Biological and Environmental Research

Program Mission

For over 50 years the Biological and Environmental Research (BER) program has been advancing environmental and biomedical knowledge that promotes national security through improved energy production, development, and use; international scientific leadership that underpins our nation's technological advances; and research that improves the quality of life for all Americans. BER supports these vital national missions through competitive and peer-reviewed research at National Laboratories, universities, and private institutions. In addition, BER develops and delivers the knowledge needed to support the President's National Energy Plan and provides the science base in support of the Energy Policy Act of 1992.

Overview:

The Biological and Environmental Research (BER) program supports fundamental research in climate change, environmental remediation, genomics, proteomics, radiation biology, and medical sciences. BER supports leading edge research facilities used by public and private sector scientists across the range of BER disciplines. BER works with other federal agencies to coordinate research across all of its programs. BER validates its long-range goals through its advisory committee, the Biological and Environmental Research Advisory Committee (BERAC).

The Opportunity:

With the 21st Century dawns what most have called the "biological century" – an era when advances in biology, spurred by achievements in genomic research, including the sequencing of the human genome, will bring revolutionary and unconventional solutions to some of our most pressing and expensive challenges in health, energy, the environment, and national security. We will understand how living organisms interact with and respond to their environments so well that we will be able to use biology to produce clean energy, remove excess carbon dioxide from the atmosphere, and help clean up the environment. Our understanding of global climate change and our ability to predict climate over decades to centuries will enable us to develop science based solutions to reduce and minimize the impacts of climate change and to better plan for our Nation's future energy needs. BER will lead the way in discovering innovative approaches along unconventional paths to energy independence and environmental cleanup.

The Challenges:

Understanding and predicting climate – Can we understand the factors that determine Earth's climate well enough so that we can predict climate decades to centuries in the future? Advanced climate models are needed to describe and predict the roles of oceans, the atmosphere, ice and land masses on climate. So too, the role of clouds in controlling solar and thermal radiation onto and away from the Earth needs to be understood since it is the single largest uncertainty in climate prediction. Moreover, the impacts of excess carbon dioxide in the atmosphere from human sources, including energy use, on Earth's climate and ecosystems need to be determined and possible mitigation strategies developed.

A cleaner environment – Microbes have a remarkable capacity to thrive in almost every environment imaginable, even when heavily contaminated. Can we use Nature's own solutions to clean up sites contaminated from years of weapons research? These solutions seem ever closer as we study the molecular details of nature's own clean up strategies.

Technology for a healthier Nation – At the crossroads of the physical and biological sciences is the promise of remarkable technology for tomorrow's medicine. Developments in imaging technology have the potential to revolutionize all of medical imaging with increases in sensitivity, ease of use, and patient comfort. Technological wonders are on the horizon, like an artificial retina that will give vision to the blind.

A new biology – Can we understand the workings of biological systems well enough so that we can use Nature's own principles of design to solve energy and environmental challenges? Understanding nature's array of multi protein molecular machines, each with exquisitely precise and efficient functions and controls, will enable us to use and even redesign these molecular machines to address DOE and National needs.

The Investment Plan:

BER will continue its investments in core technologies and fundamental science needed to address these daunting challenges. We believe that the most important scientific advances in the 21st century will occur at the interfaces between scientific disciplines such as biology, physics, chemistry, engineering, and information science.

Of highest priority will be the development of a new research infrastructure needed to understand fundamental biological principles underlying the function and control of biological systems. A combination of novel, state-of-the-art user facilities coupled with large, well-integrated, interdisciplinary research teams will form the basis of a new approach for studying complex biological systems and for using those systems to solve problems in energy and the environment. Our ability to predict climate on global and regional scales and to develop strategies for the removal of excess carbon dioxide, a contributor to global warming, from the atmosphere will depend on the continued development of novel research tools and a close integration of experimental and computational sciences research. Because of DOE's diverse capabilities across a range of scientific disciplines, from engineering to chemistry to biology to computing, continued investments in advanced medical concepts will continue to provide the medical community with novel devices and technologies to improve our Nation's health.

The Benefits:

Basic biological and environmental research has broad impacts on our health, our environment, and our energy future. An ability to predict long-range and regional climate enables effective planning for future needs in energy, agriculture and land and water use. Biotechnology solutions are possible for DOE energy, environmental, and national security challenges by understanding complex biological systems and developing computational tools to model and predict their behavior. Understanding the global carbon cycle and the associated role and capabilities of microbes can lead to solutions for reducing carbon dioxide concentrations in the atmosphere. Biological solutions can be developed to help clean up metals and radionuclides contaminating former DOE weapons sites. Both normal and abnormal health - from development to cancer to brain function – can be understood using radiotracers and advanced imaging instruments. Understanding the biological effects of low doses of radiation can lead to the development of science-based health risk policy to better protect workers and citizens.

How We Work:

BER uses a variety of mechanisms for conducting, coordinating, and funding biological and environmental research. BER is responsible for planning and prioritizing all aspects of supported research, for conducting ongoing assessments to ensure a comprehensive and balanced portfolio that addresses DOE and National science needs, and for coordinating its research programs with those of other federal agencies. BER regularly seeks advice on its research programs from the scientific community and from its diverse stakeholders. BER supports research at national laboratories, universities, research institutes, and in private companies and maintains a strong research infrastructure across the biological and environmental sciences most relevant to the BER program.

Advisory and Consultative Activities:

To ensure that resources are allocated to the most scientifically relevant and promising research, BER actively seeks external input using a variety of advisory bodies. BER regularly compares its programs to the scientific priorities recommended by the BERAC and by the standing committees created by the Office of Science and Technology Policy. BER staff and BERAC both interact with and receive feedback from other programs and advisory committees across the Department including, Advanced Scientific Computing Research, Basic Energy Sciences, Environmental Management, Energy Efficiency and Renewable Energy, Nuclear Energy, Fossil Energy, and the National Nuclear Security Administration. BER program coordination across federal agencies also benefits from international and interagency working groups such as those of the International Human Genome Project, the U.S. Global Change Research Program, and the National Institutes of Health Bioengineering Consortium. Finally, BER consults regularly with groups like JASON and The Washington Advisory Group (WAG), involving physicists, mathematicians, engineers, etc., to receive feedback on BER program elements such as the Atmospheric Radiation Measurement (ARM) program, climate change prediction activities, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), and the Human Genome program.

Facility Operations Reviews:

BER facility operations are monitored by peer reviews and user feedback. BER facility operations have also been reviewed by BERAC and by an Office of Science and Technology Policy (OSTP) interagency working group evaluating structural biology user facilities. The Office of Science's Construction Management Support Division has reviewed BER's Joint Genome Institute. BER manages these facilities in a manner that meets user requirements as indicated by achieving performance specifications while protecting the safety of workers and the environment. Facilities are operated reliably and according to planned schedules. Facilities are also maintained and improved to remain at the cutting edge of technology and scientific capability.

Program Reviews:

Effective program review, peer review, and user feedback are critical tools for BER to measure performance of research programs, research projects, and user facilities. The quality and scientific relevance of the BER program and its individual research projects are maintained by rigorous peer reviews conducted by internationally recognized scientific experts. The criteria for determining scientific quality and relevance include scientific merit, appropriateness of the proposed approach, requested level of funding, and research facilities, and qualifications of the principal investigator. BER expects the highest quality research and, when necessary, takes corrective management actions based on results of the reviews. A measure of the quality of the BER research is the sustained achievement in advancing scientific knowledge. This is demonstrated by the publication of research results in the leading refereed scientific journals pertinent to BER-related research fields, by invited participation at national and international scientific conferences and workshops, and by honors received by BER-supported researchers.

At the highest level, regular reviews of individual BER program elements and of the entire BER research program are conducted by BERAC. As noted above, BER also benefits from interagency and international reviews of programs such as the Human Genome Program, the Global Change Research Program, and the structural biology research program, including reviews by Boards and Committees of the National Academy of Sciences.

BER goes one step further in conducting program reviews. Panels of distinguished scientists are regularly charged with evaluating the quality of individual programs and with exploring ways of entraining new ideas and research performers from different scientific fields. This strategy is based on the conviction that the most important scientific advances of the new century will occur at the interfaces between scientific disciplines, such as biology and information science. Groups like JASON and The Washington Advisory Group (WAG), involving physicists, mathematicians, engineers, etc., are among the organizations that study BER program elements, such as the Atmospheric Radiation Measurement (ARM) program, climate change prediction activities, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), and the Human Genome program. The BER program is ideally positioned to facilitate and foster interactions between the physical sciences, the computational sciences, and the life sciences and aggressively pursues every opportunity to nurture collaborations at the interfaces between these scientific domains.

Planning and Priority Setting:

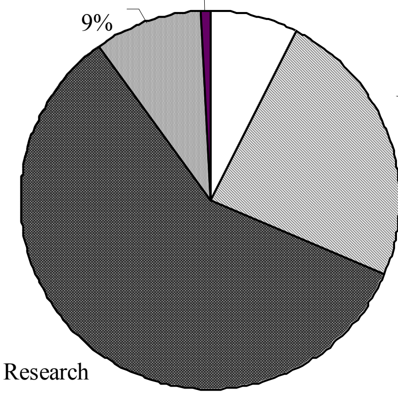
BER prides itself on supporting research and developing new research initiatives that lead the way across many fields of science and that effectively bring together many different disciplines, including biology, chemistry, engineering, computing, and the physical sciences. Peer reviews and user feedback are incorporated as BER anticipates and plans for the future needs of DOE research in the life and environmental sciences. This includes: planning for future directions, opportunities, and initiatives within the BER research portfolio; maintaining the flexibility to quickly move into promising new areas; contributing to the health of the educational pipeline in critical subfields and disciplines; planning for upgrades at existing facilities to expand the research capabilities or operational capacity; ensuring the proper balance between facilities and research; and planning for future facilities necessary to advance the science in areas relevant to BER's mission with strong involvement of the research community.

BER planning and priority setting are also key BERAC activities and part of BER's interagency coordination. Individual BER program elements, e.g., human genome, low dose radiation research, Genomes to Life, bioremediation research, and global climate change develop long-range program plans through coordinated efforts with BERAC and with other federal agencies.

How We Spend Our Budget:

The BER budget has three major components: basic research at universities (31%); basic research at national laboratories (53%); and user facility support (6%). Research at national laboratories also includes support for high throughput DNA sequencing at the Joint Genome Institute, Atmospheric Radiation Measurement Infrastructure, Unmanned Aerial Vehicles, and other elements that represent a research infrastructure for the scientific community, and primarily university scientists. BER's user facilities include the infrastructure at synchrotron and neutron sources for structural biology and operation and equipment for the Environmental Molecular Sciences Laboratory.

BIOLOGICAL AND ENVIRONMENTAL RESEARCH
FY 2004



Research:

In FY 2004, the BER program will support fundamental research in climate change, environmental remediation, genomics, proteomics, radiation biology, and medical sciences at 223 public and private research institutions in 43 states and at 16 DOE laboratories in 10 states. This research will be conducted in 1020 different research projects by over 2275 researchers and students. In addition to the principal investigator for each research project funded by BER, individual projects typically have between 1 and 20 additional PhD-level scientists who are funded collaborators. Information on scientific collaborators is not routinely tracked.

- ***University Research:*** University researchers play a critical role in the BER program, conducting fundamental research and developing the next generation of scientists for the nation's biological and environmental research efforts. BER will continue its commitment to and dependence on scientists at the Nation's universities. In general, BER-supported research at universities and research institutions are single investigator projects. Approximately half of BER basic research funding supports university-based activities directly and indirectly. University scientists are the major scientific users at BER facilities and other enabling research infrastructure such as the ARM program.

  All research projects supported by the BER program undergo regular peer review and evaluation based on the procedures set down in 10 CFR Part 605 for the extramural grant program (http://www.sc.doe.gov/production/grants/merit.html). Peer review of BER projects is performed to provide an independent assessment of the scientific and/or technical merit of the research by peers having knowledge and expertise equal to that of the researchers whose work they review.

- ***National Laboratory Research:*** Research projects at national laboratories are more often multi-investigator team projects that take advantage of unique resources, capabilities, or facilities found at the national laboratories. Researchers at the national laboratories collaborate extensively with academic researchers supported by BER as well as with academic users of the BER facilities and research infrastructure including the Environmental Molecular Sciences Laboratory, Atmospheric Radiation Measurement, Free Air Carbon Dioxide Enhancement, and AmeriFlux sites, Natural and Accelerated Bioremediation Research Field Research Center, the Joint Genome Institute, and the structural biology user facilities at the synchrotron and neutron sources.

All research projects supported by the BER program undergo regular peer review and evaluation. BER research at the DOE Laboratories and scientific user facilities undergoes peer review and evaluation in a similar procedure to that used for university-based research

Program Strategic Performance Goals

Progress toward accomplishing BER's strategic goals will be measured by Program Strategic Performance Goals, Indicators and Annual Targets, as follows:

SC3-1: Identify and characterize the multiprotein molecular machines that carry out the biological functions of cells and determine the biochemical capabilities of complex microbial communities, information needed to develop biotechnology solutions for clean energy, carbon sequestration, and environmental cleanup.

Performance Indicator

Number of complex microbial communities and multiprotein molecular machines that can be characterized per year.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Determined DNA sequence from 41 microbes important for energy and environmental cleanup. [Exceeded Goal]	Develop methods for sequencing DNA from complex microbial communities. (SC3-1)	Determine biochemical capabilities of a complex microbial community needed to develop biological solutions for environmental cleanup. (SC3-1)

SC3-2: Determine the response of the Earth system to different levels of greenhouse gases in the atmosphere.

Performance Indicator

Climate model resolution.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Develop and test a fully coupled atmosphere-ocean-land-sea ice climate model that has twice the spatial resolution of coupled models available in 2000 as part of Climate Modeling and Prediction research. Support multi-disciplinary teams of scientists at multiple institutions using DOE supercomputers to perform model simulations, diagnostics, and testing. [Goal Met]	Improve precision of climate models – deliver a cloud submodel to reduce uncertainty in the atmospheric energy budget by 10 % and increase resolution of atmospheric/ocean submodels to 150 km & sea ice submodel to 75 km for a fully coupled climate model. (SC3-2)	Implement a climate model with new cloud model components developed using Atmospheric Radiation Measurement (ARM) data, which will be used to predict regional and global climate change. (SC3-1)
Completed analysis of physical factors that govern CO_2 and water vapor flux dynamics at AmeriFlux sites. Study identified improvements for low flux measurement, which continues to be under-estimated and may introduce bias of as much as $\pm$ 20% in estimates of net ecosystem exchange (NEE) of CO_2 for example. [Goal Met]	Document a range of net annual carbon gain in deciduous forest sites in eastern North America of 2 to 4 metric tons of carbon per hectare. (SC3-2)	Deliver quantitative estimates of net annual carbon exchange between the atmosphere and terrestrial ecosystems at five AmeriFlux sites in North America. (AmeriFlux is a network of research sites that measure exchange of CO_2, energy, and water between the atmosphere and terrestrial ecosystems.) (SC3-2)
		Establish a model terrestrial ecosystem containing simplified but hierarchical communities (higher plants, consumers of plant production, and soil microorganisms) and begin characterization of the proteome of the major species. (SC3-2)

SC3-3: Develop and demonstrate novel solutions to DOE's most challenging problems, including: 1) in situ treatment of contaminant plumes such as bioremediation and environmental reactive barriers; 2) new treatment options for complex wastes; 3) novel disposal options for complex wastes (e.g. alternative to borosilicate glass) and cost-effective contaminant plume characterization and monitoring techniques for long-term stewardship of sites; 4) improved predictive capabilities for contaminant fate and transport; and 5) basis for accurate assessment of risk factors.

Performance Indicator

Advanced environmental cleanup approaches delivered.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Radiation resistant superbug, *D. radiodurans* changes mobile uranium and technetium in ground water into an immobile state. [Goal Met]	Identify naturally occurring microbial populations responsible for transformation of metals and radionuclides at DOE contaminated sites. (SC3-3)	Quantify rates of immobilization of metals and radionuclides by natural populations of microorganisms at DOE contaminated sites and identify environmental factors regulating their community structure and function. (SC3-3)
Developed a portable immunoassay that determines the quantity and species of uranium. [Goal Met]	Field test novel, long-term monitoring systems for DOE contaminated sites that are less invasive and require minimal human resources. (SC3-3)	Use experimental results from Hanford subsurface contaminant flow and transport studies to verify model improvement. (SC3-3)

SC3-4: Develop innovative radiopharmaceuticals for diagnosis and treatment of human disease and develop novel imaging instrumentation and technologies to precisely visualize and measure biological functions, including gene expression, and more accurately detect human disease.

Performance Indicator

Number of novel imaging devices delivered.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Developed novel radiopharmaceutical tracers to image the brain in obesity and addictive disorders. [Goal Met]	Establish new infrastructure in radiochemistry to develop novel radiopharmaceuticals needed to image changes in the brains of patients with mental and neurological diseases. (SC3-4)	Develop 2-4 novel radiopharma-ceuticals to be used to image the brains of patients suffering from mental, neurological diseases and cancer. (SC3-4)
Developed PET and technetium radiotracers that will be used to detect expression of specific genes. [Goal Met]	Develop technology to image gene expression in real time using *in vitro* systems – precursor of a new medical imaging tool for disease diagnosis and monitoring treatment efficacy. (SC3-4)	Develop technology to detect steady state levels of the products produced by genes in real time and complete first image of the expression of one gene using cells in culture.
Development of a low-density microelectronic array (prototype artificial retina) that was inserted into the eye of a dog. [Goal Met]	Design an artificial retina – a microelectronic array to be used for the treatment of blindness. (SC3-4)	Complete fabrication of prototype micro array for use as an artificial retina. (SC3-4)

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Development and modeling of the platform for a small biosensor for rapid diagnosis of specific infectious diseases. [Goal Met]	Design a small biosensor device for rapid diagnosis of specific infectious diseases, using tuberculosis as a model organism. This technology will have broad application including, for example, in vivo monitoring of blood glucose in diabetics. (SC3-4)	Complete fabrication of a compact device for the rapid diagnosis of tuberculosis. (SC3-4)

SC7-3: Manage facilities operations and construction to the highest standards of overall performance using merit evaluation with independent peer review. (BER)

Performance Indicator

Average operational downtime of facilities will not exceed 10% of total time scheduled, and construction and upgrades of facilities will be within 10% of baseline schedule.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Construction initiated on Laboratory for Comparative and Functional Genomics at Oak Ridge. [Goal Met]	Complete construction of Laboratory for Comparative & Functional Genomics at Oak Ridge. (SC7-1)	Begin operation of Laboratory for Comparative & Functional Genomics at Oak Ridge. (SC7-1)
Doubled capacity of the Production Genomics Facility (PGF) to sequencing 8 billion base pairs of DNA. [Exceeded Goal]	Increase capacity of Production Genomics Facility (PGF) to sequence 17 billion base pairs of DNA per year, an increase of approximately 50% from FY 2002. (SC7-1)	Begin operation of Production Genomics Facility as a user facility. (SC7-1)
Environmental Molecular Sciences Laboratory developed a new type of mass spectrometer that is 1000 times more sensitive than existing systems for identifying the proteome of organisms. [Goal Met]	Environmental Molecular Sciences Laboratory 's (EMSL) new high performance computer is fully operational. (SC7-1)	The Environmental Molecular Sciences Laboratory's 900 MHz Nuclear Magnetic Resonance (NMR) instrument will be fully operational and have an established user base. (SC7-1)
		Average operational downtime of BER facilities will not exceed 10% of total time scheduled. (SC7-1)

Program Assessment Rating Tool (PART) Assessment

The Office of Management and Budget's (OMB) PART assessment of the BER 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." BER was rated lower for planning and results because of BER's "current lack of adequate long-term and annual performance measures" though it was acknowledged that "the program has made significant strides toward developing such measures despite the problems inherent in measuring and predicting scientific progress."

The BER program was found to be focused, well managed, and to have played a leading role in the genomics revolution. BER's coordination of research with other federal research agencies was acknowledged. The regular review of the BER program by panels of outside experts was also acknowledged. At OMB's suggestion, BER is examining its use of these outside expert panels and will identify by the end of FY 2003 ways to improve the efficiency of these reviews.

To address OMB's concern for BER's "current lack of adequate long-term and annual performance measures," BER is working with SC, the Chief Financial Officer, and OMB to reform its performance measures and goals to more accurately predict future scientific progress in a scientifically justifiable and meaningful manner.

BER LEADERSHIP AND UNIQUE ROLES

The BER program has a broad range of unique roles for the Department and the national and international scientific communities including:

- Manage research on microbes for energy and the environment and work with the Advanced Scientific Computing Research program to develop the computational methods and capabilities needed to advance understanding of complex biological systems, predict their behavior, and use that information to address DOE needs.
- Provide the facilities, instrumentation, and technology needed to (1) characterize the multiprotein complexes that result in microbial products and processes of use to DOE, and (2) determine the functional repertoire of complex microbial communities that can be used to address DOE needs.
- Develop cutting edge technologies, facilities, and resources, including animal models, for the Human Genome Project.
- Provide world leadership in low dose radiation research.
- Provide world-class structural biology user facilities and unique computational and experimental structural biology research emphasizing protein complexes involved in recognition and repair of DNA damage and remediation of metals and radionuclides.
- Provide world leadership in ground-based measurement of clouds and atmospheric properties to resolve key uncertainties in climate change, through the Atmospheric Radiation Measurement (ARM) program.
- Develop advanced predictive capabilities using coupled climate models on massively parallel computers for decade-to-century long simulations of climate change.
- Support fundamental research on carbon sequestration to develop technologies that enhance the uptake of carbon in terrestrial and ocean ecosystems.
- Provide world-class scientific user facilities for environmental and climate change research.

- Provide world leadership in radiopharmaceutical development for wide use in the medical and research communities.
- Maintain world leadership in instrumentation development for medical and biological imaging.
- Enable interdisciplinary teams of scientists to use the unique resources in physics, chemistry, material sciences, and biology at the National Laboratories to develop novel medical applications.
- Manage the Environmental Management Science Program (EMSP) in consultation with the Office of Environmental Management (EM) to identify and select the appropriate fundamental research activities.
- Ensure that the rights and welfare of human research subjects at the Department are protected while advances in biomedical, environmental, nuclear, and other research lead to discoveries that benefit humanity.

