of the FY 2002 subprojects is also separately requested in FY 2004.

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 in FY 2002 and requested in FY 2003 for LBNL, ORNL, and LANL/SNL. Construction funding was also requested for ORNL in FY 2003. In FY 2004, PED funding is requested for BNL, while construction funds are requested for ORNL, LBNL, and LANL/SNL.

FY 2002 Proposed Design Projects

FY 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.

[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.

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	7,300	83,700 [a]

Fiscal Year	Appropriations	Obligations	Costs
2002	500 [b]	500 [b]	38 [b]
2003	6,800 [b]	6,800 [b]	5,972 [b]
2004	0 [b]	0 [b]	1,290 [b]

The proposed Molecular Foundry at LBNL will be a new structure near the National Center for Electron Microscopy. The project includes an approximately 80,000 gross square foot research building, a separate approximately 5,000 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.

[a] The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

[b] The FY 2003 Request included $500,000 for FY 2002, $6,800,000 for FY 2003, and $1,000,000 for FY 2004. The current funding plan eliminates the PED funding in FY 2004. The project is now proposed for construction 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		
2Q 2004	3Q 2005	N/A	N/A	6,000	70,000-85,000 [a]

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	0 [b]	0 [b]	0 [b]
2003	0 [b]	0 [b]	0 [b]
2004	3,000 [b]	3,000 [b]	3,000 [b]
2005	3,000	3,000	3,000

The Center for Functional Nanomaterials will include class 10 clean rooms, general laboratories, wet and dry laboratories for sample preparation, fabrication, and analysis. Included 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, and 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 “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 or requested for this project in FY 2003. Based on the review of a revised proposal, PED funding is requested in FY 2004.

[a] The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

[b] 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, $3,000,000 of PED funding is requested in FY 2004.

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	2,500 [a]	64,000 [b]

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	1,500 [b]	1,500 [b]	1,342 [b]
2003	1,000 [b]	1,000 [b]	1,158 [b]

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. Based on the results of a review, this project is proposed for construction funding in FY 2003.

[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 will be funded at $1,500,000 in FY 2002 and $1,000,000 in FY 2003.

[b] The full TEC Projection (design and construction) in the FY 2002 PED datasheet is a preliminary estimate based on conceptual data. The TEC displayed above is the TEC displayed in the FY 2003 construction datasheet for this project (03-R-312).

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		
3Q 2002	2Q 2004	3Q 2004	3Q 2007	4,200	73,800 [a]

Fiscal Year	Appropriations	Obligations	Costs
2002	1,000 [b]	1,000 [b]	167 [b]
2003	3,200 [b]	3,200 [b]	4,033 [b]

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 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. 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; the Microelectronics Development Laboratory and the Compound Semiconductor Research Laboratory at SNL.

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.

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[a] The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline. CINT combines the projects identified as the “Synthesis and Characterization Laboratory” at LANL and the “Nanofabrication and Integration Laboratory” at SNL described separately in FY 2002.

[b] 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 $3,200,000 in FY 2003.

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 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 [1]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	15,000	11,250
Design Management costs (15% of TEC)	3,000	2,250
Project Management costs (10% of TEC)	2,000	1,500
Total Design Costs (100% of TEC)	20,000	15,000
Total, Line Item Costs (TEC)	20,000	15,000

5. Method of Performance

Design services will be obtained through competitive and/or negotiated 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 2002	FY 2003	FY 2004	Outyears	Total
Facility Cost						
PED	0	1,547	11,163	4,290	3,000	20,000
Other project costs [2]						
Conceptual design cost	1,370	440	0	0	0	1,810
Total, Other Project Costs	1,370	440	0	0	0	1,810
Total, Project Costs	1,370	1,987	11,163	4,290	3,000	21,810

[1] 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.

[2] 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; and Project 04-R-314, Center for Integrated Nanotechnologies.

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

(Changes from the FY 2003 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

The Total Estimated Cost has increased by $2,500,000 due to FY 2004 fiscal constraints that deferred some design work from FY 2004 to FY 2005.