Significant Program Shifts

For FY 2004, BER will focus on:

- Research to create the new generation of sophisticated high-throughput technologies that are required for translating the new biology, making them widely and readily available, and using them effectively to serve the community of national laboratories, academic, and industrial researchers. Research needed to develop these technologies is currently being funded as part of the Genomes to Life program. This research will be a key component of the design and development of future facilities needed in the Genomes to Life program for conducting Systems Biology research.
- With the completion of the high quality DNA sequence of human chromosomes 5, 16, and 19, DNA sequencing capabilities at the JGI will emphasize the DNA sequencing needs of the broader research community. Sixty percent of the JGI's sequencing capacity of 1 billion base pairs per month will be available to all scientists as a user service as determined by scientific peer review of nominations for DNA sequencing targets. The remaining sequencing capacity will continue to address DOE research on microbes for energy and the environment.
- In FY 2004, BER will continue to contribute to the Administration's Climate Change Research Initiative (CCRI) to deliver information useful to policy makers. The BER contribution to the CCRI will primarily be through focused research on the carbon cycle to help resolve the North American carbon sink question –What fraction of the excess carbon dioxide emissions are taken up by the U.S. terrestrial ecosystem? BER will also contribute to the CCRI in other areas, including climate change modeling, atmospheric composition, and regional impacts of climate change.
- In FY 2004, BER will initiate new ecological research to understand how the scales of response of complex ecosystems to the environment, including their underlying causal mechanisms and pathways, are linked, ranging from the proteomes of individual species to the whole ecosystem. The focus initially will be on understanding the linkages of scales in model terrestrial ecosystems containing simplified but hierarchical communities (higher plants, consumers of plant production, and soil microorganisms). A key environmental factor such as temperature that is known to affect ecosystem functioning (e.g., carbon and nutrient cycling) will be experimentally manipulated and proteomic responses of individual species and the whole ecosystem will be measured. Advanced biologically based computational algorithms and ecosystem models will be developed to establish whether and how proteomic changes (in either single species or whole systems) explain the

responses and behavior of complex ecosystems. Tools and principles developed from this research will have broad generality and eventual application to problems in carbon sequestration, ecological risk assessment, environmental restoration and cleanup, and early detection of ecological responses to climate change and other environmental perturbations caused by energy production and use.

- Bioremediation research will continue its focus on the biotransformation of radionuclides and metals at contaminated DOE sites, the community of microbes that affect the transformations in subsurface environments at the sites, and the development of strategies for using bioremediation to clean up or stabilize these contaminants at DOE sites.
- In FY 2003 the Environmental Management Science Program and the Savannah River Ecology Laboratory were transferred from the Office of Environmental Management (EM) to the Office of Science. BER manages these research activities according to Office of Science principles, with extensive input from EM.
- In FY 2003, $20,000,000 was proposed for transfer to the Department of Homeland Security to determine the DNA sequences of potential biothreat agents, to develop technologies to determine and compare the function of the genes coded for by these DNA sequences, and to develop computational tools and databases for the DNA sequencing and annotation of potential biothreat agents. These activities will be budgeted by the Department of Homeland Security in FY 2004.

Genomes to Life Research

The FY 2004 budget includes funds for the continued expansion of the Genomes to Life program—a program at the forefront of the biological revolution—a systems approach to biology at the interface of the biological, physical, and computational sciences to address DOE's energy, environment, and national security mission needs. This research will continue to more fully characterize the inventory of multiprotein molecular machines found in selected DOE-relevant microbes and higher organisms and to determine the diverse biochemical capabilities, especially as they relate to potential biological solutions to DOE needs, found in populations of microbes isolated from DOE-relevant sites. In FY 2004, new capabilities will be developed for high throughput protein production and diverse imaging capabilities needed to characterize multiprotein complexes and gene regulatory networks and capabilities in high throughput proteomics will be enhanced well beyond current potential. Also in FY 2004, research and development that underpins future facilities needed by the Genomes to Life program will be conducted. Antiterrorism-related activities have been transferred to the Department of Homeland Security.

Climate Change Science Program

In 2003, the Administration launched a new Climate Change Research Initiative (CCRI) that is intended to focus research on areas where substantial progress in understanding and predicting climate change, including its causes and consequences, is likely over the next five years. DOE, in conjunction with its interagency partners, including NSF, NASA, NOAA, USDA, Interior, and EPA, will continue to focus its Climate Change Research in specific areas relevant to the CCRI. These areas include climate modeling, climate processes, carbon cycling, atmospheric composition, and regional impacts. The deliverables from this research will be targeted at information useful to policy makers. In FY 2004, DOE will also continue to contribute research to the CCRI research area for which additional funding was requested by the Administration for DOE in FY 2003, specifically carbon cycle research to resolve the magnitude and location of the North American carbon sink.

Scientific Discovery through Advanced Computing (SciDAC)

The Scientific Discovery through Advanced Computing (SciDAC) activity is a set of coordinated investments across all Office of Science mission areas with the goal of achieving 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 together with 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 Biological and Environmental Research request includes funds to maintain support of the Department's major scientific user facilities. Facilities include structural biology research beam lines at the synchrotron light sources and neutron sources and the operation of the William R. Wiley Environmental Molecular Sciences Laboratory where research activities underpin long-term environmental remediation and other DOE missions in energy and national security. With this funding, BER will provide for the operation of the facilities, assuring access for scientists in universities, federal laboratories, and industry. BER will also leverage both federally and privately sponsored research to maintain support for and operation of these facilities.

BER will maintain and operate EMSL and the structural biology user facilities so that the unscheduled operating downtime will be less than 10%, on average, of total scheduled operating time.

User Statistics for the Environmental Molecular Sciences Laboratory[a]

	FY 2000	FY 2001	FY 2002	FY 2003	FY 2004
Maximum hours	4,365	4,365	4,365	4,365	4,365
Scheduled hours	3,130	3,130	4,275	4,365	4,365
Unscheduled Downtime	5%	5%	5%	5%	5%

[a] Scientists use or remotely access some of the more than 100 instrumentation/computer systems in the EMSL 24 hours/day while other instruments are used only 10-12 hours/day. Maximum hours identified above are therefore based on a 12-hour day average estimate. Scheduled hours and downtime for each of the 100 instrument systems are also unique. As a result, the scheduled hours identified above are based on a 10-hour day average estimate. None of the major instrument systems within the EMSL have experienced any significant unscheduled downtimes.

User statistics for BER structural biology user facilities at DOE neutron and light sources are included as part of the user statistics collected and reported by the Basic Energy Sciences program and are not repeated here.

Construction and Infrastructure:

BER will meet the cost and schedule milestones for construction of facilities and major items of equipment with 10% of baseline estimates.

Construction of Laboratory for Comparative and Functional Genomics at Oak Ridge National Lab

	FY 2000	FY 2001	FY 2002	FY 2003	FY 2004
Total Project Cost	$520,000	$2,495,000	$11,405,000	0	0
Cost Variance	0	0	0	0	0
Schedule Variance	0	0	+$10,000,000[a]	-$10,000,000[a]	0
Major Milestones Completed	-	-	Construction started in 3rd quarter	Construction to be completed in 4th quarter	-

[a] Full funding for the construction of the Laboratory for Comparative and Functional Genomics was provided in FY 2002. By the end of FY 2003 construction of the Laboratory will be completed on schedule. This new facility will replace a 50-year old animal facility with rapidly escalating maintenance costs that is still in use at Oak Ridge National Laboratory.

Funding for capital equipment is increased to provide the capabilities essential for initiating the Genomes to Life program. For all other BER activities the capital equipment is held at near the FY 2003 level.

The BER program, as part of its responsibilities as landlord for the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge Institute for Science and Education (ORISE), provides funding for the general plant projects (GPP) and general plant equipment (GPE). In addition to the general-purpose line item projects funded out of the Science Laboratories Infrastructure program, GPP and GPE represent the capital investment funding provided by the Department for the general laboratory infrastructure. This ensures that the PNNL and ORISE infrastructures will continue to enable the Department's mission activities at these sites.

Workforce Development

Workforce development is an integral and essential element of the BER mission to help ensure a science-trained workforce, including researchers, engineers, science educators, and technicians. The research programs and projects at the National Laboratories, universities, and research institutes actively integrate undergraduate and graduate students and post-doctoral investigators into their work. This "hands-on" approach is essential for the development of the next generation of scientists, engineers, and science educators. Specific fellowship programs are also sponsored by BER to target emerging areas of need. Over 1,500 graduate students and post-doctoral investigators will be supported at universities and at National Laboratories in FY 2003. This number includes some 600 graduate students and post-doctoral investigators who conducted their research at the EMSL in FY 2002. BER will continue its support for graduate students and post-doctoral investigators in FY 2004. The number of graduate students and post-doctoral investigators will remain approximately at the FY 2003 level.

Graduate students and postdoctoral investigators use Office of Science user facilities. For example, they use the structural biology experimental stations on the beam lines at the synchrotron light sources and the instruments at the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). Using these unique research tools enables the graduate students and post-doctoral investigators to participate in and conduct leading edge research. Approximately half of all of the facility users are graduate students and post-doctoral investigators. The graduate students and post-doctoral investigators are supported by resources from a wide variety of sponsors, including BER, other Departmental research programs, other federal agencies, and U.S. and international private institutions. Graduate students and post-doctoral investigators at the synchrotron light sources are included in the Basic Energy Sciences (BES) user facility statistics and are thus not included here. As noted above, some 600 graduate students and post-doctoral investigators conducted their research at the EMSL in FY 2002.

BER will continue its commitment to and dependence on research scientists at the Nation's universities. Approximately half of BER basic research funding directly or indirectly supports university-based activities. University scientists are the major users at BER facilities and other enabling research infrastructure. University-based scientists are an integral part of research programs across the entire range of the BER portfolio. These scientists are funded through individual peer-reviewed grants and as members of peer-reviewed research teams involving both national laboratory and university scientists.

University-based scientists are the principal users of BER user facilities for structural biology at the synchrotron and neutron sources. They are also users of the Environmental Molecular Sciences Laboratory, and the Natural and Accelerated Bioremediation Research (NABIR) program's Field Research Center. University scientists also form the core of the Atmospheric Radiation Measurement (ARM) science team that networks with the broader academic community as well as with scientists at other agencies, such as the National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration. In addition, university-based scientists are funded through Requests for Applications across the entire BER program including genomics, structural biology, low dose radiation research, global change research, bioremediation research, medical imaging, and radiopharmaceutical development. Furthermore, university scientists work in close partnership with scientists at National Laboratories in many BER programs including genomics, and carbon sequestration research.

DOE-BER Human Capital

	FY 2000	FY 2001	FY 2002	FY 2003	FY 2004
# University Grants	532	579	628	630[a]	630[a]
Size / Duration	$302,000/yr	$287,000/yr	$309,000/yr	$300,000/yr[a]	$300,000/yr[a]
	3 years	3 years	3 years	3 years	3 years
# Lab Projects	379	397	392	395[a]	400[a]
# Permanent PhDs[b]	1310	1370	1427	1491[a]	1489[a]
# Postdocs[c]	251	274	357	373[a]	372[a]
# Graduate Students[c]	438	443	491	481[a]	488[a]
# PhDs awarded[d]	NA[d]	NA[d]	NA[d]	NA[d]	NA[d]

[a] Estimated. Information on the number of research projects funded, the size of those projects, or the number of personnel involved cannot be known prior to the receipt of research applications or proposals, their peer review, and the completion of funding decisions.

[b] Estimated. Information is not readily available on the total number of permanent PhDs associated with each research project. In addition to the principal investigator for each research project funded by BER, individual projects typically have between 1 and 20 additional PhD-level scientists who are funded collaborators. Information on scientific collaborators is not routinely tracked.

[c] Estimated for national laboratory projects.

[d] Information is not available on the number of PhDs awarded as a result of BER funded research at universities or national laboratories. Data will be collected in the future.

Funding Profile

(dollars in thousands)

	FY 2002 Comparable Appropriation	FY 2003 Request	FY 2004 Request	$ Change	% Change
Biological and Environmental Research					
Life Sciences	186,384	190,878	201,408	+10,530	+5.5%
Climate Change Research	125,847	137,959	142,959	+5,000	+3.6%
Environmental Remediation	111,849	109,530	109,320	-210	-0.2%
Medical Applications and Measurement Science	118,640	45,848	45,848	0	--
Subtotal, Biological and Environmental Research	542,720	484,215	499,535	+15,320	+3.2%
Construction	11,405	0	0	0	--
Total, Biological and Environmental Research	554,125[abcd]	484,215[b]	499,535	+15,320	+3.2%

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 $12,972,000 which was transferred to the SBIR program and $776,000 which was transferred to the STTR program.
[b] Excludes $2,128,000 in FY 2002 and $20,000,000 in FY 2003 and FY 2004 for Homeland Security activities that are funded in a separate Department of Homeland Security budget.
[c] Excludes $249,000 for the FY 2002 rescission contained in Section 1403 of P.L. 107-226 Supplemental Appropriations for further recovery from the response to terrorist attacks on the United States.
[d] Excludes $50,000 transferred to Safeguards and Security for a FY 2002 reprogramming.

Funding By Site[a]

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory	23,545	19,245	19,717	+472	+2.5%
Sandia National Laboratories	5,334	3,757	5,846	+2,089	+55.6%
Albuquerque Operations Office	900	850	850	0	--
Total, Albuquerque Operations Office	29,779	23,852	26,413	+2,561	+10.7%
Chicago Operations Office					
Ames Laboratory	830	512	555	+43	+8.4%
Argonne National Laboratory – East	24,446	22,970	23,295	+325	+1.4%
Brookhaven National Laboratory	23,749	16,248	14,964	-1,284	-7.9%
Chicago Operations Office	137,618	46,146	50,394	+4,248	+9.2%
Total, Chicago Operations Office	186,643	85,876	89,208	+3,332	+3.9%
Federal Energy Technology Center	625	0	0	0	--
Idaho Operations Office					
Idaho National Engineering & Environmental Laboratory	2,428	2,205	3,400	+1,195	+54.2%
Idaho Operations Office	14,242	12,552	12,283	-269	-2.1%
Total, Idaho Operations Office	16,670	14,757	15,683	+926	+6.3%
Oakland Operations Office					
Lawrence Berkeley National Laboratory	72,102	42,786	53,055	+10,269	+24.0%
Lawrence Livermore National Laboratory	27,539	28,199	36,502	+8,303	+29.4%
Stanford Linear Accelerator Center	4,435	5,550	3,675	-1,875	-33.8%
Oakland Operations Office	54,058	38,386	47,293	+8,907	+23.2%
Total, Oakland Operations Office	158,134	114,921	140,525	+25,604	+22.3%

[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.

	(dollars in thousands)				
	FY 2002	FY 2003	FY 2004	$ Change	% Change
Oak Ridge Operations Office					
Oak Ridge Inst. For Science & Education	5,850	4,761	4,550	-211	-4.4%
Oak Ridge National Laboratory	58,549	37,495	38,448	+953	-2.5%
Thomas Jefferson National Accelerator Facility	832	500	0	-500	-100.0%
Oak Ridge Operations Office	869	352	352	0	--
Total, Oak Ridge Operations Office	66,100	43,108	43,350	+242	+0.6 %
Richland Operations Office					
Pacific Northwest National Laboratory	86,047	77,677	81,105	+3,428	+4.4%
Richland Operations Office	100	0	0	0	--
Total, Richland Operations Office	86,147	77,677	81,105	+3,428	+4.4%
Savannah River Operations Office					
Westinghouse Savannah River	239	0	0	0	--
Savannah River Operations Office	8,754	6,326	8,015	+1,689	+26.7%
Total, Savannah River Operations Office	8,993	6,326	8,015	+1,689	+26.7%
Washington Headquarters	1,034	117,698	95,236	-22,462	-19.1%
Total, Biological and Environmental Research	554,125 [abcd]	484,215 [b]	499,535	+15,320	+3.2%

[a] Excludes $12,972,000 which was transferred to the SBIR program and $776,000 which was transferred to the STTR program.

[b] Excludes $2,128,000 in FY 2002 and $20,000,000 in FY 2003 and FY 2004 for Homeland Security activities that are funded in a separate Department of Homeland Security budget.

[c] Excludes $249,000 for the FY 2002 rescission contained in Section 1403 of P.L. 107-226 Supplemental Appropriations for further recovery from the response to terrorist attacks on the United States.

[d] Excludes $50,000 transferred to Safeguards and Security for a FY 2002 reprogramming.

Site Description

Ames Laboratory

Ames Laboratory is a Multiprogram Laboratory located on 10 acres in Ames, Iowa. At Ames, BER supports research into new biological imaging techniques such as the study of gene expression in real time and fluorescence spectroscopy to study environmental carcinogens.

Argonne National Laboratory

Argonne National Laboratory (ANL) in Argonne, Illinois, is a Multiprogram Laboratory located on a 1,700 acre site in suburban Chicago. ANL has a satellite site located in Idaho Falls, Idaho. At ANL, BER supports the operation of a high-throughput national user facility for protein crystallography at the Advanced Photon Source. In support of climate change research, ANL coordinates the operation and development of the Southern Great Plains, Tropical Western Pacific, and North Slope of Alaska ARM sites. The principal scientist for the Atmospheric Chemistry program is at ANL, providing broad scientific integration to the program. Research is conducted to understand the molecular control of genes and gene pathways in microbes. ANL, in conjunction with ORNL and PNNL and six universities, co-hosts the terrestrial carbon sequestration research center, Carbon Sequestration in Terrestrial Ecosystems (CSiTE).

Brookhaven National Laboratory

Brookhaven National Laboratory (BNL) is a Multiprogram Laboratory located on a 5,200 acre site in Upton, New York. BER supports the operation of beam lines for protein crystallography at the National Synchrotron Light Source for use by the national biological research community, research in biological structure determination, and research into new instrumentation for detecting x-rays and neutrons. Research is also conducted on the molecular mechanisms of cell responses to low doses of radiation.

The radiotracer chemistry, radiopharmaceutical technology, and magnetic resonance imaging research and development programs support applications of novel techniques for imaging brain function in normal and diseased states, and to study the biochemical basis of disease.

Climate change research at BNL include the operation of the ARM External Data resource that provides ARM investigators with data from non-ARM sources, including satellite and ground-based systems. BNL scientists form an important part of the science team in the Atmospheric Sciences program, providing special expertise in atmospheric field campaigns and aerosol research. BNL scientists play a leadership role in the development of, and experimentation at, the Free-Air Carbon Dioxide Enhancement (FACE) facility at the Duke Forest used to understand how plants respond to elevated carbon dioxide concentrations in the atmosphere.

Idaho National Engineering and Environmental Laboratory

Idaho National Engineering and Environmental Laboratory (INEEL) is a Multiprogram Laboratory located on 572,000 acres in Idaho Falls, Idaho. Using unique DOE capabilities such as advanced software for controlling neutron beams and calculating dose, BER supports research into boron chemistry, radiation dosimetry, analytical chemistry of boron in tissues, and engineering of new systems for application of this treatment technique to tumors, including brain tumors. Research is also supported into the analytical chemistry of complex environmental and biological systems using the technique of mass spectrometry.

Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory (LBNL) is a Multiprogram Laboratory located in Berkeley, California. The Laboratory is on a 200 acre site adjacent to the Berkeley campus of the University of California. LBNL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing techniques and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. The laboratory also conducts research on the molecular mechanisms of cell responses to low doses of radiation and on the use of model organisms to understand and characterize the human genome.

LBNL operates beam lines for determination of protein structure at the Advanced Light Source for use by the national and international biological research community, research into new detectors for x-rays, and research into the structure of proteins, including membrane proteins.

The nuclear medicine program supports research into novel radiopharmaceuticals for medical research and studies of novel instrumentation for imaging of living systems for medical diagnosis.

LBNL supports the Natural and Accelerated Bioremediation Research (NABIR) program and the geophysical and biophysical research capabilities for NABIR field sites. BER supports research at LBNL into new technologies for the detailed characterization of complex environmental contamination. LBNL also develops scalable implementation technologies that allow widely used climate models to run effectively and efficiently on massively parallel processing supercomputers. The carbon cycle field experiment at the ARM Southern Great Plains site is maintained and operated by LBNL.

Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory (LLNL) is a Multiprogram Laboratory located on an 821 acre site in Livermore, California. LLNL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. LLNL also conducts research on the molecular mechanisms of cell responses to low doses of radiation, and on the use of model organisms to understand and characterize the human genome.

Through the program for Climate Model Diagnostics and Intercomparison, LLNL provides the international leadership to understand and improve climate models. Virtually every climate modeling center in the world participates in this unique program.

Los Alamos National Laboratory

Los Alamos National Laboratory (LANL) is a Multiprogram Laboratory located on a 27,000 acre site in Los Alamos, New Mexico. LANL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. One of LANL's roles in the JGI involves the production of high quality "finished" DNA sequence. LANL also conducts research on the molecular mechanisms of cell responses to low doses of radiation and on research to understand the molecular control of genes and gene pathways in microbes. Activities in structural biology include the operation of an experimental station for protein crystallography at the Los Alamos Neutron Science Center for use by the national biological research community and research into new techniques for determination of the structure of proteins.

LANL provides the site manager for the Tropical Western Pacific ARM site. LANL also has a crucial role in the development, optimization, and validation of coupled atmospheric and oceanic general circulation models using massively parallel computers.

LANL also conducts research into advanced medical imaging technologies for studying brain function and research into new techniques for rapid characterization and sorting of mixtures of cells and cell fragments.

Oak Ridge Institute for Science and Education

Oak Ridge Institute for Science and Education (ORISE) is located on a 150 acre site in Oak Ridge, Tennessee. ORISE coordinates several research fellowship programs for BER. ORISE also coordinates activities associated with the peer review of most of the research proposals submitted to BER.

ORISE conducts research into modeling radiation dosages for novel clinical diagnostic and therapeutic procedures.

Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) is a Multiprogram Laboratory located on a 24,000 acre site in Oak Ridge, Tennessee. ORNL has a leadership role in research focused on the ecological aspects of global environmental change. The Throughput Displacement Experiment at the Walker Branch Watershed is a unique resource for long term ecological experiments. ORNL is the home of the newest FACE experiment supported by BER. ORNL also houses the ARM archive, providing data to ARM scientists and to the general scientific community. ORNL scientists provide improvement in formulations and numerical methods necessary to improve climate models. ORNL scientists make important contributions to the NABIR program, providing special leadership in microbiology applied in the field. ORNL also manages the NABIR Field Research Center, a field site for developing and testing bioremediation methods for metal and radionuclide contaminants in subsurface environments.

ORNL conducts research on widely used data analysis tools and information resources that can be automated to provide information on the biological function of newly discovered genes identified in high-throughput DNA sequencing projects. The laboratory also uses mice as model organisms to understand and characterize the human genome.

ORNL conducts research into the application of radioactively labeled monoclonal antibodies in medical diagnosis and therapy, particularly of cancer, as well as research into new instrumentation for the analytical chemistry of complex environmental contamination using new types of biosensors.

ORNL recently has upgraded the High Flux Isotope Reactor (HFIR) to include a cold neutron source that will have high impact on the field of structural biology. BER is developing a station for Small Angle Neutron Scattering at HFIR to serve the structural biology community.

ORNL, in conjunction with ANL and PNNL and six universities, co-hosts a terrestrial carbon sequestration research center, CSiTE.

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. PNNL is home to the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). PNNL scientists, including EMSL scientists, play important roles in both supporting the NABIR program and in performing research for NABIR.

PNNL operates the unique ultrahigh field mass spectrometry and nuclear magnetic resonance spectrometry instruments at the Environmental Molecular Sciences Laboratory for use by the national research community.

PNNL provides the lead scientist for the Environmental Meteorology Program, the G-1 research aircraft, and expertise in environmental field campaigns. PNNL provides the planning and interface for the Climate Change Prediction Program with other climate modeling programs. The ARM program office is located at PNNL, as is the ARM chief scientist and the project manager for the ARM engineering activity; this provides invaluable logistical, technical, and scientific expertise for the program.

PNNL conducts research into new instrumentation for microscopic imaging of biological systems and for characterization of complex radioactive contaminants by highly automated instruments.

PNNL conducts research on the molecular mechanisms of cell responses to low doses of radiation and on the development of high throughput approaches for characterizing all of the proteins (the proteome) being expressed by cells under specific environmental conditions.

PNNL, in conjunction with ANL and ORNL and six universities, co-hosts a terrestrial carbon sequestration research center, CSiTE.

PNNL also conducts research on the integrated assessment of global climate change.

In March 2001 the University of Maryland and Pacific Northwest National Laboratory created a Joint Global Change Research Institute in College Park, Maryland. The Institute investigates the scientific, social, and economic implications of climate change, both nationally and globally. BER funding supports research grants to the university and research projects to PNNL that have been successfully peer reviewed in open competition.

Sandia National Laboratory

Sandia National Laboratory (SNL) is a Multiprogram Laboratory, with a total of 3,700 acres, located in Albuquerque, New Mexico, with sites in Livermore, California and Tonopah, Nevada. SNL provides the site manager for the North Slope of Alaska ARM site. The chief scientist for the ARM-UAV program is at SNL, and SNL takes the lead role in coordinating and executing ARM-UAV missions. The laboratory conducts advanced research and technology development in robotics, smart medical instruments, microelectronic fabrication, and computational modeling of biological systems.

To support environmental cleanup, SNL conducts research into novel sensors for analytical chemistry of contaminated environments.

SNL conducts computational and biological research in support of the Genomes to Life research program.

Savannah River Site

The Savannah River Site complex covers 198,344 acres, or 310 square miles encompassing parts of Aiken, Barnwell and Allendale counties in South Carolina bordering the Savannah River. At the Savannah River Site, BER supports the Savannah River Ecology Laboratory (SREL), a research unit of the University of Georgia operating at the site for over forty years. The SREL conducts research aimed at reducing the cost of environmental cleanup and remediation while ensuring biodiversity to the restored environment.

BER supports the Savannah River Ecology Laboratory through a cooperative agreement with the University of Georgia. The ecological research activity is aimed at reducing the cost of cleanup and remediation while ensuring biodiversity to the restored environment.

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, and is the home of the Stanford Synchrotron Radiation Laboratory (SSRL). The Stanford Synchrotron Radiation Laboratory was built in 1974 to utilize 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. The facility is now comprised of 25 experimental stations and is used each year by over 700 researchers from industry, government laboratories and universities. Through the Stanford Linear Accelerator Center, BER (in coordination with the National Institutes of Health) is funding the operation of nine SSRL beam lines for structural biology. This program involves synchrotron radiation-based research and technology developments in structural molecular biology that focus on protein crystallography, x-ray small angle scattering diffraction, and x-ray absorption spectroscopy for determining the structures of complex proteins of many biological consequences.

Thomas Jefferson National Accelerator Facility

The Thomas Jefferson National Accelerator Facility (TJNAF) is a basic research laboratory located on a 200 acre site in Newport News, Virginia. BER supports the development of advanced imaging instrumentation at TJNAF that will ultimately be used in the next generation medical imaging systems.

All Other Sites

The BER program funds research at 223 institutions, including colleges/universities, private industry, and other federal and private research institutions located in 43 states.

BER supports a broad range of peer-reviewed research at America's universities, including institutions that traditionally serve minority communities. BER research opportunities are announced through public solicitations in the Federal Register for research applications from universities and the private sector.

BER's Life Sciences research is conducted at a large number of universities. For example research is conducted in support of high-throughput human DNA sequencing at the JGI, on the sequencing of entire microbial genomes with value to the DOE mission, to understand the molecular control of genes and gene pathways in microbes, on the use of model organisms to understand and characterize the human genome, and on the molecular mechanisms of cell responses to low doses of radiation.

In structural biology, universities provide new imaging detectors for x-rays, research in computational structural biology directed at the understanding of protein folding, and research into new techniques such as x-ray microscopy.

Peer-reviewed projects are supported in each element of the Climate Change Research subprogram, with very active science teams, in particular, in the Atmospheric Chemistry Program and the ARM program. Academic investigators are also essential to the Integrated Assessment portfolio.

In the NABIR program, academic and private sector investigators are performing research in areas that include mechanistic studies of bioremediation of actinide and transition metal contamination, the structure of microbial communities in the presence of uranium and other such contaminants, gene function in microorganisms with degradative properties, geochemical and enzymatic processes in microbial reduction of metals, and the use of tracers to monitor and predict metabolic degradative activity.

In the nuclear medicine program, universities conduct research into new types of radiopharmaceuticals, particularly those based on application of concepts from genomics and structural biology. BER places emphasis on radiopharmaceuticals that will be of use in advanced imaging techniques such as positron emission tomography. The research supports new instrumentation for medical imaging. The BER Measurement Science program supports research into novel types of biosensors for medical imaging and application in analytical chemistry of contaminated environments.

Life Sciences

Mission Supporting Goals and Measures

The goal of the Life Sciences subprogram is to deliver fundamental knowledge of biological systems that can be used to address DOE needs in clean energy, carbon sequestration, and environmental cleanup. Fundamental research is supported in structural biology, genomics, and the health effects of low dose radiation. Human, animal, and microbial DNA sequencing is used to understand the genetic and environmental basis of normal and abnormal biological function, from human genes that make some people more sensitive to the adverse effects of low doses of radiation to the biochemical capabilities of complex microbial communities that could be used to produce clean energy or sequester atmospheric carbon dioxide. Scientific tools and resources are developed and made widely available for determining protein structures and genomic DNA sequences and for understanding the structure, function, and regulation of multiprotein complexes from DOE-relevant organisms – information that can then be used to develop biotechnology solutions for DOE needs. Finally, low dose radiation research provides knowledge underpinning rigorous, cost-effective standards to protect the health of cleanup workers and the public and for science-based decisions on DOE site cleanup. In FY 2003 $20,000,000 related to genomic analysis of potential biothreat agents was transferred to the Department of Homeland Security.

BER supports research in five areas of the Life Sciences: structural biology; low dose radiation; molecular/systems biology; human genome; and biological research.

- BER develops and supports user facilities for the Nation's structural biologists at synchrotron, nuclear magnetic resonance (NMR), and neutron sources. BER also determines the structures of proteins important for the bioremediation of metals and radionuclides or of proteins that are involved in the repair of DNA damage.
- BER supports research on the biological effects of low doses of ionizing radiation and works closely with scientists, regulators, and the public to ensure that the research results are available to develop a better scientific basis for adequately protecting people from the adverse effects of ionizing radiation.
- BER supports systems biology research in the Genomes to Life program by developing the experimental and, together with the Advanced Scientific Computing Research program, computational resources, tools, and technologies needed to understand the complex behavior of complete biological systems – from single microbes to complex microbial communities. This information can be used to develop innovative solutions for energy production, waste cleanup, and carbon management.
- BER takes advantage of the remarkable high throughput and cost-effective DNA sequencing capacity it developed as part of the International Human Genome Project to meet future DNA sequencing needs of DOE and other agencies. BER also develops resources, tools, and technologies needed to analyze and interpret DNA sequence data from entire organisms and to study the ethical, legal, and social implications (ELSI) of information and data resulting from genome projects.

- BER develops resources, tools, and technologies to understand the function of human genes that it identifies as part of the International Human Genome Project using model organisms such as the mouse, *Fugu* (the puffer fish), and *Ciona* (the sea squirt).

The Life Sciences subprogram provides fundamental knowledge building to long-term outcomes that underpin the Program Strategic Performance Goals and the Office of Science's Strategic Objectives. Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This program was reviewed as part of a BERAC review of the entire BER program in FY 2001. The next scheduled comprehensive review of the Life Sciences subprogram by BERAC will be in FY 2004. The following are recent scientific accomplishments that highlight program progress.

- *First Tree Genome to be Sequenced.* The genome of *Populus balsamifera* ssp. *trichocarpa,* commonly known as the black cottonwood, a species of Poplar tree will be the first tree genome ever sequenced. Scientists working on tree genetics and tree productivity and product utilization are highly enthusiastic about the sequencing of this tree species because it represents an important first step in understanding the genome of a common, commercially important tree species with potential impacts that could include improved carbon sequestration and biomass for energy. This effort is being led by a consortium of scientists from the University of Washington, Oregon State University, Pennsylvania State University, the British Columbia Genome Sequence Center, the Swedish University of Agricultural Sciences, the National Center for Genome Research in New Mexico, the DOE Joint Genome Institute (JGI), the Oak Ridge National Laboratory, and other institutions. The sequencing will be carried out at DOE's high throughput DOE sequencing facility, the JGI.
- *Pufferfish Helps Scientists Understand the Human Genome.* The first public assembly of an animal genome, the genome of the Japanese pufferfish *Fugu rubripes,* has been completed by the DOE JGI. Although the *Fugu* genome contains essentially the same genes and regulatory sequences as the human genome, it carries those genes and regulatory sequences in approximately 365 million bases as compared to the 3 billion bases that make up human DNA. With far less so-called "junk DNA" to sort through, the information can then be used to help identify genes and regulatory sequences in the human genome. This effort was led by an international research consortium that included the JGI, the Singapore Biomedical Research Council's Institute for Molecular and Cell Biology, the Human Genome Mapping Resource Centre of the United Kingdom's Medical Research Council, the Cambridge University Department of Oncology, and the Institute for Systems Biology in Seattle, Washington. The consortium's sequencing efforts were bolstered by two US companies, Celera Genomics of Rockville, Maryland and Myriad Genetics, Inc. of Salt Lake City, Utah.
- *First ever DNA sequence of an algae.* The genomic DNA sequence of a unicellular green algae has been determined by the JGI – the first algae to be sequenced. Chlamydomonads have a 100 million base pair genome (compared to 3 billion for humans and 365 million for the *Fugu* described above) and are a genus of unicellular green algae (Chlorophyta) found nearly everywhere - in soil, fresh water, oceans, and even in snow on mountaintops. Algae in this genus have a cell wall, a chloroplast for photosynthesis, an "eye" that perceives light, and two flagella with which they can swim using a breast-stroke type motion. More than 500 different species of Chlamydomonas have been described. The most widely used laboratory species is *Chlamydomonas reinhardtii.* DOE is interested in *Chlamydomonas* because of its widespread global distribution and its ability to carry out photosynthesis, the most powerful biological technology for carbon dioxide capture from the atmosphere.

- *First DNA sequence of a marine diatom.* The first ever genomic DNA sequence of a marine diatom, *Thalassiosira pseudonann*, has been determined by the JGI. Diatoms, or marine phytoplankton, are important model organisms for carbon sequestration and are found in all of Earth's oceans. They display an incredible and intriguing variety of shapes and are major players in the Earth's carbon cycle responsible for much of the ocean's ability to move carbon dioxide captured in the near surface regions by photosynthesis to deep ocean compartments. The shapes, growth rates, and carbon management processes of diatoms are all under genetic control and could be exploited to enhance its carbon processing capabilities as a step towards partial mitigation of global warming. Additionally, the silicate shells of many diatoms are engineering and material science marvels and could provide important insights for nanoscience activities.

- *JAZZing up genomes.* Because of the sequencing process, the DNA sequences of organisms large and small are determined in hundreds or thousands of small pieces. A new graphical algorithm, JAZZ, has been developed for stitching these pieces back together into a complete DNA sequence. JAZZ has been used at the JGI to put together the genomes of many microbes, a fungal genome, the genomes of the sea squirt C*iona intestinalis* and the pufferfish *Fugu rubripes*.

- *Another record-breaking year of microbial DNA sequencing.* The JGI has again surpassed expectations in microbial DNA sequencing in FY 2002 by determining high quality draft sequences of 41 microbes important to DOE needs in energy, environmental cleanup, and counter terrorism. Twelve of these organisms are pathogens or their close genetic relatives that were sequenced as part of a coordinated interagency effort to quickly characterize as many potential threat agents as possible.

- *International Scientists Celebrate at Sea Squirt Genome Jamboree*. Fifty scientists from around the world gathered in San Francisco to celebrate, by staying glued to their computers to analyze the DNA sequence of *Ciona intestinalis*, a sea squirt. *Ciona* is an organism with the smallest genome of any experimentally manipulable chordate and is a good system for exploring the evolutionary origins of the chordate lineage, from which vertebrates, including man, sprouted. The complete genome sequence of *Ciona* was determined by DOE's JGI and will provide a foundation for genome-scale analysis of regulatory networks through development. Genes that have survived in humans since the sea squirt's evolution have surely been preserved for good reasons. By comparing the human genome to the genomes of different creatures, researchers can pinpoint which genes have survived hundreds of millions of years of evolution. Those that have survived throughout evolution are likely to have important functions. In other words, they compare these animal genomes to the human genome to see the similarities and differences—and eventually discover the secrets of evolution and disease.

- *First Call for Candidate Microbes for DNA Sequencing*. DOE's JGI will now be available as a resource to all scientists for determining the DNA sequences of microbes or communities of microbes relevant to DOE mission needs including waste remediation, carbon management, and energy production. Microbes nominated by scientists for genomic sequencing will be prioritized by a panel of scientific experts, including representatives from the American Society for Microbiology. All DNA sequence data determined by the JGI will be publicly available to all scientists. This call for nominations for DNA sequencing at the JGI is the first in what is anticipated to be an ongoing series of public calls for DNA sequencing that will effectively make the JGI's considerable DNA sequencing capabilities available to scientists as a public resource.

- *New Neutron User Facility for Structural Biologists* - DOE user facilities for structural biologists at the synchrotron light sources enable scientists to determine high resolution electron density maps of protein crystals needed to determine their three dimensional structure. In some cases, neutrons provide additional information critical to understand protein structure by providing vital insights into the locations of hydrogen bonds and the nature of macromolecular-solvent interactions. A new protein crystallography station at the Los Alamos Neutron Science Center (LANSCE) will be available by the end of 2002. This is the only neutron crystallography station for structural biologists in the U.S.
- *New Ultrasensitive Mass Spectrometer for Proteomics* - Pacific Northwest National Laboratory has developed a new electrospray ionization fourier transform ion cyclotron resonance mass spectrometer (ICR), the highest field and most sensitive ICR mass spectrometer currently available. This new machine is approximately 1000 fold more sensitive than conventional instruments, has a resolution 100-1000 fold greater than conventional instruments and can measure peptides at a level less than or equal to 1 part per million. At this level, most peptides are unique and can be assigned to a specific protein in the genome. In contrast, conventional instruments measure at approximately the 500 parts per million level.

Subprogram Goals

Identify and characterize the multiprotein molecular machines that carry out the biological functions of cells and determine the biochemical capabilities of complex microbial communities, information needed to develop biotechnology solutions for clean energy, carbon sequestration, and environmental cleanup.

Performance Indicator

Number of complex microbial communities and multiprotein molecular machines that can be characterized per year.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Structural Biology – Basic Research)	(Structural Biology – Basic Research)	(Structural Biology – Basic Research)
New research emphasis in Structural Biology basic research. First awards given based on competitive peer review. [Goal Met]	Develop one new computational model that can successfully predict which proteins interact with protein complexes involved in DNA damage recognition and repair or bioremediation of metals and radionuclides from analysis of DNA sequence.	Develop two new computational models that can successfully predict which proteins interact with protein complexes involved in DNA damage recognition and repair or bioremediation of metals and radionuclides from analysis of DNA sequence. Demonstrate accuracy of new model from FY 2003 by experimentally determining the fraction of proteins known to interact with these complexes that are correctly predicted by the model.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Microbial Genomics)	(Microbial Genomics)	(Microbial Genomics)
Determined high quality draft sequences of 41 microbes important to DOE needs in energy and environmental cleanup. [Exceeded Goal]	Draft genomic sequence of more than 30 microorganisms of high DOE relevance and scientific research; improve the computational tools for predicting gene function; and develop methods for sequencing unculturable microbes and microbial consortia.	Determine the frequency of lateral gene transfer among 5 different groups of microbes, improve the efficiency of computational tools for predicting the function of newly identified microbial genes by 50%, and develop new strategies for the rapid comparison of closely related microbial DNA sequences that are twice as efficient as current methods
(Carbon Sequestration Research)	(Carbon Sequestration Research)	(Carbon Sequestration Research)
The first ever genomic DNA sequence of a marine diatom, *Thalassiosira pseudonann*, has been determined by the JGI, well ahead of the original schedule for completion. [Goal Met]	Complete DNA sequence of a member of the genus *Populas* (trees like poplar, aspen, etc.). In addition, determine the draft DNA sequence of *Thalassiosira*, a diatom important in oceanic sequestration.	Identify genes and proteins in the poplar that are important for carbon utilization and initially characterize microbes that live in the poplar rhizosphere.
(Genomes to Life)	(Genomes to Life)	(Genomes to Life)
New research program in FY 2002.	In conjunction with ASCR and using data produced by BER and BES-sponsored microbial cell project researchers, develop new computational tools for the analysis and simulation of biological processes. For 3-5 of the over 70 microbial genomes sequenced by DOE, begin the difficult, comprehensive integration of genomic, biochemical, structural and physiological information on DOE relevant functionalities (e.g., bioremediation, carbon sequestration and/or biomass to fuel). Develop working conceptual and numerical models to describe these functionalities. Sequence one or more consortia of microorganisms that will provide information on how microbes function and interact in the environment, such as at DOE legacy waste sites.	Produce 1000 distinct proteins in quantities of 2 milligrams each in highly purified form and use those proteins to develop tags that enable detection and imaging of 500 of these molecules. These capabilities will be used to address the following GTL goals: (1) imaging the molecular machines of life; (2) imaging to characterize gene regulatory networks; and (3) imaging to characterize complex microbial communities in model and natural environments at the molecular level.

Characterize the biological effects of low doses of ionizing radiation (less than annual DOE exposure limit) to assist policy makers in developing science-based health protection standards to protect DOE cleanup workers and the public and to strengthen the scientific basis for making decisions on radiation exposure limits for DOE site cleanup operations.

Performance Indicator

Eighty percent of all new research projects will be peer reviewed and deemed excellent and relevant, and ongoing projects will be subject to triennial peer review with merit evaluation.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Low Dose Radiation Research)	(Low Dose Radiation Research)	(Low Dose Radiation Research)
BERAC report (March 2001) states that "the program has gotten off to an excellent start and is funding a number of scientifically sound and important projects."	Research results will be incorporated into the National Academy of Sciences Biological Effects of Ionizing Radiation VI report.	By the end of FY 2004, the program will demonstrate for the first time the effects of ionizing radiation on neighbors of irradiated cells in vivo.

Develop high throughput methods for rapidly predicting, characterizing, and understanding the control and functions of genes identified from genomic DNA sequencing.

Performance Indicator

DNA base pairs sequenced per year.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Human Genome)	(Human Genome)	(Human Genome)
The first public assembly of an animal genome, the genome of the Japanese pufferfish *Fugu rubripes,* has been completed by the DOE JGI. With far less so-called "junk DNA" to sort through, the information can then be used to help identify genes and regulatory sequences in the human genome. [Goal Met] A new graphical algorithm, JAZZ, has been developed for stitching small pieces of DNA sequence back together into a complete DNA sequence. JAZZ has been used at the JGI to put together the genomes of many microbes, a fungal genome, the genomes of the sea	Establish at least 30 diverse collaborations for high throughput DNA sequencing with scientists outside the JGI and with programs at other federal agencies.	Produce 12 billion base pairs of high quality DNA sequence at the JGI. Approximately 7.2 billion base pairs of the total will be genomes for outside users based on a peer-review selection process. The remaining sequencing capacity will be used to complete the draft sequence and assembly of the *Xenopus* (frog) genome, a model organism for the Human Genome Project, that will contribute to understanding human development.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
squirt *Ciona intestinalis*, and the pufferfish *Fugu rubripes*. [Goal Met] As of July 2002 the Department of Energy' Joint Genome Institute (JGI) has completed the high quality sequencing of human chromosome 19 and approximately 80% of human chromosome 16. The JGI has also produced seven billion bases of sequences completing the draft sequencing of *Fugu* (the pufferfish) and Ciona (the sea squirt) as its contribution to the Human Genome Program. [Goal Met]		

Manage all BER facility operations to the highest standards of overall performance, using merit evaluation with independent peer review.

Performance Indicator

Average operational downtime of BER facilities will not exceed 10% of total time scheduled.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Structural Biology – Infrastructure) New neutron crystallography user facility opened at LANL's LANSCE. An estimated 2000 users used the structural biology instruments at the DOE national user facilities (end of year data not yet available for FY 2002). [Goal Met]	(Structural Biology – Infrastructure) More than 2,500 highly satisfied users will use the structural biology instruments at the DOE national user facilities. Ten external user groups will use the LANSCE protein crystallography station. The installation of the new station at HFIR for use by structural biologists to determine the structures of protein complexes will be completed.	(Structural Biology – Infrastructure) More than 3,000 highly satisfied users will use the structural biology instruments at the DOE national user facilities. Have five structural biology user groups from outside ORNL complete experiments at the HFIR by the end of FY 2004. Add at least 4000 new structure data sets to the Protein Data Bank during FY 2004. Produce a pixel array detector, with at least 100x100 pixel size, deployed at a DOE synchrotron by the end of FY 2004 (TEC less than $1 million).