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 (Current Estimate)	1Q 2003	4Q 2006	N/A	N/A	$36,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2003	6,000	6,000	5,500
2004	7,500	7,500	7,000
2005	20,,000	20,000	21,000
2006	2,500	2,500	2,500

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.

[a] The full TEC Projection (design and construction) ranges between $200,000,000 and $240,000,000. This is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source. 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 beams 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, this latter activity will be limited to 30 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 70 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 radio-frequency 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^{12}-10^{13} 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 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one-third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120-meter undulator and associated equipment. Two new experimental buildings, the Near Hall and the Far Hall will be constructed. They will be connected by the beam line tunnel, and the Far Hall will provide laboratory and office space for LCLS users.

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	25,125
Design Management costs	5,000	5,025
Project Management costs	5,000	3,350
Total Design Costs	36,000	33,500
Total, Line Item Costs (TEC)	36,000	33,500

5. Method of Performance

A Conceptual Design Report (CDR) for the project has been completed and reviewed. Key design activities will be identified in the areas of the injector, undulator, x-ray optics and experimental halls that will reduce the risk of the project and accelerate the startup. Also, the management systems for the project will be put in place and proven during the Project Engineering Design (PED) phase. These activities will be managed by an LCLS project office in the Stanford Synchrotron Radiation Laboratory (SSRL) Division of SLAC. Portions of the project will be executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL).

[a] This cost estimate includes design phase activities only. Construction activities will be requested to be funded in FY 2005.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2002	FY 2003	FY 2004	Outyears	Total
Facility Cost						
PED	0	0	5,500	7,000	23,500	36,000
Other project costs						
Conceptual design cost	0	1,500	0	0	0	1,500
Research and development costs	0	0	0	2,000	4,000	6,000
NEPA documentation costs	0	0	0	0	0	0
Other project related costs	0	0	0	0	0	0
Total, Other Project Costs	0	1,500	0	2,000	4,000	7,500
Total Project Cost (TPC)	0	1,500	5,500	9,000	27,500	43,500

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

(Changes from FY 2003 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 (Current Estimate)..................................	2Q2002	1Q2003	3Q2003	4Q2006	$64,000	$65,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering & Design (PED)			
2002	1,500[a]	1,500[a]	1,342[a]
2003	1,000[a]	1,000[a]	1,158[a]
Construction			
2003	24,000[a]	24,000[a]	7,100[a]
2004	20,000	20,000	28,000
2005	17,500	17,500	19,700
2006	0	0	6,700

[a] Funding of $1,000,000 in FY 2003 and $2,000,000 in FY 2004 was identified in the FY 2002 President's Request for this project. Based on the results of peer review, this project is now proposed for PED funding of $1,500,000 in FY 2002 and $1,000,000 in FY 2003 and construction funding of $24,000,000 beginning in FY 2003.

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 scope of this project is to construct the Center for Nanophase Materials Sciences. The engineering effort includes preliminary and final design. The project also includes procurement of an initial set of experimental capital equipment and construction of facilities. While no FY 2002 PED funds were identified for this project on the FY 2002 PED Project Data Sheet (02-SC-002, Project Engineering Design (PED), various locations), SC plans to allocate FY 2002 and FY 2003 PED funding to complete design of the CNMS. FY 2003 construction funding will be used to initiate construction and equipment procurement.

4. Details of Cost Estimate[1]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design Costs	1,700	1,700
Design and Project Management Costs	300	300
Total, Design Costs	2,000	2,000
Construction Phase		
Improvements to Land	500	500
Buildings	19,700	19,700
Special Equipment[2]	26,000	26,000
Utilities	500	500
Inspection, design and project liaison, testing, checkout and Acceptance	1,800	1,800
Construction and Project Management	1,700	1,700
Total, Construction Costs	50,200	50,200
Contingency (23.5% of Construction Costs)	11,800	11,800
Total, Line Item Costs (TEC)	64,000	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.

[1] 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.