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Structural Biology	29,536	27,847	27,809	-38	-0.1%
Molecular and Cellular Biology	55,041	71,195	93,500	+22,305	+31.3%
Human Genome	90,075	76,805	64,572	-12,233	-15.9%
Health Effects	11,732	10,260	10,260	0	0%
SBIR/STTR	0	4,771	5,267	+496	+10.4%
Total, Life Sciences	186,384	190,878	201,408	+10,530	+5.5%

Detailed Program Justification

(dollars in thousands)

	FY 2002	FY 2003	FY 2004
Structural Biology	**29,536**	**27,847**	**27,809**
▪ **Basic Research**	**12,307**	**12,547**	**12,509**

In FY 2004, BER will continue to invest in structural biology research relevant to DOE missions. In carrying out their functions within cells, proteins form complexes with other proteins (forming molecular machines) and interact with a variety of structural and regulatory molecules on which proteins carry out their functions. Understanding how molecular machines carry out their biological functions requires that we observe dynamic changes in protein structure and study protein modifications, translocations, and subcellular concentrations. Starting with DNA sequencing information, research is supported to predict or identify the proteins that are involved in the recognition or repair of radiation-induced DNA damage or in the bioremediation of metals and radionuclides that could lead to reduced clean up costs; and to determine the high-resolution three-dimensional structures of those proteins. To fully understand the mechanisms underlying the behavior of the molecular machines that carry out these functions, research is conducted and computer simulation models are developed: (1) on the dynamic changes in protein structure associated with protein modification and with protein-protein and protein-nucleic acid interactions that occur in these molecular machines; (2) to develop instrumentation that enables imagery of molecular machines in real-time at high levels of resolution; and (3) to precisely measure their intracellular compartmentalization and translocation.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Infrastructure Development**	**17,229**	**15,300**	**15,300**

BER develops beamlines and instrumentation at the Department's national user facilities for the Nation's structural biologists and supports access by these scientists to these experimental stations. It coordinates with the NIH and the NSF management of experimental stations at DOE synchrotrons [Advanced Photon Source (APS), Advanced Light Source (ALS), Stanford Synchrotron Radiation Laboratory (SSRL) and National Synchrotron Light Source NSLS)] and neutron beam sources [the Los Alamos Neutron Science Center (LANSCE) and High Flux Isotope Reactor (HFIR) at ORNL]. User statistics for all BER structural biology user facilities are included in BES facility user reports. BER also supports access to unique high performance mass spectrometry and nuclear magnetic resonance spectrometry user facilities at the EMSL that are used for both proteomic and structural biology research. DOE investment in structural biology facilities is having a large impact on basic research investments being made by other agencies. These facilities will be used to conduct the research described above. In addition, DOE investments in structural biology user facilities at synchrotron light sources and at the EMSL have enabled the National Institute of General Medical Sciences at the National Institutes of Health (NIH) to make a large investment (over $30,000,000 per year from FY 2001 to FY 2005) in pilot projects for NIH's Protein Structure Initiative to develop high throughput methods for determining protein structure. Six of the nine pilot projects funded by NIH include partners from DOE Laboratories and nearly all make heavy use of DOE user facilities. BER also supports development of new instrumentation that will make more effective use of the intense x-ray beams at the DOE synchrotrons. A new x-ray detector technology is being supported in cooperation with the NIH called the pixel-array detector (PAD). This technology would allow much more rapid acquisition and read-out of x-ray crystallographic data and would enable collection of complete data sets for protein structure determination in minutes, avoiding problems with decomposition of the protein crystals that occur over longer time periods. The total estimated cost for each detector is estimated at less that $1,000,000.

Molecular and Cellular Biology	**55,041**	**71,195**	**93,500**
▪ **Microbial Genomics**	**10,997**	**10,987**	**9,838**

Microbial genomics research underpins DOE research programs - Fundamental microbiology research will continue to underpin DOE's need to exploit the capabilities of microbes to address mission needs. Begun in 1994 with DOE's first sequencing of a complete microbial genome, microbial genomics research continues to provide support for individual investigator initiated projects that provide a fundamental understanding of microbes.

Microbial genomics research serves to strengthen the fundamental research foundation that underpins other BER and DOE programs, including: Genomes to Life; bioremediation research; and carbon sequestration. The underlying scientific justification remains a central principle of the BER genome programs – complete genomic sequences yield answers to fundamental questions in biology. Knowing the complete DNA sequence of a microbe provides important insights to the biological capabilities of that organism and is the first step in developing strategies to more efficiently detect, counteract, use, or reengineer that microbe to address DOE needs.

Microbial genomics research includes:

Development of novel strategies to obtain and compare microbial DNA sequences. Research is being conducted on new methods to accelerate sequence comparisons without resequencing the entire genome of the related organism from scratch. Emphasis is being placed on novel uses of proven technologies with a particular emphasis on the identification of specific DNA sequence features that are associated with phenotypic differences between the microbes being compared.

Research on microbial genomic plasticity, including the normal ability of microbes to exchange genetic information in nature. Current microbial DNA sequence data strongly suggest that entire blocks of genes have been transferred between microbes during evolution. Research is being conducted to assess the frequency, mechanisms, and circumstances of lateral gene exchanges among microbes. This understanding is important for interpreting microbial DNA sequence data and for designing novel strategies for using microbes to address DOE mission needs.

Development of bioinformatics tools for analyzing microbial DNA sequence information. More than a third of the more than 100 publicly available genomic sequences of archaea and bacteria are a result of DOE Microbial Genome program funding. Novel computational tools are being developed to increase the value of microbial genomic information, such as identifying distant relationships of genes, understanding microbial evolution, predicting gene function, identifying and modeling gene expression networks, and extracting longer stretches of useable DNA sequence from raw sequence data.

In FY 2003 $2,128,000 was transferred for genomic analysis of potential biothreat agents to the Department of Homeland Security.

The research activities in this subprogram are carried out at National Laboratories, universities, and at private institutions and are selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
▪ **Carbon Sequestration Research**	**7,057**	**7,138**	**7,127**

Microbes and plants play substantial roles in the global cycling of carbon through the environment. In FY 2004 the program continues to leverage new genomic DNA sequence information on microbes important to the global carbon cycle by characterizing key biochemical pathways or genetic regulatory networks in these microbes. The information on the DNA sequence, key reaction pathways, and genetic regulatory networks will be used to develop strategies to use microbes and other organisms capable of carbon sequestration more efficiently or to even reengineer these organisms to enhance their capacity to sequester excess atmospheric carbon.

Research will also leverage the genomic DNA sequence of the poplar tree, completed in FY 2003, by developing high throughput experimental and computational methods for understanding the poplar genome and proteome, especially as related to carbon utilization. Research will also focus on microbes that live in the poplar rhizosphere (root zone) with the intent of understanding the role

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

that these microbes play in the transfer of carbon between the roots and the soil. The program will emphasize organisms and pathways that serve to increase long-term carbon storage over organisms and pathways that would serve to decrease carbon storage. A goal is to identify strategies that would lead to increased carbon storage in the poplar rhizosphere and surrounding soil, such as manipulation of the soil chemical environment to promote certain microorganisms or particular metabolic pathways.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
■ **Genomes to Life**	**18,696**	**34,547**	**59,039**

Genomes to Life is a program at the forefront of the biological revolution - a systems approach to biology at the interface of the biological, physical, and computational sciences. It will take advantage of solutions that nature has already devised to solve many of our most pressing and expensive problems. It will help us design and use complex systems to produce clean energy, mitigate climate change, and clean up the environment.

This new biological era – the era of systems biology – will enable us to understand entire living organisms and their interactions with the environment. Scientists have long tried to understand the workings of individual genes or small groups of genes. This new era in biology will focus on entire networks of genes and even biological systems – small, single celled organisms at first and later more complex creatures including humans.

This dramatic advance is possible, in large part, because of the scientific and technical successes of the Human Genome Project. Information and technology now available to all scientists working on the human genome and on a growing list of other organisms from microbes to plants to mice gives us new perspectives on the inner workings of biological systems and provides opportunities to use this knowledge to solve problems confronting DOE.

Genomes to Life offers the possibility of biotechnology solutions that can give us abundant sources of clean energy yet control greenhouse gases like carbon dioxide, a key factor in global climate change, and that can help us clean up past contamination of the environment.

Genomes to Life is a comprehensive, systems-level, interdisciplinary research program at the interfaces of the biological, physical, and computational sciences. It will require development of novel capabilities for new high throughput biological research, e.g., for protein production, molecular imaging, small molecule production, and proteomics. It will involve a well integrated mix of experimental and computational science that will, in the end, enable us to predict responses of biological systems to their environments and to use that predictive capability to generate solutions to complex and expensive DOE and National challenges including –

- *Clean Energy* - Within 10 years advances in systems biology, computation, and technology may contribute to increased biology-based energy sources. In the long-term, they could contribute to energy security through a major new bioenergy industry.

- *Reduced Carbon Dioxide in the Atmosphere* - Within 10 years advances in systems biology, computation, and technology may help us understand earth's carbon cycle and design ways to enhance carbon dioxide (CO_2) capture. In the long-term, they could help us stabilize atmospheric carbon dioxide to counter global warming.
- *Cleanup of the Environment* - Within 10 years advances in systems biology, computation, and technology may lead to cost-effective ways for environmental cleanup. In the long-term, new technology could save billions in waste cleanup/disposal.

Over billions of years of evolution, nature has created a remarkable array of molecular machines and complex microbial community structures with exquisitely diverse, precise, and efficient functions and controls. The goal of Genomes to Life is to understand the nature and control of these molecular machines and of complex microbial communities so well that we can use and even redesign them to address DOE and National needs. Success in Genomes to Life will be measured by scientific breakthroughs that lead to predictive computational models for –

- Natural, multiprotein molecular machines of complex living systems.
- Complex networks that control the assembly and operation of these machines.
- The organization and biochemical capabilities of complex microbial communities.

The overriding goal of this long-term research program is to understand biology well enough to be able to predict the behavior and responses of biological systems – from cells to organisms so that they can best be used to address DOE mission needs in energy, the environment, and national security. This research will lead to greatly improved computational strategies, tools and resources that are central to the success of Genomes to Life and, indeed, to all of biology, and that will be developed in partnership with the Advanced Scientific Computing Research program.

The broad goals of this research are shared with other agencies, such as the National Institutes of Health, the National Science Foundation, the Department of Agriculture, the Environmental Protection Agency, and private sector companies and will require coordination exceeding that of the Human Genome Project. The program will focus on scientific challenges that can be uniquely addressed by DOE and its National Laboratories in partnership with scientists at universities and in the private sector and will focus on high throughput genomic-scale activities (e.g., DNA sequencing, complex computational analysis, imaging, and genomic protein-expression experimentation and analysis) that are beyond the reach of individual investigators or even small teams.

Multidisciplinary research teams funded in FY 2003 will pursue the characterization of the biochemical capabilities of microbial communities. *In FY 2004, the program will increase its emphasis on research to characterize the function and control of molecular machines and on the development of broad capabilities for large scale protein production and diverse imaging approaches for these molecular machines. In FY 2004, the program will also increase its emphasis on high throughput DNA sequencing of microbes and microbial communities. This DNA sequence information will continue to serve as the core of biological information needed to understand the*

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

control and function of molecular machines and complex microbial communities. DNA sequencing for the Genomes to Life program will be conducted at the Joint Genome Institute's Production Sequencing Facility.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
■ **Human Frontiers Science**	**1,000**	**1,000**	**0**

BER has completed its funding of the Human Frontiers Science program, an international program of collaborative research to understand brain function and biological function at the molecular level.

	FY 2002	FY 2003	FY 2004
■ **Low Dose Radiation Research**	**17,291**	**17,523**	**17,496**

The goal of the Low Dose Radiation Research program is to support research that will help determine health risks from exposures to low levels of ionizing radiation, information that is critical to adequately, and appropriately, protect people and to make the most effective use of our national resources.

BER will continue to emphasize the use of new tools such as microbeam irradiators developed in the program in prior years that enable scientists to irradiate specific parts of an individual cell such as the nucleus or the cytoplasm, the use of molecular tools such as gene and protein expression chips to describe biological responses to low doses of radiation, and the characterization of individual susceptibility to radiation.

In FY 2004, emphasis will be placed on the development and use of experimental systems that enable scientists to make a transition from the use of highly quantifiable but less relevant *in vitro* systems for studying low doses of radiation to *in vivo* systems that are more relevant to human risk from exposure to low doses of radiation but in which it has been very difficult to quantify results.

BER will continue to forge closer, more productive linkages between experimentalists and risk modelers, a relationship that lies at the critical interface between experimental science, risk analysis, and development of better risk management policies.

In particular, research will focus on:

- *Bystander effect* – the response of cells that are not directly traversed by radiation but respond with gene induction and/or production of potential genetic and carcinogenic changes. It is important to know if bystander effects can be induced by exposure to low LET (linear energy transfer) radiation delivered at low total doses or dose-rates. This bystander effect potentially "amplifies" the biological effects (and the effective radiation dose) of a low dose exposure by effectively increasing the number of cells that experience adverse effects to a number greater than the number of cells directly exposed to radiation. Scientists will be challenged to determine if bystander effects to low doses of ionizing radiation occur *in vivo*.

(dollars in thousands)

FY 2002	FY 2003	FY 2004

- *Genomic instability* – is the loss of genetic stability, a key event in the development of cancer, induced by radiation and expressed as genetic damage that occurs many cell divisions after the insult is administered. Current evidence suggests that DNA repair and processing of radiation damage can lead to instability in the progeny of irradiated cells and that susceptibility to instability is under genetic control but there is virtually no information on the underlying mechanisms. Its role in radiation-induced cancer remains to be determined experimentally. It is also important to determine if genomic instability occurs at low total doses (<10 rads) or low dose rates. Scientists will be challenged to determine if low doses of radiation induce genomic instability *in vivo*.
- *Adaptive response* – is the ability of a low dose of radiation to induce cellular changes that reduce the level of subsequent radiation-induced or spontaneous damage. If low doses of radiation regularly and predictably induce a protective response in cells to subsequent low doses of radiation or to spontaneous damage, this could have a substantial impact on estimates of adverse health risk from low dose radiation. The generality and the extent of this apparent adaptive response needs to be quantified and extended to *in vivo* systems.
- *Endogenous versus low dose radiation induced damage* – The program will continue to investigate the similarities and differences between endogenous oxidative damage and damage induced by low levels of ionizing radiation as well as an understanding of the health risks from both. This information was not previously attainable because critical resources and technologies were not available. Today, technologies and resources such as those developed as part of the human genome program and at the National Laboratories have the potential to detect and characterize small differences in damage induced by normal oxidative processes and low doses of radiation. Research in this aspect of the program will be concluded by the end of FY 2004.
- *Genetic factors that affect individual susceptibility to low dose radiation* – Research is also focused on determining whether genetic differences make some individuals more sensitive to radiation-induced damage since these differences could result in individuals or sub-populations that are at increased risk for radiation-induced cancer.
- *Mechanistic and risk models* – Novel research is supported that involves innovative collaborations between experimentalists and modelers to model the mechanisms of key radiation-induced biological responses and to describe or identify strategies for developing biologically-based risk models that incorporate information on mechanisms of radiation-induced biological responses. This has been the most difficult and challenging component of the program. In FY 2004, a comprehensive effort will be undertaken to identify innovative new research strategies that will determine the extent to which the development of biologically-based risk models for low dose radiation is a possibility. This will involve interactions between experimental and computational scientists and with scientists at regulatory agencies responsible for developing risk policy.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

- Information developed in this program will provide a better scientific basis for making decisions with regard to remediating contaminated DOE sites and for determining acceptable levels of human health protection, both for cleanup workers and the public, in a more cost-effective manner. University scientists, competing for funds in response to requests for applications, conduct a substantial fraction of the research in this program.
- The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
Human Genome	**90,075**	**76,805**	**64,572**

In FY 2003 $13,765,000 was transferred for genomic analysis of potential biothreat agents to the Department of Homeland Security.

	FY 2002	FY 2003	FY 2004
▪ **Joint Genome Institute**	**57,200**	**57,200**	**51,480**

With the completion of the high quality DNA sequences of human chromosomes 16 and 19 in CY 2002 (with chromosome 5, DOE's share of the international effort to sequence the human genome), the Joint Genome Institute (JGI) will continue, at a reduced level, to use its DNA sequencing capacity to address the challenges of understanding the human genome, to address DOE mission needs in energy, carbon sequestration, and bioremediation, and as a resource for our Nation's scientists. *Beginning in FY 2004, the JGI will devote 60% of its sequencing capacity to peer reviewed sequencing needs of the broader scientific community, including the needs of other agencies. DNA sequencing targets will be chosen using a process of peer review of requests for sequencing submitted by individual scientists and other federal agencies. Forty percent of the JGI's DNA sequencing capacity will be used to address DOE sequencing needs, including BER programs such as carbon sequestration research and bioremediation research, and other DOE and national needs. The substantial high throughput DNA sequencing needs of the Genomes to Life Program are supported directly by the Genomes to Life Program and are not included in funds for the Joint Genome Institute.*

The JGI is a virtual research institute principally comprised of research programs at DOE national laboratories (LLNL, LANL, LBNL, PNNL, ORNL) and a significant partnership with Stanford University. The JGI's DNA sequencing factory is located in Walnut Creek, California.

	FY 2002	FY 2003	FY 2004
▪ **Tools for DNA Sequencing and Sequence Analysis**	**30,396**	**16,900**	**11,245**

BER continues to develop the tools and resources needed by the scientific, medical, and private sector communities to fully exploit the information contained in the first complete human DNA sequence. As a result of the success in sequencing the human genome, several research activities were reduced or eliminated in FY 2003 (e.g., optical mapping of chromosomes, gene library preparation, gene sequencing, etc.). Unimaginable amounts of DNA sequencing, at dramatically increased speed and reduced cost, will still be required in the future for medical and commercial purposes and to understand the information in the DNA sequence that has already been determined. In FY 2004, BER continues research to further improve the efficiency and cost effectiveness of its

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

own DNA sequencing factory at the JGI by improving the reagents used in DNA sequencing and analysis (including genome assembly and annotation); decreasing the costs of sequencing; increasing the speed of DNA sequencing; and developing more robust computational tools for genome-wide data analysis.

Use of sequence information to understand human biology and disease will also require new strategies and tools capable of high-throughput, genome-wide experimental and analytic approaches. In FY 2004, BER will continue efforts to develop high-throughput approaches for analyzing gene regulation and function.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

- **Ethical, Legal, and Societal Issues (ELSI)** **2,479** **2,705** **1,847**

The DOE and NIH human genome programs agreed at the outset to dedicate a fraction of their human genome program funding to understanding the ELSI associated with the genome program. DOE's ELSI research program represents three percent of the DOE human genome program. The DOE ELSI program supports research focused on issues of: (1) the use and collection of genetic information in the workplace especially as it relates to genetic privacy; (2) the storage of genetic information and tissue samples especially as it relates to privacy and intellectual property; (3) genetics and ELSI education; and (4) the ELSI implications of advances in the scientific understanding of complex or multigenic characteristics and conditions.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

A table follows displaying both DOE and NIH genome funding.

U.S. Human Genome Project Funding

	(dollars in millions)			
	Prior Years	FY 2002	FY 2003	FY 2004
DOE Total Funding (FY 87-01)	864.5	90.1	76.8	64.6
NIH Funding (FY 88-01)	2,241.6	431.0[a]	467.0 [a]	TBD
Total U.S. Funding	3,106.1	521.1	543.8	TBD

[a] Estimate from NIH.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Health Effects	**11,732**	**10,260**	**10,260**
▪ **Functional Genomics Research**	**11,732**	**10,260**	**10,260**

Understanding the structure and function of the human genome. – Many individual genes, large families of genes, and the regulatory networks that control these genes have been conserved during evolution in organisms as diverse as yeast and humans. Thus, model organisms including *Fugu* (puffer fish), *Ciona* (sea squirt), and mouse can be used to efficiently understand the organization, regulation, and function of much of the human genome. Functional genomics research is a key link between human genomic sequencing, that provides a complete parts list for the human genome, and the development of information (a high-tech owner's manual) that is useful in understanding normal human development and disease processes. The mouse continues to be a major focus of our efforts and is an integral part of our functional genomics research program. This effort is greatly enhanced by the completion of the Center for Comparative and Functional Genomics at Oak Ridge National Laboratory in FY 2003 that will serve as a national focal point for high throughput genetic studies using mice. BER creates and genetically characterizes new mutant strains of mice that serve as important models of human genetic diseases and for understanding gene function. It also develops high-throughput tools and strategies to characterize these mutant strains of mice. This mouse genetics research provides tools useful to the entire scientific community for decoding the functionality of the human genome as human DNA sequence becomes available. Research to develop new high-throughput strategies for using model organisms such as the mouse, *Fugu*, and *Ciona* to understand the function of human genes increases in FY 2004.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

In FY 2003 $4,107,000 was transferred for genomic analysis of potential biothreat agents to the Department of Homeland Security.

	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**4,771**	**5,267**

In FY 2002 $4,458,000 and $256,000 were transferred to the SBIR and STTR programs, respectively. FY 2003 and FY 2004 amounts are estimated requirements for continuation of these programs.

	FY 2002	FY 2003	FY 2004
Total, Life Sciences	**186,384**	**190,878**	**201,408**

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Structural Biology	
▪ Maintain structural biology research at near FY 2003 levels.	-38
Molecular and Cellular Biology	
▪ Decrease in Microbial Genomics research decreases capability to obtain and compare microbial DNA sequences	-1,149
▪ Maintains carbon sequestration research at near FY 2003 level................................	-11
▪ Increase for Genomes to Life research with focus on characterization of molecular machines and on development of broad capabilities for large scale protein production and diverse imaging approaches. Increase in high throughput DNA sequencing of individual microbes and microbial communities. Funding provided for Homeland Security in FY 2003 is budgeted by the Department of Homeland Security in FY 2004.	+24,492
▪ BER Human Frontier Science Program completed ………………………………..	-1,000
▪ Maintains Low Dose Radiation Research at near FY 2003 levels.............................	-27
Total, Molecular and Cellular Biology	+22,305
Human Genome	
▪ Decrease in JGI and Tools for Sequencing and Sequencing Analysis reflects completion of human DNA sequencing for the International Human Genome Program and support for DNA sequencing needs of the Genomes to Life program within that program. JGI DNA sequencing capacity is shifted to address the needs of the broader scientific community.	-11,375
▪ Decrease in ethical, legal, and societal issues program (approximately 3% of human genome funding) due to overall decrease in human genome funding	-858
Total, Human Genome	-12,233
SBIR/STTR	
Increase in SBIR/STTR due to increase in research funding for the Life Sciences program and increased STTR allocation..	+496
Total Funding Change, Life Sciences	+10,530

Climate Change Research

Mission Supporting Goals and Measures

The goal of the Climate Change Research subprogram is to deliver relevant scientific knowledge that will enable scientifically-based predictions and assessments of the potential effects of greenhouse gas and aerosol emissions on climate and the environment. Research will reduce and resolve key uncertainties and provide the scientific foundation needed to predict, assess, and mitigate adverse effects of energy production and use on the environment through research in climate modeling and simulation, climate processes, carbon cycle and carbon sequestration, atmospheric chemistry, and ecological science.

The Climate Change Research subprogram supports four contributing areas of research: Climate and Hydrology; Atmospheric Chemistry and Carbon Cycle; Ecological Processes; and Human Interactions. The research is focused on understanding the physical, chemical, and biological processes affecting the Earth's atmosphere, land, and oceans and how these processes may be affected, either directly or indirectly, by energy production and use, primarily the emission of carbon dioxide from fossil fuel combustion. BER has designed and planned the research program to provide the data that will enable objective assessments of the potential for, and consequences of, global warming. The BER Climate Change Research subprogram (excluding the carbon sequestration element) represents DOE's contribution to the interagency U.S. Global Change Research Program proposed by President Bush in 1989 and codified by Congress in the Global Change Research Act of 1990 (P.L. 101-606). It also contributes to the Administration's Climate Change Research Initiative (CCRI).

In FY 2003, the Administration launched a new CCRI. The CCRI is a set of cross-agency programs in areas of climate change research of high priority and where substantial progress is anticipated over the next three to five years. The specific focus areas of the research are climate forcing (atmospheric concentrations of greenhouse gases and aerosols), climate feedbacks and sensitivity, climate modeling, including enabling research, regional impacts of climate change, including environment-society interactions, and climate observations. In FY 2003 funding allows DOE to participate in one of the specific research areas: climate forcing, which includes modeling carbon sources and sinks, especially those in North America. In FY 2004 ($25,335,000) BER will continue to support research to quantify the magnitude and location of the North American carbon sink, a high priority need in the interagency Carbon Cycle Science Plan and expand its CCRI research to include climate modeling, Atmospheric Radiation Measurement, and Integrated Assessment activities.

The National Institute for Global Environmental Change (NIGEC) is integrated throughout the subprogram (FY 2004 Request is $8,749,000). NIGEC regional centers are located at the University of California, Davis (Western Region), the University of Nebraska, Lincoln (Great Plains Region), Indiana University, Bloomington (Northeast Region), Tulane University, New Orleans (Southcentral Region), and the University of Alabama, Tuscaloosa (Southeastern Region). The national NIGEC center is located at the University of California, Davis.

A major emphasis of the Climate Change Research subprogram is on understanding the radiation balance from the surface of the Earth to the top of the atmosphere and how changes in this balance due to increases in the concentration of greenhouse gases in the atmosphere may alter the climate. Much of the research is focused on improving the quantitative models necessary to predict possible climate change at global and regional scales. Research in the Atmospheric Radiation Measurement (ARM) program will continue to focus on resolving the greatest scientific uncertainty in climate change prediction – the role of clouds and their interactions with solar radiation. ARM seeks to develop a better quantitative understanding of how atmospheric properties, including the extent and type of cloud cover and changes in aerosols and greenhouse gas concentrations affect the solar and infrared radiation balance that drives the climate system. BER's Climate Modeling program develops advanced, fully coupled climate models and uses massively parallel supercomputers to simulate and predict climate and climate change, including evaluating uncertainties in climate models due to changes in atmospheric levels of greenhouse gases on decade-to-century time scales.

The Atmospheric Science program is focused on acquiring the data to understand the atmospheric processes that control the transport, transformation, and fate of energy-related chemicals and particulate matter emitted to the atmosphere. BER is emphasizing research on processes relating to new air quality standards for tropospheric ozone and particulate matter and relationships between air quality and climate change.

Research on the carbon cycle explores the movement of carbon on a global scale starting from natural and anthropogenic emissions to ultimate sinks in the terrestrial biosphere and the oceans. Experimental and modeling efforts primarily address the net exchange of carbon between major types of terrestrial ecosystems and the atmosphere. This research includes DOE's contribution to the Climate Change Research Initiative, an interagency effort on specific areas of climate change research in which substantial progress in understanding and modeling is expected over the next five years.

The BER carbon sequestration element funds basic research that seeks to exploit the biosphere's natural processes to enhance the sequestration of atmospheric carbon dioxide in terrestrial and marine ecosystems. It also seeks the understanding needed to assess the potential environmental implications of purposeful enhancement and/or disposal of carbon in the terrestrial biosphere and at the surface or deep ocean. The carbon sequestration activities include research to identify and understand the environmental and biological factors or processes that limit carbon sequestration in these systems and to develop approaches for overcoming such limitations to enhance sequestration. The research includes studies on the role of ocean and terrestrial microorganisms in carbon sequestration.

The Ecological Processes research is focused on experimental and modeling studies to understand and simulate the effects of climate and atmospheric changes on the biological structure and functioning of terrestrial ecosystems. The research also seeks to identify the potential feedback effect of ecosystem responses on climate and atmospheric composition. The research emphasizes major field studies of intact ecosystems using experimental manipulations of, for example, carbon dioxide and ozone concentrations and precipitation, and using data from these experiments to develop, test, and improve models for simulating and predicting ecosystem responses.

Within Ecological Processes, new research will be initiated to develop a mechanistic understanding of how complex ecosystems respond to environmental changes, including the causal mechanisms and pathways underlying observed responses. The focus will be on documenting and understanding the causal mechanisms and pathways of biological and ecological responses ranging from the proteome of individual species to the whole ecosystem. The initial focus will be to understand the responses of a model terrestrial ecosystem containing simplified but hierarchical communities (higher plants, consumers of plant production, and soil microorganisms) to changes in a key environmental factor such as temperature that is known to affect ecosystem functioning (e.g., carbon and nutrient cycling). Advanced biologically based computational algorithms and ecosystem models will be developed to establish whether and how changes in the proteome, in either single species or whole systems, can explain the responses and behavior of complex ecosystems.

The Human Interactions research is focused on improving methods and models that can be used to assess the economic and societal costs and benefits of both human-induced climate change and possible response options or strategies for mitigating or adapting to climate change. It also includes support to archive and analyze climate change data and make it available for use by the broader climate change research community.

The Climate Change Research subprogram provides fundamental knowledge building to long-term outcomes that underpin the Program Strategic Performance Goals and the Office of Science's Strategic Objectives. Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This program was examined as part of a BERAC review of the entire BER program in FY 2001. The next scheduled comprehensive review of the Climate Change Research subprogram by BERAC will be in FY 2005. The following are recent scientific accomplishments that highlight program progress.

- *Model results provide further evidence that 20th century warming is caused by greenhouse gas.* Scientists from BER's Climate Change Prediction Program have provided further evidence that the observed climate warming in the twentieth century is due to human induced forcing of the climate system. The scientists compared results from two ensembles of twentieth century climate simulations with observational temperature records. The climate forcing conditions in the climate model used to produce one ensemble included all known sources of natural variability, including temporal changes in solar output and the cooling effects of volcanic dust. A model used to produce a second series of runs also included anthropogenic effects on the atmosphere, i.e., increased greenhouse gas concentrations and aerosols. The ensemble from the model that included anthropogenic forcings closely matched the observed record and was a statistically significant 0.3 C warmer at the end of the century than the runs from the model that contained only natural variability.
- *Anomalous Absorption of Solar Radiation Question is Resolved.* BER's Atmospheric Radiation Measurement (ARM) program resolved a long-standing scientific question concerning the transfer of solar radiation through the atmosphere. A considerable body of scientific literature indicates that measurements of the absorbed solar energy in cloudy atmospheres exceed theoretical calculations. A group of papers published in 1995 claimed that the ratio of measured to calculated absorption was as large as 1.4 or 1.5. If the ratio were this large, it would require a substantive reevaluation of our understanding of atmospheric radiation physics because such a large increase could not be explained by any reasonable extrapolation of currently understood physics. To test this, the ARM Program conducted field campaigns utilizing ground and aircraft borne instruments coordinated with satellite measurements. Results show that measured solar absorption in a cloudy atmosphere is within a few to 15% of absorption computed from state-of-the-art radiative transfer models. These results indicate that anomalous absorption occurs only at the level of 15% or less and can be explained by conventional atmospheric physics.

- *ARM Develops New Parameterization for Ice Crystals in Cirrus Clouds.* Using detailed information from the Atmospheric Radiation Measurement (ARM) site in the Southern Great Plains, ARM researchers have improved how the scattering of sunlight by ice crystals in cirrus clouds is represented in models. The new parameterization was incorporated into a model that simulates the atmosphere over the ARM site. Actual measurements from the ARM sites were used to assess the realism of the model simulations, and the model version that used the new treatment showed excellent agreement. Comparison between the new model and a numerical weather forecasting model with observations also shows that the new model is more accurate. The use of the new cloud parameterization improved the computed rates at which the atmosphere cools radiatively by as much as 20 percent when averaged over a season. Larger improvements occurred for specific days.
- *New Understanding of Air Pollution Phenomena Leads to Advances in Air Pollution Control Strategies.* Through coordinated field research, laboratory measurements, and modeling studies in a variety of areas around the U.S. such as Nashville, Phoenix, Salt Lake City, and Houston, the Atmospheric Sciences Program (ASP) provided new insights into the diversity of factors that affect air quality and showed that a "one-approach-fits-all" strategy for air quality management does not work. The research demonstrated that reducing industrial emissions of volatile organic compounds in Houston could reduce ozone concentrations there, but this strategy would be less effective in the southeastern U.S., where reactive volatile organic compounds tend to be dominated by natural emissions from vegetation. In Phoenix, on the other hand, emissions of hydrocarbons from vegetation and industrial sources are minimal, so the focus should be on reducing emissions from vehicles. Since most of the emissions associated with energy production and use are to the atmosphere, understanding how such emissions are transported, transformed, and removed from the atmosphere is essential for understanding their environmental consequences, in terms of air quality, climate change, and health effects. Research results from the Atmospheric Science Program are provided well beyond the research community, both to industry and to state authorities for use in assessing and developing air pollution control strategies.
- *New Method Developed for Measuring Total Soil Carbon.* Laser-induced breakdown spectroscopy (LIBS) is a new method for measuring soil carbon content that significantly advances research on the cycling and sequestration of carbon in soil. LIBS was developed by researchers at the Los Alamos National Laboratory and further tested by ORNL and USDA/ARS Laboratories The method directly measures soil carbon by "shooting" a small laser beam into the soil matrix in the field, and spectra of soil organic matter broken down by the laser are resolved to estimate the quantity of carbon present in the soil matrix. LIBS analyzes the sample in less than one minute, and results exhibit excellent precision and accuracy when correlated with conventional dry-combustion techniques for measuring soil carbon content. The field-portable LIBS device has been tested with a number of natural soil configurations and morphologies, and has been found to perform faster and more efficiently than conventional approaches. LIBS offers the potential of revolutionizing soil carbon measurement, where fast determinations are useful for many practical applications of soil carbon inventory, management and sequestration. Research is continuing jointly with the USDA to determine effects of other soil properties such as texture, mineralogy and moisture content on performance of LIBS.

- *Iron Fertilization Makes Ocean Bloom.* The Southern Ocean Fertilization Experiment (SOFeX) jointly funded by BER and the National Science Foundation demonstrated that carbon fixation by ocean phytoplankton in the Southern Ocean south of New Zealand is iron limited and can be enhanced by fertilizing ocean surface water with iron. Data from SOFeX demonstrate that iron fertilization may offer a potential approach for enhancing carbon sequestration in the ocean by increasing the rate of carbon fixation by ocean phytoplankton. The SOFeX data will be used to constrain estimates of the amount of carbon in particles, including phytoplankton that is exported downward into the deep ocean where it is isolated from the atmosphere, a prerequisite for ocean carbon sequestration. In January-February 2002, over 100 scientists and 3 research vessels fertilized the surface ocean water in two 15 square kilometer study areas with dissolved iron and inert chemical tracers. The latter was to tag the ocean water in the two areas fertilized so as to be able to distinguish the areas and volumes of water fertilized from those not fertilized. Addition of the iron produced a bright green phytoplankton bloom in the two areas fertilized that could be seen from space by ocean color satellites, evidence that the addition of iron enhances the growth and carbon fixation by phytoplankton in the Southern Ocean.

- *First Field Test of Multiple Ecological Models with Three Years of Independent Data.* BER's Program on Ecosystem Research recently completed a rigorous evaluation and testing of nine terrestrial ecosystem models in collaboration with NASA, NSF, and the Canadian government by comparing model simulations with independent field data. It was discovered that more complex models tended to provide more accurate predictions of short-term (i.e., daily) water and carbon dioxide exchange rates, but that model complexity was apparently unrelated to accuracy of monthly and annual predictions. This type of model evaluation is essential to understanding uncertainties and limitations of ecological models used to predict and assess effects of global and regional environmental changes on the structure and functioning of terrestrial ecosystems. Several model improvements have already resulted from this work.

  The models (which represented a wide range of model complexity) were compared to three years of field data collected on ecosystem water use, net primary production, gross primary production, net ecosystem production, and soil carbon dioxide release in a boreal spruce forest. This was the most extensive test of forest ecosystem models using independent field data conducted to date, and represented forest responses to natural climatic variability in interior Canada.

Subprogram Goals

Determine the response of the Earth system to different levels of greenhouse gases in the atmosphere.

Performance Indicator

Climate model resolution.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Climate and Hydrology) A new coupled model was released in May 2002, with an average resolution of 280 km in the atmosphere and 60 km in the ocean. The previous version had a resolution of 280 km and 200 km, respectively. An 800-year equilibrium climate simulation was executed at the National Energy Research Supercomputer Center. [Goal Met] Addition of new cloud submodel for cirrus clouds improved climate model computed rates at which atmosphere cools radiatively by 20%. [Goal Met]	(Climate and Hydrology) Increase the realism of the coupled modeling system through both increases in spatial resolution and improvements in the physical parameterizations. More objective and systematic methods for evaluating model performance will be implemented and applied to the model components (atmosphere, ocean, land and sea ice) as well as to the coupled modeling system. Model productivity will be increased by completing a larger number of scenarios of climate change forcing and making the results available to researchers in the broader community. This will be made possible by a significant effort in software engineering and algorithm development so that the model is able to exploit new computing technology rapidly and efficiently.	(Climate and Hydrology) By the end of 2004, incorporate climate data rapidly into climate models to allow testing of the performance of submodels (e.g., cloud resolving module) and model parameters by comparing model simulations with real world data from the ARM sites**.**
(Atmospheric Chemistry & Carbon Cycle) Coordinated field and laboratory measurements and modeling experiments in diverse regions demonstrate that regional air quality management strategies must be designed for the specific regional environment, e.g., one size does not fit all. [Goal Met]	(Atmospheric Chemistry & Carbon Cycle) Evaluate preliminary findings from field measurement campaigns in both atmospheric chemistry and environmental meteorology and the extent to which scientific results are incorporated into models to predict and assess air quality. Produce quality micrometeorological data, net carbon dioxide exchange data, and biometric data from 20 of 45 active AmeriFlux sites, and synthesize results from these sites.	(Atmospheric Chemistry & Carbon Cycle) The program will incorporate respiration functions into biophysical carbon cycle models for terrestrial ecosystems calculating carbon exchange for three woody ecosystems. Independent data will be used to evaluate model improvement.
Data from the Southern Ocean Iron Fertilization Experiment demonstrated that iron added to the ocean may enhance carbon sequestration by ocean phytoplankton. [Goal Met]	Analyze and publish results from the Southern Ocean Iron Fertilization Experiment (SOFeX) that will study the export of particulate organic carbon below the mixed layer in high and low silicate waters following the experimental addition of iron to a large area of the ocean's surface.	Data from the Southern Ocean Iron Fertilization Experiment (SOFEX) will be incorporated into coupled biogeochemical models to evaluate the effectiveness of ocean fertilization as a carbon sequestration strategy. New field studies will be initiated to examine the fate of carbon exported from the surface ocean to intermediate depths (100m-1000m) and the carbon sequestration potential.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
New method developed for measuring soil carbon will provide faster and more accurate measurement of soil carbon, data that are needed for carbon cycle modeling in diverse ecosystems. [Goal Met]	Apply an ecosystem framework to estimate annual rates of actual carbon gain by vegetation and soil. Enhanced sequestration will be estimated relative to baseline carbon quantities established for the range of ecosystems investigated by the CSiTE Consortium.	CSiTE will estimate the biophysical potential of terrestrial carbon sequestration for one specific region of the U.S. New field data, analysis of full carbon accounting, and improved carbon cycle models will demonstrate how existing carbon stocks of terrestrial vegetation and soil could be increased.
(Ecological Processes)	(Ecological Processes)	(Ecological Processes)
Nine ecological models tested with three years of independent field data provide the framework for understanding model limits for predicting ecosystem responses to environmental change. [Goal Met]	Complete synthesis of data collected during 8-9 years of a unique experimental manipulation of precipitation received by a large-statured forest on the Oak Ridge reservation in a published book. This will include using the data collected in the experiment to evaluate (test) up to 15 ecosystem models.	Establish a model terrestrial ecosystem in a controlled and controllable environment that contains simplified but hierarchical communities (higher plants, consumers of plant production, and soil microorganisms) and begin the characterization of the proteome of the major species.
(Human Interactions)	(Human Interactions)	(Human Interactions)
Integrated assessments provided a basis for quantifying the potential significance of enhancing carbon sequestration in terrestrial ecosystems, ocean, and/or geologic formations with the goal of reducing CO_2 concentrations. Sequestration strategies that have limited lifetimes, either because of constraints on the amount of carbon sequestered or on the expected residence time before re-release, can be compared economically with other strategies that may be more expensive, such as premature replacement of capital stocks. [Goal Met] 15 undergraduate summer fellowships were awarded. In addition, 27 graduate students were supported, 7 first year, 6 second year, 7 third year, and 7 fourth year students. All granduate and undergraduate students worked with DOE-funded scientists and/or at DOE facilities. [Goal Met]	Integrate a new land and ocean carbon sub-model in one of the two large integrated assessment models. The submodel includes a detailed representation of direct human influence (mainly agriculture and forestry) on the terrestrial biosphere. In addition to providing a more accurate representation of the global carbon cycle, the change will ensure consistent accounting of carbon-sink projects and the carbon uptake that occurs as a result of other land-use change and the effects of climate change and carbon fertilization. The other integrated assessment model will simulate the effect of 1) climate on crop yields and 2) the amount of crop and pasture land necessary to provide (a) a sufficient diet in developing countries under climate change and (b) the likely increase in dietary requirements as developing countries become richer.	Performance will be measured by the sustaining the number, quality, and diversity of students enrolled in the program and by end-of-summer evaluations by students and their mentors.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
	Performance will be measured by the number, quality, and diversity of students enrolled in the program and by end-of-summer evaluations by students and their mentors.	

Manage all BER facility operations to the highest standards of overall performance, using merit evaluation with independent peer review.

Performance Indicator

Average operational downtime of BER facilities will not exceed 10% of total time scheduled.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Climate and Hydrology)	(Climate and Hydrology)	(Climate and Hydrology)
ARM instruments averaged over a 95% up time in 2002 and successfully completed 7 IOP's. [Goal Met]	Achieve a downtime of less than five percent for the principal ARM instruments and successfully conduct five IOPs across the three ARM sites.	Achieve a downtime of less than five percent for the principal ARM instruments and successfully conduct five IOPs across the three ARM sites.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Climate and Hydrology	70,353	74,669	74,559	-110	-0.1%
Atmospheric Chemistry and Carbon Cycle	34,735	37,764	37,707	-57	-0.2%
Ecological Processes	12,817	13,888	18,726	+4,838	+34.8%
Human Interaction	7,942	8,084	8,071	-13	-0.2%
SBIR/STTR	0	3,554	3,896	+342	+9.6%
Total, Climate Change Research	125,847	137,959	142,959	+5,000	+3.6%

Detailed Program Justification

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Climate and Hydrology	**70,353**	**74,669**	**74,559**
▪ **Climate Modeling**...	**26,999**	**27,181**	**27,138**

Model based climate prediction provides the most scientifically valid way of predicting the impact of human activities on climate for decades to centuries in the future. BER will continue to develop, improve, evaluate, and apply the best coupled atmosphere-ocean general circulation models (GCMs) that simulate climate variability and climate change over these time scales. The goal is to achieve statistically accurate forecasts of future climate over regions as small as river basins using ensembles of model simulations. The ensembles will accurately incorporate the dynamic and thermodynamic feedback processes that influence climate, including clouds, aerosols, and greenhouse gas forcing. Current predictions are limited by the inadequacy of computational resources and uncertainties in the model representations of key small-scale physical processes, especially those involving clouds, evaporation, precipitation, and surface energy exchange. BER will address both the computational and scientific shortcomings through an integrated effort. Support will continue to provide climate modelers access to the high-end computational resources needed to complete ensembles of climate simulations using present and future models. BER will emphasize research to develop and employ information technologies that can quickly and efficiently work with large and distributed data sets of both observations and model predictions to produce quantitative information suitable for the study of regional climate changes. BER will continue to fund the multi-institutional research consortia established in FY 2001 to further the development of comprehensive coupled GCMs for climate prediction that are of higher resolution and contain accurate and verified representations of clouds and other important climate processes. In FY 2004, BER will continue the partnership with the Advanced Scientific Computing Research program. This includes applying the computing resources for climate simulation and continuing climate model development and application through the use of collaboratory technologies. Additionally, BER will emphasize data assimilation methods so as to quickly make use of the high quality observational data streams provided by ARM, satellite and other USGCRP climate data programs to evaluate model performance.