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

6. Schedule of Project Funding

	Prior Years	FY 2002	FY 2003	FY 2004	Outyears	Total
Project Cost						
Facility Cost						
Design	0	1,342	1,158	0	0	2,500
Construction	0	0	7,100	28,000	26,400	61,500
Total, Line item TEC	0	1,342	8,258	28,000	26,400	64,000
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 [1]	95	225	100	250	175	845
Total, Other Project Costs	250	225	100	250	175	1,000
Total, Project Cost (TPC)	250	1,567	8,358	28,250	26,575	65,000

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 (operating from FY 2006 through FY 2046)	$18,000	$18,000

[1] 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.

8. Design and Construction of Federal Facilities

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088, "Federal Compliance with Pollution Control Standards"; section 19 of the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, and the related Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); and the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. This project will be located in an area not subject to flooding determined in accordance with the Executive Order 11988. DOE has reviewed the U.S. General Services Administration (GSA) inventory of Federal Scientific laboratories and found insufficient space available, as reported by the GSA inventory.

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

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)*	3Q2002	1Q2004	2Q2004	2Q2006	$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	6,800	6,800	5,972
2004	0	0	1,290
Construction			
2004	35,000	35,000	16,660
2005	32,000	32,000	32,500
2006	9,400	9,400	26,640
2007	0	0	600

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 80,000 gross square foot research building, a separate approximately 5,000 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.

4. Details of Cost Estimate[1]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary Design & Final Design	4,300	N/A
Design Management costs	1,650	N/A
Total, Design Costs	5,950	N/A
Construction Phase		
Building & Improvements to land	43,300	N/A
Special Equipment[2]	15,300	N/A
Inspection, design and project liaison, check out	1,700	
Construction Management & Project Management	2,150	N/A
Total, Construction Costs	62,450	N/A
Contingencies		
Design Phase	1,330	N/A
Construction Phase	13,970	N/A
Total, Contingencies (18.3% of TEC)	15,300	N/A
Total, Line Item Costs (TEC)	83,700	N/A

5. Method of Performance

An Architect - Engineering firm (AE) with appropriate multi-disciplinary design experience will prepare a building program and design criteria with the support of the LBNL Facilities Department. The AE will also prepare Title I and II design and 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 will be based on competitive bidding of the Construction General Conditions. The CM contract will have an option for management

[1] This cost estimate is based on conceptual data. The annual escalation rates assumed in the FY 2003 estimate for FY 2002 through FY 2006, are 2.6%, 2.8%, 2.8%, 2.9% and 2.9% respectively.

[2] Initial research equipment including testing and acceptance.

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.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Years	FY 2002	FY 2003	FY 2004	Outyears	Total
Facility Cost						
PED	0	38	5,972	1,290	0	7,300
Construction	0	0	0	16,660	59,740	76,400
Total, Line Item TEC	0	38	5,972	17,950	59,740	83,700
Other Project Costs						
Conceptual design cost	290	440	0	0	0	730
NEPA Documentation Costs	0	40	0	0	0	40
Other project-related costs[1]	120	30	0	0	380	530
Total, Other Project Costs	410	510	0	0	380	1,300
Total, Project Costs (TPC)	410	548	5,972	17,950	60,120	85,000

7. Related Annual Funding Requirements

(FY 2006 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs	$18,000	N/A
Total related annual funding (operating from FY 2006 through FY 2046)	$18,000	N/A

[1] Includes preconceptual data and documentation required for CD-1 and for commissioning and startup. Experimental research will begin at the time of beneficial occupancy of the facility. These experimental research costs are not part of the TPC and will be funded by the BES program.

8. Design and Construction of Federal Facilities

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088A Federal Compliance with Pollution Control Standards, the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, the Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. The project will be located in an area not subject to flooding determined in accordance with Executive Order 11988. The scientific research which will take place in this facility requires a unique research facility and location as described in Section 3.

04-R-314, The Center for Integrated Nanotechnologies (CINT) Facility, Sandia National Laboratories Albuquerque, New Mexico, and Los Alamos National Laboratory Los Alamos, New Mexico

1. Construction Schedule History

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

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering and Design (PED)			
2002	1,000	1,000	167
2003	3,200	3,200	4,033
Construction			
2004	29,850	29,850	20,000
2005	35,300	35,300	31,300
2006	4,450	4,450	18,300

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 will be a distributed center operated jointly by Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL). CINT will include a Core Facility in Albuquerque, a Gateway to Sandia, and a Gateway to Los Alamos.