For CCRI the research will provide ensemble projections of multi-century climate change using the Community Climate System Model through the Climate Change and Assessment Working Group. Additionally, the program will provide the infrastructure for major model evaluation and model improvement research through the coordination of model intercomparisons and the maintenance of model testbeds for parameterization testing. In FY 2004 ($15,347,000) climate model experiments will provide scenarios, such as carbon dioxide (CO_2) stabilization scenarios.

In FY 2004 BER’s SciDAC program ($7,776,000) is focused on improving the models used for climate simulation and prediction. A major effort is dedicated to providing a robust and extensible software engineering framework for the Community Climate System Model, a code used by hundreds of researchers on many different high-end computing platforms. Additional research will

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

provide the prototype climate model of the future that will explore approaches to climate simulation and prediction for the next ten years.

The research activities in this subprogram are carried out at National Laboratories, universities, and at private institutions and are selected through competitive and peer-reviewed processes.

In FY 2004, NIGEC will continue to support research to evaluate the reliability of using isotopic signatures of trace gases in ice cores for interpreting past climate variation and change and the relationship between greenhouse gas concentrations and climate change (FY 2004 Request is $2,187,000).

▪ **Atmospheric Radiation Measurement (ARM) Research**	**13,310**	**13,310**	**13,247**

In FY 2004, the principal goal of the ARM scientific enterprise continues to be the development of an improved understanding of the radiative transfer processes in the atmosphere and to formulate better parameterizations of these processes in climate prediction models, referred to as General Circulation Models (GCMs). ARM research supports about 50 principal investigators involved in studies of cloud physics and the interactions of solar and infrared radiation with water vapor and aerosols (including black soot). University scientists form the core of the ARM science team that networks with the broader academic community as well as with the scientists at the DOE National Laboratories and with federal scientists at NASA, NOAA, and DOD. ARM scientists pursue research as individuals and as members of teams and contribute both to the production of ARM data, e.g., as designers of cutting-edge remote sensing instrumentation, as well as consumers of the data produced at the three ARM sites. To facilitate the knowledge transfer from the ARM program to the premier modeling centers, the ARM program supports scientific "Fellows" at the NSF's National Center for Atmospheric Research, the NOAA's National Center for Environmental Prediction, and the European Center for Medium-Range Weather Forecasting in the U.K. In addition, a model parameterization testbed initiated in FY 2003 will be continued to enable the testing and improvement of submodels by rapidly incorporating data from the ARM sites into the models to enable diagnostic tests and intercomparisons of model simulations with real world data.

▪ **Atmospheric Radiation Measurement (ARM) Infrastructure** ..	**27,306**	**31,441**	**31,441**

In FY 2004, the Atmospheric Radiation Measurement (ARM) infrastructure program will continue to develop, support, and maintain the three ARM sites and associated instrumentation. BER will continue to operate over two hundred instruments (e.g., multifilter shadowband radiometers for aerosol measurements, Raman Lidar for aerosol and cloud measurements, radar wind profiler systems, radar cloud measurement systems, sky imaging systems, arrays of pyranometers, pyrgeometers, and pyrheliometers for atmospheric and solar radiation measurements, and standard meteorological measurement systems for characterization of the atmosphere) at the Southern Great Plains site and will continue operations at the Tropical Western Pacific station and at the North Slope site in Alaska. The ARM program will continue to provide data to the scientific community through the ARM Archive.

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

The ARM data streams will continue to be enhanced periodically by additional measurements at the ARM sites during intensive field campaigns referred to as Intensive Operation Periods (IOPs). Ranging from two weeks to two months, the campaigns bring together teams of scientists testing cutting edge remote sensing instruments and coordinate measurements with airborne and satellite observations. The ARM sites have become major testbeds of research in atmospheric processes serving as scientific user facilities for hundreds of scientists from universities and government laboratories. For example, both DOD and NASA have used the ARM sites to "ground truth" their satellite instruments.

The UAV program will conduct a major field campaign in conjunction with the ARM program to measure the effect of cirrus clouds on the absorption and scattering of downwelling radiation over the Western Tropical Pacific ARM-CART site.

The CCRI ARM program will deploy a mobile climate observatory to provide new atmospheric measurements needed to fill data gaps and will develop the corresponding data products needed for evaluating and modeling the effects of atmospheric processes and properties on the radiation balance and for developing and evaluating the models. In FY 2004 ($4,100,000) a mobile Cloud and Radiation Testbed (CART) facility will be deployed in a selected data poor region (e.g., tropics) or a region that represents a location of opportunity for measuring the effects of atmospheric conditions on the radiation balance that are currently poorly understood (e.g., direct and indirect effects of aerosols). The mobile site will be instrumented for cloud and radiation measurements. The primary siting criterion is to provide those measurements needed to address specific modeling needs that presently cannot be addressed by the permanent ARM sites. Activities will be coordinated with other U.S. agencies and international partners, such as Australia, Japan, China, and European countries. Data products will be developed through collaborations with model developers. In FY 2004 the criteria for data products for evaluating precipitation processes will be established.

The research activities in this subprogram are carried out at National Laboratories, universities, and at private institutions and are selected through competitive and peer-reviewed processes.

- **Atmospheric Radiation Measurement (ARM)/Unmanned Aerial Vehicles (UAV)** **2,738** **2,737** **2,733**

  The UAV program will conduct one major field campaign in conjunction with the ARM program to provide high altitude measurements of cloud properties and radiation balance.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Atmospheric Chemistry and Carbon Cycle	**34,735**	**37,764**	**37,707**
▪ **Atmospheric Science**	**13,161**	**12,571**	**12,551**

The Atmospheric Science project will continue to acquire data to understand the atmospheric processes that control the transport, transformation, and fate of energy-related chemicals and particulate matter. Emphasis is placed on processes relating to new air quality standards for tropospheric ozone and particulate matter and relationships between air quality and climate change. Field and laboratory studies will continue to be conducted in both atmospheric chemistry and environmental meteorology and acquired data will be used to develop and validate predictive models of atmospheric processes. The research will include studies of chemical and physical processes affecting air pollutants such as sulfur and nitrogen oxides, tropospheric ozone, gas-to-particle conversion processes, and the deposition and resuspension of associated aerosols. It also includes studies to improve understanding of the meteorological processes that control the dispersion of energy-related chemicals and particulates in the atmosphere. Much of this effort involves multi-agency collaboration, and university scientists play key roles. New information will document both the contribution of energy production to regional haze in the U.S. and the relationship between urban and regional air pollution processes and continental, intercontinental, and global scale phenomena. The information is essential for assessing the effects of energy production on air quality and will contribute to the evaluation of science-based options for minimizing the impact of energy production on visibility.

In FY 2004 BER will continue the Tropospheric Aerosol Program (TAP) to quantify the impacts of energy-related aerosols on climate, air quality, and human health. TAP will be closely coupled with other components of DOE's climate change research, especially the Atmospheric Radiation Measurement (ARM) program. TAP will also be broadly coordinated with the air quality and global change research communities, including collaborations with the EPA, NASA, and NOAA and with the DOE Office of Fossil Energy's Airborne Fine Particulate Matter (PM) Research program. Regional patterns of aerosol distribution will be related to sources and sinks and the information will feed the models that simulate the impacts of aerosols on air quality and climate.

In FY 2004 the Atmospheric Sciences subprogram will, in general, focus on the evaluation of findings from field measurement campaigns in both atmospheric chemistry and environmental meteorology.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

In FY 2004, NIGEC will support research to quantify the effects of natural processes on atmospheric composition, including the exchange of energy-related trace gases between the atmosphere and the terrestrial biosphere (FY 2004 Request is $2,187,000).

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Terrestrial Carbon Processes and Ocean Sciences**	**13,056**	**16,636**	**16,613**

In FY 2004, BER will continue supporting the AmeriFlux program, a network of approximately 25 research sites that measure the net exchange of CO_2, energy, and water between the atmosphere and major terrestrial ecosystems in North America. These measurements are linked to field measurement campaigns across North America that will test how well point measurements represent larger areas and allow the estimation of carbon sources and sinks on a regional basis. This research supports the interagency Carbon Cycle Science Plan. The fluxes of other greenhouse gases, e.g., methane and nitrous oxide, will also be measured at 5 to 10 AmeriFlux sites.

BER will also continue research to refine and test carbon cycle models (based on mechanistic representations and carbon accounting). The models will be used to estimate potential carbon sequestration in response to changes in environmental factors, including climate.

The continuing focus of the ocean science element is on using microbiology tools to determine the linkages between the carbon and nitrogen cycles involving marine microbes. This research is conducted through partnerships between institutions with a tradition of research in oceanography (such as Skidaway Institute of Oceanography, U. of Washington, U. of Delaware, Rutgers University, U. of South Florida, Princeton University), and institutions traditionally serving minority students (such as Lincoln U., Howard U., Savannah State U., U. of Puerto Rico, and San Francisco State).

In FY 2004 (FY 2003 $2,920,000; FY 2004 $2,916,000) BER CCRI activities on the carbon cycle will continue to explore the movement of carbon starting from natural and human-induced emissions to the atmosphere to ultimate sinks in the terrestrial biosphere and the oceans. The AmeriFlux sites supported by BER are essential to quantifying the net exchange of carbon between the atmosphere and major terrestrial ecosystems in North America. Hence, they are essential to documenting the magnitude and variation in the North American carbon sink and how it is affected by variation and changes in environmental factors such as climate. BER will continue measurements and process studies at the network of AmeriFlux sites across North America. This information, along with data from extensive measurements around the sites, will provide a sound scientific basis for extrapolating carbon flux measurements at AmeriFlux sites to landscape and regional scales. Hence, it will improve estimates of the magnitude of the North American carbon sink and identify the regions and ecosystem types that account for the sink. In FY 2004 the research will deliver an intercomparison of estimates of the net annual exchange of CO_2 between terrestrial ecosystems and the atmosphere for a region of the U.S. with independent estimates using atmospheric sampling and inverse modeling.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Carbon Sequestration Research**	**8,518**	**8,557**	**8,543**

In FY 2004, BER will continue support for one carbon sequestration research consortium, led by ORNL, PNNL, and ANL, and involving six collaboratory universities, that focuses on terrestrial sequestration, Carbon Sequestration in Terrestrial Ecosystems (CSiTE) ($3,000,000). The consortium develops the information to enhance the natural sequestration of carbon in terrestrial soils and vegetation. BER will also continue the support of research at universities and DOE laboratories on ocean carbon sequestration ($2,000,000). The focus of the research on terrestrial and ocean sequestration will continue to be on cellular and biogeochemical processes that control the rate and magnitude of carbon sequestration in terrestrial and oceanic systems, including the identification of pathways and processes that could be modified to enhance the net flow of carbon from the atmosphere to terrestrial plants and soils, and to the ocean surface and, ultimately, to the deep ocean. Also, BER will support the research needed to assess the environmental implications of enhancing carbon sequestration and storage in the ocean and in terrestrial systems. BER research on carbon sequestration in terrestrial ecosystems will improve the scientific understanding of mechanisms of sequestration and how to alter them to enhance sequestration. The CSiTE activity will conduct research that specifically examines those plant and soil processes that capture and retain carbon in chemical and physical forms that are resistant to decay. The data will inform new models for estimating carbon sequestration in terrestrial ecosystems. New technologies will be developed by the BER-supported ocean carbon sequestration research to facilitate the export of carbon to the deep ocean and for re-mineralization of organic carbon at depth. Such technologies are vital to assessing accurately the potential of enhancing ocean carbon sequestration. Initial *in situ* experiments will be designed to determine the feasibility and potential environmental impacts of deep ocean injection of carbon dioxide (CO_2). Associated research will include determination of chemical reactions at depth, stability of products, and effects of those products on marine organisms.

In FY 2004, university scientists will continue the analyses of research results on the effects of iron fertilization on plankton communities in the Southern Ocean. The ocean surrounding Antarctica is the largest high-nutrient, low-chlorophyll region in the world. The joint DOE-NSF Southern Ocean Iron Enrichment Experiment (SoFEX) will help scientists understand the potential to enhance ocean carbon sequestration through iron enrichment.

Ecological Processes	**12,817**	**13,888**	**18,726**

In FY 2004, new ecological research will be initiated to develop a more mechanistic understanding of the scales of response of complex ecosystems to environmental changes, including identifying the underlying causal mechanisms and pathways and how they are linked, ranging from the proteomes of individual species to the whole ecosystem. The focus initially will be on understanding the linkages of scales in model terrestrial ecosystems containing simplified but hierarchical communities (higher plants, consumers of plant production, and soil microorganisms). A key environmental factor such as temperature that is known to affect ecosystem functioning (e.g., carbon and nutrient cycling) will be experimentally manipulated and proteomic responses of individual species and the whole ecosystem will be measured. Advanced biologically based computational algorithms and ecosystem models will be

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

developed to establish whether and how proteomic changes (in either single species or whole systems) explain the responses and behavior of complex ecosystems. Tools and principles developed from this research should have broad generality and eventual application to problems in carbon sequestration, ecological risk assessment, environmental restoration and cleanup, and early detection of ecological responses to climate change and other environmental factors.

BER will continue four Free-Air Carbon Dioxide Enrichment (FACE) experiments at Duke University (North Carolina), Rhinelander (Wisconsin), Oak Ridge (Tennessee), and Mercury (Nevada) on the Nevada Test Site to improve understanding of the direct effects of elevated carbon dioxide and other atmospheric changes on the structure and functioning of various terrestrial ecosystems. Emphasis will be on understanding the cause of differential responses of plant species that may impact plant competition, succession, and productivity in terrestrial ecosystems. Research will explore changes, over time, in the elevated productivity of terrestrial plants exposed to elevated atmospheric carbon dioxide (CO_2) concentrations.

The long-term experimental investigation at the Walker Branch Watershed in Tennessee will continue to improve the understanding of the direct and indirect effects of alterations in the annual average precipitation on the functioning and structure of a southeastern deciduous forest ecosystem.

Both the FACE network and the Walker Branch Watershed represent scientific user facilities that have attracted scientists from both the academic community and government laboratories who use the facilities to develop new instrument methodologies and test scientific hypotheses related to ecosystem responses, including carbon sequestration, to climate and atmospheric changes.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

In FY 2004, NIGEC will support experimental studies to document how climate warming and increasing CO_2 levels in the atmosphere affect biophysical processes in terrestrial ecosystems (FY 2004 Request is $2,625,000).

Human Interactions	**7,942**	**8,084**	**8,071**
▪ **Human Interactions**	**7,942**	**8,084**	**8,071**

The Integrated Assessment program, with a strong academic involvement, will continue to support research that will lead to better estimates of the costs and benefits of possible actions to mitigate global climate change. The goal is to improve the integrated assessment models to include several greenhouse gases, carbon sequestration, and international trading of emission permits. The models will better represent the efficiency gains and losses of alternate emission reduction plans, including market adjustments to inter-regional differences among relative energy prices, regulations, and production possibilities in the international arena. Integrated assessment models will be modified to

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

include carbon sequestration as an alternative mitigation option. This representation will include both options to enhance natural carbon storage in the terrestrial biosphere, as well as engineering options, such as the capture of carbon dioxide and storage in geologic formations.

The research will include integrating a new land and ocean carbon sub-model in a large integrated assessment model. The submodel includes a detailed representation of direct human influence (mainly agriculture and forestry) on the terrestrial biosphere. In addition to providing a more accurate representation of the global carbon cycle, the improvement will ensure consistent accounting of carbon-sink projects and the carbon uptake that occurs as a result of other land-use change and the effects of climate change and carbon fertilization. A second integrated assessment model will be used to simulate the effect of 1) climate on crop yields and 2) the amount of crop and pasture land necessary to provide (a) a sufficient diet in developing countries under climate change and (b) the likely increase in dietary requirements as developing countries become richer.

In FY 2004, NIGEC will support research to develop and test new methods involving the use of large regional databases and coupled climate-impact-economic models to conduct integrated assessments of the effects of climate change on regionally important resources in the U.S. (FY 2004 Request is $1,750,000).

The Integrated Assessment research program will fund research to develop internally consistent sets of scenarios that can be used for national-scale decision-making. The scenarios will be evaluated in selected integrated assessment models, also funded by the Integrated Assessment program. In FY 2004 ($2,972,000) the Integrated Assessment program will produce at least four scenarios to provide alternatives to the scenarios that were published by the Intergovernmental Panel on Climate Change. These scenarios will include forecasts of such items as economic productivity, population, and energy use by global region. They will serve as input to the Integrated Assessment Models and will be used as input to decision support analysis in the new CCRI.

The Information and Integration element stores, evaluates, and quality-assures a broad range of global environmental change data, and disseminates those data to the broad research community. BER will continue the Quality Systems Science Center for the tri-lateral (Mexico, United States, and Canada) NARSTO (formally known as the North American Strategy for Tropospheric Ozone), a public partnership for atmospheric research in support of air quality management. The Center serves a diverse set of users, including academic and laboratory scientists and policy makers across North America.

The Global Change Education program supports DOE-related research in global environmental change for both undergraduate and graduate students, through the DOE Summer Undergraduate Research Experience (SURE), the DOE Graduate Research Environmental Fellowships (GREF), and collaboration with the NSF Significant Opportunities in Atmospheric Research and Science (SOARS) program.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**3,554**	**3,896**

In FY 2002 $3,152,000 and $188,000 were transferred to the SBIR and STTR programs, respectively. FY 2003 and FY 2004 amounts are the estimated requirements for continuation of these programs.

Total, Climate Change Research	**125,847**	**137,959**	**142,959**

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Climate and Hydrology	
▪ Held at near FY 2003 level. Change is due to increase in STTR allocation	-110
Atmospheric Chemistry and Hydrology	
▪ Held at near FY 2003 level. Change is due to increase in STTR allocation.	-57
Ecological Processes	
▪ The increase will support new research on scaling from the molecular level in individual organisms up to the aggregate ecosystem scale. The focus is on research to understand and model how complex ecosystems respond to the environment, including the causal mechanisms and pathways underlying observed responses, ranging from the proteome of individual species to the whole system. Tools and principles developed from this research will have eventual application to problems in carbon sequestration, ecological risk assessment, environmental restoration and cleanup, and early detection of ecological responses to climate change and other environmental perturbations caused by energy production and use.	+4,860
▪ Traditional Ecological Processes research held at near FY 2003 levels.	-22
Total, Ecological Processes	+4,838
Human Interactions	
▪ Held at near FY 2003. Decrease is due to increase in STTR allocation	-13

	FY 2004 vs. FY 2003 ($000)
SBIR/STTR	
▪ Increase in SBIR/STTR due to increase in STTR allocation and increase in research funding for the Climate Change Research program.	+342
Total Funding Change, Climate Change Research	+5,000

Environmental Remediation

Mission Supporting Goals and Measures

The mission of the Environmental Remediation subprogram is to deliver the scientific knowledge, technology and enabling discoveries in biological and environmental research to reduce the costs, risks, and schedules associated with the cleanup of the DOE nuclear weapons complex; to extend the frontiers of biological and chemical methods for remediation; to discover the fundamental mechanisms of contaminant transport in the environment; to develop cutting edge molecular tools for investigating environmental processes; and to develop an understanding of the ecological impacts of remediation activities. In addition much of the work performed for the cleanup program will provide fundamental knowledge that applies to a broad range of remediation problems, as well to the development advanced nuclear waste management approaches and predicting and avoiding environmental hazards for future nuclear energy options.

Research priorities include bioremediation, contaminant fate and transport, nuclear waste chemistry and advanced treatment options, and the operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) and the Savannah River Ecology Laboratory (SREL).

Bioremediation activities are centered on the Natural and Accelerated Bioremediation Research (NABIR) program, a basic research program focused on determining how and where bioremediation may be applicable as a reliable, efficient, and cost-effective technique for cleaning up or containing metals and radionuclides in contaminated subsurface environments. In the NABIR program, research advances will continue to be made from molecular to field scales in the Biogeochemical Dynamics element; on genes and proteins used in bioremediation through the Biomolecular Science and Engineering element; in non-destructive, real-time measurement techniques in the Assessment element; in overcoming physico-chemical impediments to bacterial activity in the Acceleration element; on species interaction and response of microbial ecology to contamination in the Community Dynamics and Microbial Ecology element; and in understanding microbial processes for altering the chemical state of metallic and radionuclide contaminants through the Biotransformation element. In analogy with the Ethical, Legal, and Social Implications component of the Human Genome program, the Bioremediation and its Societal Implications and Concerns component of NABIR is exploring societal issues surrounding bioremediation research and promoting open and interactive communication with stakeholders to help ensure understanding and acceptance of bioremediation as a potential solution to remediating contaminants. All NABIR elements and EMSL activities have a substantial involvement of academic scientists.

The Clean Up Research and Environmental Management Science Programs (EMSP) focus on a variety of solutions for the DOE weapons complex cleanup effort. Three primary elements include: contaminant fate and transport in the subsurface, nuclear waste chemistry and advanced treatment option, and novel characterization and sensor tools. In addition, studies on bioremediation of organic contaminants are conducted in EMSP, complementing the NABIR program, which focuses on metals and radionuclides. This program works closely with related programs in the Basic Energy Sciences program and with related programs of other agencies. The SREL is managed through a cooperative agreement with the University of Georgia and performs ecological research aimed at ensuring that environmental cleanup operations do not disturb the biodiversity at the restored environment.

Within Facility Operations, support of the EMSL national user facility operations is focused on providing advanced molecular tools to the scientific community in such areas as environmental remediation sciences, biology and genomics, and atmospheric science. In FY 2004, unique EMSL facilities, such as the newly upgraded Molecular Science Computing Facility, the new (in FY 2003) 900 MHz NMR, and the High-Field Mass Spectrometry Facility will expand both their scientific scope and their user base.

The Environmental Remediation subprogram provides fundamental knowledge building to long-term outcomes that underpin the Program Strategic Performance Goals and the Office of Science's Strategic Objectives. Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This program was reviewed as part of a BERAC review of the entire BER program in FY 2001. The next scheduled comprehensive review of the Environmental Remediation Sciences subprogram by BERAC will be in FY 2003. The following are recent scientific accomplishments that highlight program progress.

- *EMSP Project Results in Commercialized D&D Tool for use at DOE Sites.* An Environmental Management Science Program project "Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces" has just been licensed and is being commercialized by APJet Inc. The project, collaboration between Los Alamos National Laboratory (LANL) and University of California, Los Angeles (UCLA), began at LANL out of basic research on cold plasmas at atmospheric pressures. The commercialized product will be used for removing contaminants from surfaces during D&D operations at DOE sites.
- *Theoretical Work Results in Advanced Separations Agents for Nuclear Wastes.* Using theoretical methods and the computing capabilities at EMSL, a new class of designer molecules that are highly organized for selective complexation with transuranic elements has been designed. In this EMSP project, preliminary experimental results suggest that these new molecules, called bicyclic diamides exhibit distribution coefficients for certain transuranics that are 10 *million times* larger than conventional diamides used in the current Purex process for separating transuranics from high-level nuclear waste media.
- *Some Microorganisms can "sniff out," produce flagella, and swim toward metal oxides.* Natural and Accelerated Bioremediation Research Program (NABIR) funded studies show that microorganisms that use insoluble metal oxides to drive energy metabolism play important roles in the bioremediation of metal and organic contaminants in groundwater. Although iron oxides are often present in subsurface environments, microbes must find and access these insoluble substrates to live. A surprising finding in the genetic code of a common bacterium, *Geobacter*, led to the discovery of an unusual strategy for survival in subsurface environments. The genome of *Geobacter metallireducens* was sequenced through the Microbial Genome Program at the Joint Genome Institute. The sequence data revealed that *Geobacter,* previously thought to be immobile, can produce flagella that allow it to swim toward metal oxides. Thus, *Geobacter* appears to have a built-in sensor that allows it to "sniff out" and find metals oxides. *Geobacter* is of great interest to the DOE because it can precipitate uranium, and therefore offers a potentially efficient and economic solution to removing uranium from contaminated groundwater through *in situ* immobilization.

- *Innovative Sensors for Field Detection of Environmental Contaminants Developed*. A novel handheld sensor for detecting uranium in the environment has been developed in the NABIR program using a monoclonal antibody with specificity for uranium and an instrument developed by Sapidyne Instruments, Inc. The prototype "immunosensor" has been shown to detect soluble uranium oxide at extremely low concentrations (2.5 to 24 ppb). These portable sensors yield reliable data in real time (< 1 hour), are field ready (simple, durable, accurate) and inexpensive (<$5,000 per instrument). Work is underway to develop new monoclonal antibodies for chromium and mercury for detection in the environment.
- *EMSL Users and Scientists Conduct Computational Science Studies with New Linux-Based Supercomputer* - A new 8.3 teraflop, Linux-based supercomputer at the EMSL has been made available for grand challenge teams of scientists to apply computational science to study complex chemical problems that form the basis for new discoveries in areas such as subsurface transport, atmospheric chemistry, materials design, life sciences and systems biology, and combustion. The new massively parallel system is more than 30 times faster, has 50 times more disk space and holds 10 times as much memory as EMSL's original supercomputer.
- *900 MHz Nuclear Magnetic Resonance (NMR) Spectrometer at the EMSL Provides Improved Resolution of Protein Structures* - EMSL users and scientists are obtaining high resolution data on the atomic structures of large and unstable proteins using EMSL's 900 MHz wide-bore NMR. Because certain types of proteins are difficult to crystallize, and therefore not amenable to structure determination using DOE's light sources, the EMSL's 900 MHz NMR is proving to be the only alternative to resolving the structure of these "difficult" proteins. In addition, because the proteins are examined in a solution state, the resolved structures may be more "realistic" than crystallized samples.

Subprogram Goals

Develop and demonstrate novel solutions to DOE's most challenging problems, including 1) in situ treatment of contaminant plumes such as bioremediation and environmental reactive barriers, 2) new treatment options for complex wastes, 3) novel disposal options for complex wastes (e.g. alternative to borosilicate glass); cost-effective contaminant plume characterization and monitoring techniques for long-term stewardship of sites, 5) improved predictive capabilities for contaminant fate and transport, and 6) basis for accurate assessment of risk factors.

Performance Indicator

Advanced environmental cleanup approaches delivered.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(NABIR & Bioremediation Research)	(NABIR & Bioremediation Research)	(NABIR & Bioremediation Research)
Using data from genomic sequences of key bioremediation microorganisms such as *Geobacter, Deinococcus* and *Shewanella*, a molecular level understanding of the detection and transformation of metals and radionuclides is being achieved. Physiological studies of microorganisms have shown that common soil microorganisms produce organic compounds that interact with radionuclides, including plutonium. Research at Uranium Mill Tailings Remedial Action sites has demonstrated the potential to use biostimulation to reduce and immobilize uranium in the subsurface. In partnership with EM-50, two new projects have been initiated at Hanford to study the use biostimulation (addition of nutrients) to remove chromium and technetium from ground water. [Goal Met]	Complete two critical field experiments at the NABIR Field Research Center near the Y-12 area at the Oak Ridge Reservation. The first experiment will use "push-pull" technology to probe the structure and function of undisturbed microbial communities in the subsurface contaminated with uranium and nitrate. This will be the first time this new technology has been tested in a radionuclide-contaminated site. The second experiment will provide valuable information on the use of bioremediation to remove uranium from groundwater in which nitrate is a co-contaminant-- a common problem at DOE sites Demonstrate, in partnership with the Office of Environmental Management, the reliability of new biologically based technologies for monitoring radionuclides contaminants and the microbial communities that can bioremediate those contaminants. These include antibody-based sensors for detecting uranium and certain metals, as well as nucleic acid based technologies for assessing the structure and function of microbial communities in contaminated environments.	By the end of FY 2004, demonstrate whether certain nutrient additions stimulate subsurface microorganisms to immobilize uranium, thereby reducing its concentration and transport in soil water and groundwater. The field experiment will be in a contaminated subsurface environment where the co-contaminant nitrate is also present and will confirm the potential of biotechnology for environmental remediation of radionuclides. Successful demonstrate, in partnership with the Office of Environmental Management's Science and Technology program, the reliability of new biologically based technologies for monitoring radionuclide contaminants and the microbial communities that can bioremediate those contaminants. These include antibody-based sensors for detecting uranium and certain metals, as well as nucleic acid based technologies for assessing the structure and functioning of microbial communities in contaminated environments.
(Environmental Management Science Program)	(Environmental Management Science Program)	(Environmental Management Science Program)
Performed analysis of program scope and management and developed a strategic plan for incorporating EMSP into Environmental Remediation Sciences in preparation for the FY 2003 transfer from the Office of Environmental Management as requested in the President's FY 2003 budget. [Goal Met]	Begin integration of EMSP into Environmental Remediation Sciences, including coordination with ongoing NABIR research. Develop two new activities with EMSP: (1) develop plan with SRS and EMSP investigators for a Bioremediation Project at the Savannah River Site. Assess the needs for user facilities and capabilities for	Complete integration of EMSP into Environmental Remediation Sciences, including coordination with ongoing NABIR research. Initiate R&D projects to support SRS Bioremediation Project. Start development of user facility enhancements.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
	environmental research, including the synchrotron light sources, neutron scattering facilities, and computation centers.	
(Savannah River Ecology Laboratory)	(Savannah River Ecology Laboratory)	(Savannah River Ecology Laboratory)
Performed analysis of program scope and management and developed strategic plan for incorporating SREL into Environmental Remediation Sciences in preparation for the FY 2003 transfer from the Office of Environmental Management as requested in the President's FY 2003 budget. [Goal Met]	Develop a plan, working with the University of Georgia and the Savannah River Site to increase the scope of ecology research and education programs at SREL.	Initiate new peer reviewed ecology research programs at the Savannah River site and new education programs at SREL.

Manage all BER facility operations to the highest standards of overall performance, using merit evaluation with independent peer review.

Performance Indicator

Average operational downtime of BER facilities will not exceed 10% of total time scheduled.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Environmental Molecular Sciences Laboratory)	(Environmental Molecular Sciences Laboratory)	(Environmental Molecular Sciences Laboratory)
First phase of new high performance computer delivered and meeting performance benchmarks, achieving 1 Tflop in FY 2002. The number of FY 2002 users increased by approximately 10% over FY 2001. Unscheduled downtimes on the major instrument / computer systems did not exceed 10%. Successful receipt and testing of the 900 MHz NMR was completed. [Goal Met]	(1) Initiate operation of a new high performance computer at the EMSL reaching 9 Tflop performance and (2) unscheduled operational downtime on EMSL instrumentation and computational resources will not exceed 10 percent.	(1) Full operation at 9 Tflop of the new supercomputer at the EMSL and (2) unscheduled operational downtime on EMSL instrumentation and computational resources not to exceed 10 percent.

Funding Schedule

	(dollars in thousands)				
	FY 2002	FY 2003	FY 2004	$ Change	% Change
Bioremediation Research	29,320	30,700	29,867	-833	-2.7%
Clean Up Research	44,915	38,190	39,470	+1,280	+3.4%
Facility Operations	37,614	37,948	37,138	-810	-2.1%
SBIR/STTR	0	2,692	2,845	+153	+5.7%
Total, Environmental Remediation	111,849	109,530	109,320	-210	-0.2%

Detailed Program Justification

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Bioremediation Research	**29,320**	**30,700**	**29,867**
▪ **NABIR and Bioremediation Research**	**23,365**	**24,720**	**24,097**

In FY 2004, NABIR will continue to increase the understanding of the intrinsic bioremediation (natural attenuation) of DOE relevant metal and radionuclide contaminants, as well as of manipulated, accelerated bioremediation using chemical amendments. Laboratory and field experiments will be conducted to explore the fundamental mechanisms underlying chemical processes and complexation/transformation of contaminants. The NABIR Field Research Center is in operation at the Oak Ridge National Laboratory. Field site characterization of this Field Research Center and distribution of research samples to investigators will continue. In FY 2004, science elements in the NABIR program continue fundamental research on the following subjects: (1) Biotransformation (microbiology to elucidate the mechanisms of biotransformation of metals and radionuclides); (2) Community Dynamics and Microbial Ecology (structure and activity of subsurface microbial communities); (3) Biomolecular Science and Engineering (molecular and structural biology to enhance the understanding of bioremediation and identify novel remedial genes); (4) Biogeochemical Dynamics (dynamic relationships among *in situ* geochemical, geological, hydrological, and microbial processes); and (5) Assessment (measuring and validating the biological and geochemical processes of bioremediation). University scientists continue to form the core of the NABIR science team that networks with the broader academic community as well as with scientists at the National Laboratories and at other agencies.

The NABIR Field Research Center (FRC) is located near the Y-12 area at the Oak Ridge Reservation and is the site of field-scale, hypothesis-driven research on the bioremediation of metals and radionuclides. Researchers are characterizing and modeling the subsurface water flow, contaminant transport and biogeochemical processes at the FRC. These experiments will be completed and

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004

written up for peer-reviewed publication in FY 2003. In FY 2004, field experiments will continue. These combine both microbiological and chemical treatment of uranium and the common co-contaminant, nitrate.

The NABIR program will continue to take advantage of recently completed genome sequence of important metal and radionuclide-reducing microorganisms to study the regulation and expression of genes that are important to bioremediation. In FY 2004, researchers working on sequenced microorganisms such as *Geobacter sulfurreducens, Desulfovibrio vulgaris*, and *Shewanella onediensis* will use state-of-the-art nucleic acid based microarrays to identify environmental factors affecting genetic regulation of uranium reduction.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

In FY 2004, the activities are reduced to enhance funding for Savannah River Ecology Laboratory.

	FY 2002	FY 2003	FY 2004
■ **General Plant Projects (GPP)**	**4,791**	**4,811**	**4,811**

The General Plant Projects (GPP) funding is continued for minor new construction, other capital alterations and additions, and for buildings and utility systems such as replacing piping in 30 to 40-year old buildings, modifying and replacing roofs, and HVAC upgrades and replacements. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting the requirements for safe and reliable facilities operation. This subprogram includes stewardship GPP funding for Pacific Northwest National Laboratory (PNNL) and for Oak Ridge Institute for Science and Education (ORISE). The total estimated cost of each GPP project will not exceed $5,000,000. The effort will continue rehabilitation and upgrade of research facilities in the 300 area of the PNNL, including beginning the replacement of process water piping in a 40 year old building used for biological research, refurbishing 20-year old office and laboratory space, and reconfiguring space in several 40+ year old buildings to better accommodate current scientific research projects.

	FY 2002	FY 2003	FY 2004
■ **General Purpose Equipment (GPE)**...	**1,164**	**1,169**	**959**

The General Purpose Equipment (GPE) funding will continue to provide general purpose equipment for PNNL and ORISE such as information system computers and networks, and instrumentation that supports multi-purpose research.

	FY 2002	FY 2003	FY 2004
Clean Up Research	**44,915**	**38,190**	**39,470**
■ **Clean Up Research**..	**790**	**2,463**	**2,448**

The modest program in clean up research will continue to be managed together with the EMSP program. The focus will continue on biophysical and chemical characterization of environmental contaminants in support of field and laboratory studies of contaminant transport and bioremediation.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
▪ **Environmental Management Science Program**	**36,125**	**29,886**	**29,246**

The goal of the Environmental Management Science Program (EMSP), transferred in FY 2003 from Environmental Management to the BER program, is to support basic research that improves the science base underpinning the clean up of DOE sites. Traditional clean up strategies may not work or be cost effective for many of the challenges that threaten the successful closure of DOE sites. The EMSP, through its support of basic research aims to develop and validate technical solutions to complex problems, provide innovative technical solutions where there are none, and lead to future risk reduction and cost and time savings. It is the intent or the expectation of the EMSP that the basic research projects funded are directed toward specific issues and uncertainties at the DOE sites. EMSP research will focus on contaminant fate and transport in the subsurface, nuclear waste chemistry and advanced treatment options, and novel characterization and sensor tools. In addition, studies on bioremediation of organic contaminants are conducted in EMSP, complementing the NABIR program, which focuses on metals and radionuclides.

EMSP projects will continue to be funded through a competitive peer review process. The most scientifically meritorious research proposals and applications will be funded based on availability of funds and programmatic relevance to ensure a complete and balanced research portfolio that addresses DOE needs. Research will be funded at universities, national laboratories, and at private research institutes and industries. This research will be conducted in collaboration with the Office of Environmental Management.

In FY 2004, the activities are reduced to enhance funding for the Savannah River Ecology Laboratory.

▪ **Savannah River Ecology Laboratory**...	**8,000**	**5,841**	**7,776**

This activity supports, through a cooperative agreement with the University of Georgia, a long-term (40+ years) ecological research activity aimed at reducing the cost of clean up and remediation while ensuring biodiversity at the restored environment. Peer-reviewed research will be supported to assess the ecological risks of environmental contaminants and remediation activities. Characterizing and understanding the impacts of environmental contamination on intact, living ecosystems is a complex and long-term process since the research is dependent on natural cycles of growth, reproduction, and normal environmental variation. A sustained investment is required to understand the complex interactions of ecosystems with environmental contaminants.

In FY 2004, new ecological research will develop the knowledge needed to understand how site environmental cleanup activities may impact biodiversity at the Savannah River Site and other DOE sites. This will continue a broad educational component at the site including opportunities for K-12, undergraduate, and graduate students, and post doctoral fellows.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Facility Operations: William R. Wiley Environmental Molecular Sciences Laboratory (EMSL)..	**37,614**	**37,948**	**37,138**
▪ **Operating Expenses**	**33,808**	**35,959**	**35,149**

The EMSL is a scientific user facility located at the Pacific Northwest National Laboratory focused on conducting interdisciplinary, collaborative research in molecular-level environmental science. Operating funds are essential and will continue to allow the EMSL to operate as a user facility, and are used for maintenance of buildings and instruments, utilities, staff support for users, environment, safety and health compliance activities, and communications. With over 100 leading-edge instruments and computer systems, the EMSL annually supports approximately 1200 users. University scientists form the core of the EMSL science team that networks with the broader academic community as well as with scientists at other agencies. EMSL users have access to unique instrumentation for environmental research, including a new Linux-based supercomputer, a 900 MHz nuclear magnetic resonance (NMR) spectrometer that adds to the suite of NMRs in EMSL, a suite of mass spectrometers, including an 11.5 Tesla high performance mass spectrometer, laser desorption and ablation instrumentation, ultra-high vacuum scanning tunneling and atomic force microscopes, and controlled atmosphere environmental chambers.

The supercomputer will continue to support two dozen "grand challenge" computational projects at the molecular level and in areas ranging from molecular geochemistry and biogeochemistry, numerical modeling of reactive transport in the subsurface, chemical processing and catalysis, aerosol formation and chemical transformations, climate modeling and simulation, and structural biology.

The research activities using EMSL are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.
BER will maintain and operate EMSL and the structural biology user facilities so that the unscheduled operating downtime will be less than 10%, on average, of total scheduled operating time.

In FY 2004, the activities are reduced to enhance funding for the Savannah River Ecology Laboratory.

▪ **Capital Equipment**..	**3,806**	**1,989**	**1,989**

Capital equipment support for the EMSL enables instrument modifications needed by collaborators and external users of the facility as well as the purchase of state-of-the-art instrumentation to keep EMSL capabilities at the leading edge of molecular-level scientific research. Increased capital equipment funding ($2,994,000) in FY 2002 supported the upgrade of user capabilities through the acquisition of additional mass spectrometers and Nuclear Magnetic Resonance (NMR) spectrometers for structural biology research.

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**2,692**	**2,845**

In FY 2002 $2,354,000 and $139,000 were transferred to the SBIR and STTR programs, respectively. FY 2003 and FY 2004 amounts are estimated requirements for continuation of these programs.

Total, Environmental Remediation	**111,849**	**109,530**	**109,320**

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Bioremediation Research	
▪ GPE funding for motor vehicles at PNNL reduced	-210
▪ Funding for NABIR reduced to accommodate increase for Savannah River Ecology Laboratory	-623
Total, Bioremediation Research	-833
Clean Up Research	
▪ Funding for Savannah River Ecology Laboratory restored to FY 2002 level	+1,935
▪ Funding for Clean Up research reduced to accommodate increase for Savannah River Ecology Laboratory	-15
▪ Funding for EMSP reduced to accommodate increase for Savannah River Ecology Laboratory	-640
Total, Clean Up Research	+1,280
Facility Operations: William R. Wiley Environmental Molecular Sciences Laboratory (EMSL)	
▪ Funding for EMSL operations reduced to accommodate increase for Savannah River Ecology Laboratory	-810
SBIR/STTR	
▪ SBIR/STTR increases due to increased STTR allocation and increase in research for Environmental Remediation.	+153
Total Funding Change, Environmental Bioremediation	-210

Medical Applications and Measurement Science

Mission Supporting Goals and Measures

The goal of the Medical Applications and Measurement Science subprogram is to deliver the scientific knowledge and discoveries that will lead to innovative diagnostic and treatment technologies for human health. The research builds on unique DOE capabilities in physics, chemistry, engineering, biology and computational science. Research will lead to new metabolic labels and imaging detectors for medical diagnosis; tailor-made radiopharmaceutical agents and beam delivery systems for treatment of inoperable cancers; and the ability to predict structure and behavior of cells and tissues to better engineer targeted drugs, biosensors, and medical implants. The basic research technologies growing out of this program offer applications for study, detection, diagnosis and early intervention of biochemical, bacterial, and viral health risks of biological, and/or gross environmental insults.

The modern era of nuclear medicine is an outgrowth of the original charge of the Atomic Energy Commission (AEC), "to exploit nuclear energy to promote human health." From the production of a few medically important radioisotopes in 1947, to the development of production methods for radiopharmaceuticals used in standard diagnostic tests for millions of patients throughout the world, to the development of ultra-sensitive diagnostic instruments, e.g. the PET (positron emission tomography) scanner, the medical applications program has led and continues to lead the field of nuclear medicine.

Today the program seeks to develop new applications of radiotracers in diagnosis and treatment driven by the latest concepts and developments in genomic sciences, structural and molecular biology, computational biology and instrumentation. Using non-invasive technologies and highly specific radiopharmaceuticals, BER is ushering in a new era of brain mapping, and highly specific disease diagnostics. New tools will enable the real-time imaging of gene expression in a developing organism.

Research capitalizes on the National Laboratories' unique resources and expertise in biological, chemical, physical, and computational sciences for technological advances related to human health. The National Laboratories have highly sophisticated instrumentation (neutron and light sources, mass spectroscopy, high field magnets), lasers and supercomputers, to name a few, that directly impact research on human health. Research is directed to fundamental studies in biological and medical imaging (including construction of an artificial retina), biological and chemical sensors, laser medicine and informatics. This research is highly complementary to and coordinated with clinical research at the National Institutes of Health (NIH) and to basic research in the NIH intramural and extramural programs.

DOE supports cutting edge, high-risk, proof-of-concept research that develops research tools with broad applications in clinical medicine and in biological research. NIH supports cutting edge, disease-specific research that uses those tools, along with many others, to determine fundamental mechanisms of human disease for better diagnosis and treatment. For example, NIH supports clinical imaging research but not research to develop radiotracers or imaging instruments, whereas DOE is the only government agency that supports research to develop imaging instruments and the radiotracers needed to carry out imaging procedures.

The philosophical differences, roles, strengths, and advantages of the DOE versus NIH medical sciences research programs are clear:

- DOE medical sciences research is built on a base of chemistry, physics, engineering, computation, and biology. NIH medical sciences research is built on a complementary base of biology and medicine. DOE research leverages the unique combination of multidisciplinary competencies available at the DOE national laboratories.
- DOE develops research tools for medicine by supporting high-risk research often based on theoretical predictions of success rather than preliminary studies that demonstrate a promise of success. As in other fields of science, high risk research often leads to spectacular advances, e.g., the human genome project and genetics. NIH develops disease-specific applications for these research tools by supporting research that is generally based on substantive preliminary studies that actually demonstrate a promise of success.

Measurement Science research emphasizes new sensor instrumentation for cleanup efforts and new imaging instrumentation having broad application in the life and medical sciences.

The Medical Applications and Measurement Science subprogram continues a substantial involvement of academic scientists along with the scientists in the National Laboratories.

The Medical Applications and Measurement Science subprogram provides fundamental knowledge building to long-term outcomes that underpin the Program Strategic Performance Goals and the Office of Science's Strategic Objectives. Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This program was examined as part of a BERAC review of the entire BER program in FY 2001. The next scheduled comprehensive review of the Medical Applications and Measurement Science subprogram by BERAC will be in FY 2006. The following are recent scientific accomplishments that highlight program progress.