The Core Facility will provide approximately 83,000 gross square feet of laboratory and office space, including state-of-the-art clean rooms with an initial set of nanofabrication and characterization equipment. This facility will also have general purpose chemistry/biology laboratories and electronic and physical measurement laboratories. Lastly, there will be offices and meetings rooms for the Center staff, SNL/LANL collaborators, Center-sponsored post docs, visiting students and faculty, and industry collaborators.

The Gateway to Sandia will focus on specialized microfabrication and nanomaterials capabilities and expertise. This gateway will utilize existing space in SNL's Integrated Materials Research Laboratory and thus will not require any construction funding. The Gateway to Los Alamos will focus on connecting CINT scientists to the extensive biosciences and nanomaterials capabilities at LANL. The facility will provide approximately 31,000 gross square feet of general purpose chemistry/biology laboratories and characterization laboratories outfitted with an initial set of scientific equipment, as well as office and interaction space.

The primary objective of CINT 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 macroworlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. The initial technical focus of CINT will be on the four thrusts that derive from expertise at SNL and LANL: nanophotonics and nanoelectronics; complex functional nanomaterials; nanomechanics; and nanoscale bio-micro interfaces.

No existing facilities at SNL or LANL satisfy the needs and objectives of CINT. The Compound Semiconductor Laboratory (CSRL) and the Microelectronic Development Laboratory (MDL) at SNL have some of the needed capabilities, but they are highly subscribed and not available for exploratory work by students and visitors and do not meet the open environment requirement for NSRCs. Likewise, the Materials Science Laboratory at LANL has some of the needed capabilities but it too is highly subscribed with programmatic deliverables and activities.

4. Details of Cost Estimate [1]

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs	2,640	N/A
Design Management Costs	540	N/A
Project Management Costs	400	N/A
Total, Design Costs	3,580	N/A
Construction Phase		
Buildings	35,990	N/A
Special Equipment[2]	15,760	N/A
Standard Equipment	1,540	N/A
Inspection, Design and Project Liaison, Testing, Checkout and Acceptance	2,900	N/A
Construction and Project Management	1,030	N/A
Total, Construction Costs	57,220	N/A
Contingencies		
Design Phase	620	N/A
Construction Phase	12,380	N/A
Total, Contingencies (17.6% of TEC)	13,000	N/A
Total, Line Item Costs (TEC)	73,800	N/A

[1] 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).

[2] 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 will be prepared by SNL personnel with external support as needed.

Performance specifications will be 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 bidders' qualifications, experience, and the quoted price.

SNL and LANL personnel will provide project management, design management, and project controls support.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Years	FY 2002	FY 2003	FY 2004	Outyears	Total
Project Cost						
Facility Cost						
Design	0	167	4,033	0	0	4,200
Construction	0	0	0	20,000	49,600	69,600
Total, Line item TEC	0	167	4,033	20,000	49,600	73,800
Other Project Costs						
Conceptual design cost	330	0	0	0	0	330
Other project-related costs [1]	45	425	0	150	1,050	1,670
Total, Other Project Costs	375	425	0	150	1,050	2,000
Total, Project Costs (TPC)	375	592	4,033	20,150	50,650	75,800

[1] Includes tasks such as NEPA documentation, 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 [1]

(FY 2006 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs	340	N/A
Annual facility maintenance/repair costs	400	N/A
Programmatic operating expenses directly related to the facility	16,920	N/A
Utility costs	840	N/A
Total related annual funding (operating from FY 2006 through FY 2046)	18,500	N/A

8. Design and Construction of Federal Facilities

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088A Federal Compliance with Pollution Control Standards, the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, the Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. The project will be located in an area not subject to flooding determined in accordance with Executive Order 11988. The scientific research which will take place in this facility requires a unique research facility and location as described in Section 3.

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