- *First technique to measure Alzheimer's disease onset.* DOE researchers at UCLA have developed an imaging technique that can detect early lesions in the brains of Alzheimer's disease before symptoms begin. The method utilizes a novel radiotracer and highly sensitive PET scanning. Early identification of Alzheimer's lesion offers the possibility of therapeutic intervention before severe brain injury and clinical debilitation occurs.
- *BNCT technology transferred to NIH for clinical trials*. DOE research at the Brookhaven National Laboratories, MIT and Harvard Medical School established the parameters of clinical safety of boron neutron capture therapy in humans. DOE has completed upgrade of the Medical Reactor at MIT; the facility now generates the most advanced neutron beam for clinical studies in the world. Using the fundamental technology developed by DOE, the National Cancer Institute has initiated a BNCT clinical trial in the treatment of brain cancer and melanoma at the MIT medical reactor.
- *Successful transfer of DOE Micro-Pet technology to industry.* DOE investigators at UCLA have successfully developed the Micro-Pet for repeated physiological imaging of small animals without sacrificing the animal. The Micro-Pet is a major advance in the study of animal models of human disease. The technology developed at UCLA has been transferred to Concorde Microsystems, Inc. of Knoxville, TN for marketing and public use.

- *Helping the blind to see.* A collaborative project between USC Doheny Eye Institute, Oak Ridge National Laboratory, Sandia National Laboratory, Argonne National Laboratory, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory is aimed at developing an artificial retina to restore the sight of patients with retinitis pigmentosa and age-related macular degeneration. A milestone was reached in which a prototype design of a high-density sensor was successfully inserted into a canine and tested successfully. Future programmatic goals include improvement in the prototype design of the retinal device and eventually implantation into the eye of a blind person.
- *New, ultra-sensitive detection of prostate cancer protein in the blood*. DOE scientists at ORNL and UC-Berkeley have developed a cancer detecting microchip that works as a sensitive assay for prostate cancer. The device utilizes a micro machine cantilever to detect prostate specific antigen and is twenty times more sensitive than currently used assays. This technology, which has been pioneered at ORNL, can be adapted to measure other clinically important molecules at high levels of sensitivity.
- *DOE technology for stroke treatment transferred to NIH.* DOE researchers at Lawrence Livermore National Laboratory have successfully completed the material design of a mechanical shape memory polymer device that can be introduced into the vessels in the brain and successfully remove a blood clot causing a stroke. This technology has the potential of significantly reducing deaths from one of the major disease killers in the United States. The DOE has successfully transferred this technology to the NIH, which will fund initial clinical evaluation of the device.
- *A Multitracer Technique for Diagnosing the Root Cause of Obesity.* Brookhaven National Laboratory (BNL) scientists have developed a multi-radiotracer (carbon-11-raclopride, fluorine-18-FDG and carbon-11 cocaine combined) PET imaging approach which shows that obese individuals have an understimulated brain dopamine system similar to drug abusers. Dopamine is a brain chemical that is important in reward and well-being. This disruption of dopamine function may account for pathological overeating, which has parallels in the drug abuser who cannot stop taking the drug even when this behavior is detrimental. This suggests that improving dopamine function may be a useful treatment strategy for obesity, a major public health problem affecting more than 25% of the United States population.
- *New Toluene Radiotracer Developed to Study Inhalant Abuse*. BNL scientists have successfully labeled the volatile chemical toluene with carbon-11 for PET imaging. Using carbon-11 toluene for PET imaging, Brookhaven scientists have shown for the first time that toluene, the most common solvent of abuse, rapidly enters the brain and localizes on the same areas of the brain that are affected by cocaine and other drugs of abuse. This new approach and the new knowledge that it is generating are an important step in understanding and eventually treating addiction to inhalants. The abuse of inhalants ("huffing") by children is a growing problem worldwide.
- *PET Imaging Study Provides New Knowledge For Improved Targeting of Attention Deficit Hyperactivity Disorder.* For more than 40 years, attention deficit hyperactivity disorder (ADHD) has been treated with Ritalin, a stimulant. Yet there have been no studies showing how Ritalin affects the human brain. Using PET imaging with radiotracers (carbon-11 raclopride, and carbon-11 cocaine) Brookhaven researchers have shown for the first time in the human brain that Ritalin elevates

dopamine, a signaling chemical that is important in regulating attention. This new knowledge will form the groundwork for designing better drugs to treat ADHD.

Subprogram Goals

Develop innovative radiopharmaceuticals for diagnosis and treatment of human disease and develop novel imaging instrumentation and technologies to precisely visualize and measure biological functions, including gene expression, and more accurately detect human disease.

Performance Indicator

Number of novel imaging devices delivered.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Novel cell-directed cancer therapies)	(Novel cell-directed cancer therapies)	(Novel cell-directed cancer therapies)
BNCT program at MIT/Harvard was successfully transferred to the National Cancer Institute for conduct of clinical trials. [Goal Met]	Number of tumor therapeutic agents that perform sufficiently well in pre-clinical evaluations to deserve consideration for clinical trials by NIH and/or private industry.	Number of tumor therapeutic agents that perform sufficiently well in pre-clinical evaluations over five years to deserve consideration for clinical trials by NIH and/or private industry and success in developing a high flux epithermal beam suitable for clinical use at the MIT reactor.
(Radiopharmaceutical design/synthesis)	(Radiopharmaceutical design/synthesis)	(Radiopharmaceutical design/synthesis)
A novel radiotracer was developed that can be used to detect early lesions in Alzheimers Disease. [Goal Met] A multi-radiotracer detection system was developed to detect biochemical abnormalities in brains of patients with obesity. [Goal Met] A toluene radiotracer was developed to study inhalant abuse. [Goal Met]	Develop unique radiopharmaceutical tracers that will enable PET medical imaging to more precisely diagnose neuro-psychiatric illnesses (Alzheimer's Disease, Parkinson's Disease, multiple sclerosis, and others) and cancer in humans. This research is closely coordinated with the NIH Institutes of Drug Abuse, of Mental Health, and of Neurological Disorders and Stroke. Develop innovative methods and instrumentation to image gene expression in real time in cells, tissues and whole organisms.	Through radiopharmaceutical and molecular nuclear medicine research, three positron emission tomography (PET) radiotracers with precise cellular, subcellular, and molecular targeting capability will be developed as potential imaging agents for nuclear medicine research and clinical use to study brain disorders due to substance abuse and mental illnesses (such as Alzheimer's and Parkinson's diseases), cancer diagnosis and treatment, heart-function-related ailments, therapeutic gene expression in the whole animals, and for monitoring progress to therapy.

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
(Imaging Sciences) Micro-PET technology was transferred to industrial partners for commercialization. [Goal Met] A prototype artificial retina device was successfully inserted into the eye of a blind person. [Goal Met] A PET imaging system was used to pinpoint abnormalities in the brains of patients with attention deficit disorder. [Goal Met] An ultra sensitive cantilever detection system, even more sensitive than currently used technology, was developed as a potential new clinical tool to detect prostate specific antigen (PSA). [Goal Met]	(Imaging Sciences) Enhance micro-PET and micro-CT scanners so that these unique and powerful tools can be used to enhance basic biomedical research in medical centers, leading to improved human health care. In close partnership with NIH, develop novel technology and instrumentation for imaging single molecules, genes, cells, organs, and whole organisms in real time under natural physiological conditions with a high degree of precision, including MRI, PET, and SPECT. Technology and detector systems will be developed to capitalize on recent findings of the human genome project that will enable imaging of gene expression in real time that will have a critical impact on biomedical research and medical diagnosis.	(Imaging Sciences) Complete the design, computational modeling and construction of a prototype high-density micro array device (artificial retina) and have implanted the test device into the canine eye. The device will receive light signals from an external camera and convert the photons to electrical signals to be transmitted to the brain. The biological compatibility and ability of the device to transmit signals to the canine brain will be measured. Complete the development of a radiotracer imaging system that approaches the fundamental limit of spatial resolution and detector sensitivity to be applied to the diagnosis of small cancers. Complete the prototype design of MRI and PET instruments capable of performing functional images on moving animals including the design of novel dipole magnets, fiber-optic arrays, miniature positron detectors, and the construction of algorithms to detect and correct for motion during image acquisition. Develop an array of biological sensors employing laser cantilever technology, protein-receptor detection systems that rely on fluorescent resonant energy transfer, and microspectroscopy platform systems.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Medical Applications	116,085	38,701	38,642	-59	-0.2%
Measurement Science	2,555	5,961	5,952	-9	-0.2%
SBIR/STTR	0	1,186	1,254	+68	+5.7%
Total, Medical Applications and Measurement Science	118,640	45,848	45,848	0	--

Detailed Program Justification

	(dollars in thousands)		
	FY 2002	FY 2003	FY 2004
Medical Applications	**116,085**	**38,701**	**38,642**
■ **Novel cell-directed cancer therapies**	**9,699**	**4,870**	**4,862**

In FY 2004, BER continues to support fundamental research on the therapeutic use of ionizing radiation that may be achieved with radionuclide therapy and novel methods of tumor targeting. Recent therapeutic successes employing antibodies or ligands linked to radionuclides has grown out of fundamental combinatorial radiochemistry supported by BER. The specific goals include the development of novel therapeutic agents and delivery techniques to target and treat cancer at the cellular level. Research will address such complex challenges as chemical ligand synthesis, tumor-targeting, and dosimetry.

Overall program objectives include: (1) techniques to ensure highly selective tumor-targeting by the proposed therapeutic agents; (2) efficient screening techniques for selecting candidate therapeutic agents for in-vivo testing; (3) research suggesting a reasonable likelihood of success for in-vivo targeting of primary tumors and their metastases in pre-clinical animal trials; (4) reliable approaches for dosimetry calculations to normal tissues and to tumor sites based on 3-dimensional modeling; (5) measurement techniques for accurately assessing the success of tumor-targeting in vivo; and (6) measurement techniques for assessing therapy effects in vivo at the molecular, cellular and metabolic levels.

The BER supported Boron Neutron Capture Therapy clinical safety studies at the Brookhaven National laboratories and at MIT/Beth Israel Hospital were completed in FY 2002. BER funding of the MIT medical reactor continues with the aim of developing the optimum neutron beam delivery for animal studies and to support NIH research trials of BNCT cancer treatment in humans.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

■ **Radiopharmaceutical Design and Synthesis**	**23,570**	**24,445**	**24,407**

In FY 2004, BER will continue to support research on radiopharmaceutical design and synthesis using concepts from genomics as well as computational biology and structural biology. BER will continue research into radiolabeling of monoclonal antibodies for cancer diagnosis and new radiotracers for the study of brain and heart function. Molecules directing or affected by homeostatic controls always interact with each other and, thus, are targets for specific molecular substrates. The substrate molecules can be tailored to fulfill a specific need and labeled with appropriate radioisotopes to become measurable in real time in the body on their way to, and during interaction with their targets, allowing the analysis of molecular functions in the homeostatic control in health and disease. The function of radiopharmaceuticals at various sites in the body is imaged by nuclear medical instruments, such as, gamma ray cameras and positron emission tomographs (PET). This type of imaging refines diagnostic differentiation between health and disease at the molecular/metabolic levels leading to more effective therapy. If labeled with high energy-emitting

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

radioisotopes, the substrate molecules, carrying the radiation dose may be powerful tools for targeted molecular therapy especially of cancer. The program will continue to support development of new radiotracer and radiopharmaceutical molecules for PET imaging applications (e.g., normal and abnormal brain biochemistries in response to normal and abnormal brain functions in health and disease).

BER will also develop nuclear medicine driven technologies to image mRNA transcripts in real time in tissue culture and whole animals. Currently the expression of endogenous genes in animals (including humans) cannot be imaged, at least not directly. However, given the astounding pace of biotechnology development, such imaging is an attainable goal. This research includes an emphasis on nucleic acid biochemistry, radioactive ligand synthesis and macromolecular interactions. It addresses the functional consequences of gene expression by targeting and perturbing the activity of a particular gene in living cells or animals. It also develops new biological applications using optical and radionuclide imaging devices for imaging specific gene expression in real time in both animals and humans. Methods such as combinatorial chemistry techniques will be used to develop antisense radiopharmaceuticals that hybridize DNA probes to RNA transcripts in highly specific ways to block their activity or function. Molecular signal amplification methods that work in vivo at the mRNA level will be developed. Drug-targeting technology will be developed to such an extent that the various biological barriers can be safely surmounted in vivo. The research will evaluate the clinical potential of real-time imaging of genes at work in cells, tissues, and whole organisms, including humans. This information will have applications ranging from understanding the development of a disease to the efficacy of treatments for the disease. This new technology will strongly impact developmental biology, genome research, and medical sciences.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
▪ **Imaging Sciences Instrumentation and Research**	**13,994**	**9,386**	**9,373**

In FY 2004, BER will emphasize support in fundamental research to facilitate the development of imaging systems relevant to solving critical problems related to the Nation's health. This program capitalizes on the unique resources at the National Laboratories in the fields of computational modeling, detector development, multimodal spectroscopy, high-field magnet development and microelectronics. Imaging instrumentation and technology being developed includes: **(**1) the development of a high-density microelectronic array (the artificial retina) that can be packaged into a tiny device to be implanted in to the back of the eye. The device will be used for the treatment of the major causes of blindness in the United States, retinitis pigmentosa and age-related macular degeneration; 2) PET and MRI instruments that will be used to study brain function in the awake individual. These imaging devices will obviate the necessity of anesthetizing animals (inducing coma) to acquire brain images and may also have great potential for use with infants; 3) a range of image detector systems that will be more sensitive and cost effective than current instrumentation used in the diagnosis of human disease; and 4) novel biosensor devices that can detect specific molecules or biological processes important in human biology and disease and convert this

(dollars in thousands)

	FY 2002	FY 2003	FY 2004

information into a measurable signal. These devices can be adapted to rapidly diagnose microorganisms in the field.

BER's imaging technology program works closely with other Federal Agencies, especially the National Institutes of Health, to help coordinate and focus the research efforts at the National Laboratories. Federal Agency partners include National Institutes of Health Biomedical Engineering Consortium (BECON) and the National Institute of Bioengineering and Bioimaging (NBIB).

The research activities in this subprogram are principally carried out at National Laboratories.

	FY 2002	FY 2003	FY 2004
▪ **Congressional Direction**	**68,822**	**0**	**0**

Congressional direction in FY 2002 for Positron Emission Tomography Center at the University of South Alabama; Gulf Coast Cancer Center and Research Institute; Center for Nuclear Magnetic Resonance Imaging at the University of Alabama Birmingham; University of South Alabama research, in cooperation with industry and the Cooperative Research Network of the National Rural Electric Cooperative Association, on a fuel cell powered home using the Smart Energy Management Control System; Library and Regional Resource Learning Center at Spring Hill College; South Alabama Medical Education Outreach Program; University of Florida Genetics Institute; Linear Accelerator for the Baystate Medical Center; Cancer Institute at New Jersey; Institute for Molecular Biosciences at the University of Arizona; Stanley Scott Cancer Center at Louisiana State University; Infotonics Center of Excellence in Rochester New York; Joint Collaboration on Advanced Nanotechnology and Sensors with the University of New Orleans, Louisiana State University, and Louisiana Tech; Breast Cancer Program at the North Shore-Long Island Jewish Health System; Functional Magnetic Resonance Imaging Machine at the University of Texas at Dallas and the University of Texas Southwestern Medical Center's Center for Brain, Cognition, and Behavior; Integrated Environmental Research and Services Program at Alabama A&M University; Energy Efficiency Initiative at the Carolinas Health Care System; Multidisciplinary Research Facility at the College of Engineering, University of Notre Dame; Linear Accelerator for the Burbank Regional Cancer Center in Fitchburg, Massachusetts; Hampshire College's National Center for Science Education; Audubon Biomedical Science and Technology Park at Columbia University; McFadden Science Center at Texas Wesleyan University; Emergency Power Supply System at Cedars-Sinai Medical Center; Rush-Presbyterian-St. Luke's Medical Center; Nanoscience Facility at Purdue University; Julie and Ben Rogers Cancer Institute; School of Public Health at the University of South Carolina; Continued Development of the Life Science Building at Brown University; Environmental Modeling at the University of North Carolina at Chapel Hill; Renovation of the Science, Technology, and Engineering Research Complex at Jackson State University; PowerGrid Simulator at Drexel University and the New Jersey Institute of Technology; Positron Emission Tomography Facility at West Virginia University; Linear Accelerator for the University Medical Center of Southern Nevada; Research Foundation of the University of Nevada-Las Vegas; University of Nevada-Las Vegas for Continued Study of the Biological Effects of Exposure to Low-level Radioactivity; Biomolecular Nuclear Magnetic Resonance Instrument at the Medical University of South Carolina; Oncology Center of the Medical University of South Carolina; National Center of Excellence in Photonics and

	FY 2002	FY 2003	FY 2004
	(dollars in thousands)		

Microsystems in New York; Institute of Comparative Genomics at the American Museum of Natural History; Inland Northwest Natural Resources Center at Gonzaga University; Hall of Paleontology at the Field Museum; Center for Catalysis at Iowa State University; Human Genome Project at the University of Southern California; Biomedical Research at Creighton University; Child Health Institute of New Brunswick, New Jersey; Oregon Renewable Energy Center; Superconductor Research at Boston College; Natural Renewable Energy Laboratory in Hawaii; Rochester Institute of Technology Microelectronics Technology Program; Operations and Capital Investment at the Mental Illness and Neuroscience Discovery Institute; and University of Missouri-Columbia to Expand the Federal Investment in the University's Nuclear Medicine and Cancer Research Capital Program.

	FY 2002	FY 2003	FY 2004
Measurement Science	**2,555**	**5,961**	**5,952**

In FY 2004, BER will continue research on new sensor instrumentation for characterizing the chemical composition of contaminated subsurface environments in support of the Department's environmental cleanup efforts of highly radioactive chemical wastes.

The research will include the development of new environmental sensors that are better, faster, and more economical than existing laboratory techniques. New field-based sensors that take advantage of novel biotechnologies will be ready for deployment. The new sensors will include antibody and nucleic acid approaches that have precedence in other applications but will be new to bioremediation at DOE legacy sites.

Research into new imaging instrumentation for life sciences and biomedical sensor applications will be continued. Capital equipment funds will be used for research to develop new instrumentation having broad application in the life and medical sciences. BER will continue research on medical applications of laser technology at the National Laboratories and at universities.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

	FY 2002	FY 2003	FY 2004
SBIR/STTR	**0**	**1,186**	**1,254**

In FY 2002 $3,008,000 and $193,000 were transferred to the SBIR and STTR programs, respectively. FY 2003 and FY 2004 amounts are estimated requirements for the continuation of these programs..

	FY 2002	FY 2003	FY 2004
Total, Medical Applications and Measurement Science	**118,640**	**45,848**	**45,848**

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Medical Applications & Measurement Science	
■ Activities will continue at near FY 2003 levels. Decrease is due to the increase in STTR allocation.	-68
SBIR/STTR	
■ SBIR/STTR increases due to STTR allocation increase	+68
Total Funding Change, Medical Applications and Measurement Science	0

Construction

Mission Supporting Goals and Measures

Construction is needed to support the research under the Biological and Environmental Research Program (BER) program. Cutting-edge basic research requires that state-of-the-art facilities be built or existing facilities modified to meet unique BER requirements.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
Construction..	11,405	0	0	0	0.0%

Detailed Program Justification

(dollars in thousands)

	FY 2002	FY 2003	FY 2004
Construction	**11,405**	**0**	**0**

- The Laboratory for Comparative and Functional Genomics at Oak Ridge National Laboratory will provide a modern research facility to help understand the function of newly discovered human genes, to support DOE research programs and to house the genetic mutant mouse lines created during the past 50 years. This new facility will replace a 50-year old animal facility with rapidly escalating maintenance costs still in use at Oak Ridge.

  BER will meet the cost and schedule milestones for construction of facilities and major items of equipment within 10% of baseline estimates.

Explanation of Funding Changes

	FY 2004 vs. FY 2003 ($000)
Construction	
▪ Funding for the construction of the Laboratory for Comparative and Functional Genomics is completed in FY 2002.	0

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	$ Change	% Change
General Plant Projects	4,991	4,811	4,811	0	--
Capital Equipment	37,263	17,047	19,625	+2,578	+15.1%
Total Capital Operating Expenses	42,254	21,858	24,436	+2,578	+11.8%

Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2002	FY 2003	FY 2004	Unapprop-riated Balance
01-E-300, Laboratory for Comparative and Functional Genomics, ORNL	13,900	2,495	11,405	0	0	0
Total, Construction		2,495	11,405	0	0	0

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.

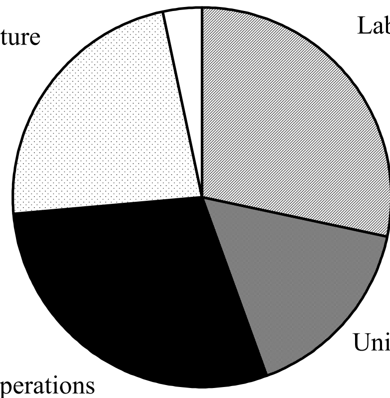
Inputs to our prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, these considerations have led to: increased investments in science at the nanoscale to take advantage of 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 4^{th} 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	Preliminary Safety Assessment Document Approved	Complete RF System Production	Approve Final Safety Assessment Document	Complete Accelerator Readiness Review
	Arc vacuum system design completed		Complete Magnet Production	Complete Vacuum System Production	Start Commissioning
	Start vacuum system production			Complete Raft Assemblies	Approve Critical Decision 4 – Start Operations
	Test magnet prototypes			Start Major Installation	
	Start magnet production				

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]

	(dollars in thousands)				
	FY 2002	FY 2003	FY 2004	$ Change	% Change
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.

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.

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.

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.

	FY 2002	FY 2003	FY 2004
▪ **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.

▪ **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
▪ **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.

Facilities	FY 2002	FY 2003	FY 2004
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.

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.

	FY 2002	FY 2003	FY 2004
▪ **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

	(dollars in thousands)	
FY 2002	FY 2003	FY 2004

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.

▪ **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.

▪ **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
	(dollars in thousands)		
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.

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.

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.

Total, Construction	**279,300**	**251,571**	**219,950**

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.

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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.

[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.