Basic Energy Sciences

Program Mission

Basic Energy Sciences (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 grow 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 mission of the BES program – a multipurpose, scientific research effort – is to foster and support fundamental research in focused areas of the natural sciences in order to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. 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.

Strategic Objectives

SC4: Provide leading scientific research programs in materials sciences and engineering, chemical sciences, biosciences, and geosciences that underpin DOE missions and spur major advances in national security, environmental quality, and the production of safe, secure, efficient, and environmentally responsible systems of energy supply; as part of these programs, by 2010, establish a suite of Nanoscale Science Research Centers and a robust nanoscience research program, allowing the atom-by-atom design of revolutionary new materials for DOE mission applications, and restoring U.S. preeminence in neutron scattering research and facilities.

SC7: Provide major advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10% of schedule; construction and upgrades are within 10% of schedule and budget; and facility technology research and development programs meet their goals.

Progress toward accomplishing these Strategic Objectives will be measured by Program Strategic Performance Goals, Indicators, and Annual Targets, as follows:

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 Indicator

Validation of results by merit review with external peer evaluation.

Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
BES used expert advisory committees and rigorous peer review committees to ascertain that the research performed by investigators in universities and DOE laboratories was focused and outstanding. An additional indicator of the success of our scientific research was the recognition through the awards received by our researchers and by the broader scientific community. (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, the relevance, and the national and international leadership of BES programs, review the chemical sciences activities using a BESAC-chartered Committee of Visitors. In addition, 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: superconductivity. Publish results and continue to structure BES programs per results. (SC4-1)	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 materials sciences and engineering activities using a BESAC-chartered Committee of Visitors. In addition, 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 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 Indicator

Validation of results by merit review with external peer evaluation.

Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
Initiated 76 grants to universities (from 417 grant applications) and 12 projects at DOE laboratories (from 46 Field Work Proposals) in selected areas of nanoscale science, engineering, and technology. (SC4-2) [Met Goal]	Begin engineering and design of three Nanoscale Science Research Centers. (SC4-2)	Begin construction of one Nanoscale Science Research Center meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheets, project number 03-R-312. Conduct engineering and design activities to establish construction baselines on the two other Nanoscale Science Research Centers. (SC4-2)
	Initiate approximately 40 grants to universities and 6 projects at DOE laboratories in selected areas of nanoscale science, engineering, and technology. (SC4-2)	Establish the instrument suites and identify fabrication capabilities for the new Nanoscale Science Research Centers based upon user community input at national workshops held in late FY 2001 and FY 2002. (SC4-2)

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 Indicator

Validation of results by merit review with external peer evaluation.

Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 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. (SC4-3)
		Establish collaborative, national R&D programs for common needs at the BES synchrotron light sources, e.g., for detectors and other components. (SC4-3)

SC7-4A: 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 Indicator

Validation of results by merit review with external peer evaluation.

Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
BES scientific user facilities were maintained and operated so that the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. The cost and schedule milestones for upgrades and construction of scientific user facilities, including the construction of the Spallation Neutron Source were met. [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. Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4A)	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. Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4A)

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
	Continue upgrades on the major components of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory (SSRL), maintaining cost and schedule within 10 percent of baselines. At the end of FY 2002, the upgrade of SPEAR 3 will be 70 percent complete. (SC7-4A)	Complete the upgrade of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory (SSRL), maintaining cost and schedule within 10 percent of baselines. (SC7-4A)

SC7-4B: 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 Indicator

Validation of results by merit review with external peer evaluation.

Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
	Continue construction of the Spallation Neutron Source (SNS), meeting the cost and timetables 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 will be 47 percent complete. (SC7-4B)	Continue construction of the Spallation Neutron Source (SNS) meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheet, project number 99-E-334. At the end of FY 2003, construction of the SNS will be 61 percent complete. (SC7-4B)
	Select and begin fabrication of one additional instrument for the SNS. (SC7-4B)	Select and begin fabrication of one additional instrument for the SNS. Select and begin upgrade/fabrication of one instrument each at the High Flux Isotope Reactor and the Manuel Lujan, Jr. Neutron Scattering Center. Commitment at the Lujan Center is conditional upon LANSCE demonstrating reliable operations as determined by a BESAC review conducted in FY 2003. (SC7-4B)

Significant Accomplishments and Program Shifts

The BES program continues as one of the Nation's largest sponsors of fundamental research in the natural sciences and is uniquely responsible for supporting research impacting energy resources, production, conversion, efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2001, the program funded research in more than 150 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 40% of the program's research activities sited at academic institutions.

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; • toughened (i.e., 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; • new commercial processes for ethanol production, pulp and paper manufacturing, and *in planta* production of oils built on foundations laid by the Energy Biosciences activities; • processes for extraction of radioactive and hazardous metal ions from solutions for nuclear fuel purification/reprocessing and for cleanup of radioactive wastes; • the atomic-level understanding of combustion processes as a result of the creation of the Combustion Research Facility, where basic, applied, and industrial research are collocated; and • a host of new instruments, e.g. instruments based on high-temperature superconductors — "superconducting quantum interference devices" or SQUIDs for short — 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 fundamental questions.

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 specimens and crystals. 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.

FY 2001 Honors and Awards

Each year, principal investigators funded by BES win dozens of major prizes and awards sponsored by professional societies and by others. In addition, many are elected to fellowship in organizations such as the National Academy of Sciences, the National Academy of Engineering, and the major scientific professional societies. Paramount among the honors are six Nobel Prizes awarded to BES principal investigators since the mid-1980s. Selected major prizes and awards for FY 2001 include:

From Acta Metallurgica, Inc. -- Acta Metallurgica Gold Medal

From ASM International -- the 2001 ASM International Gold Medal

From R&D Magazine -- R&D 100 Award for the invention of the MOLYCAST Furnace, an environmentally friendly system of new energy efficient heating elements.

From the Alexander von Humboldt Foundation of Germany -- the Humboldt Research Award

From the American Association of Engineering Societies -- the John Fritz Medal

From the American Chemical Society -- the Award in Chemistry of Materials; the Award in Colloid or Surface Chemistry; the Arthur C. Cope Scholar Award; the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry; the Nobel Laureate Signature Award for Graduate Education in Chemistry; the Award for Creative Research in Homogeneous or Hetergeneous Catalysis

*From the American Institute of Chemical Enginee*rs -- the William H. Walker Award

From the American Physical Society -- the Irving Langmuir Prize in Chemical Physics; the Herbert P. Broida Prize

From the American Vacuum Society -- the Medard W. Welch Award; the John A. Thornton Award

From the American Welding Society -- four recipients of the William Spraragen Award

From the Computing Research Association -- an Honorable Mention in the Computing Research Association's Outstanding Undergraduate Award

From the Electrochemical Society -- the David C. Graham Award in Physical Electrochemistry

From the German Society for Physical Chemistry -- the Jost Memorial Award

From the Iron and Steel Society -- the Geoffrey Belton Award

From the Japan Fine Ceramics Association -- the 2001 International Prize

From the Materials Research Society -- the Materials Research Society Medal for 2001

From the Metals, Minerals, and Materials Society -- the Robert Lansing Hardy Award

From the Samsung Foundation -- the Ho-Am Prize for Science

Twelve principal investigators were elected to the National Academy of Sciences, and six were elected to the National Academy of Engineering. Fifteen principal investigators were advanced to fellowship in the American Physical Society; seven in the American Academy of Arts and Sciences; one in the American Ceramics Society; four in the Minerals, Metals, and Materials Society; and two in the John Simon Guggenheim Memorial Foundation.

Selected FY 2001 Science Accomplishments

<u>Materials Sciences and Engineering</u>

- *Micro-size Light Emitters for Solid State Lighting Applications.* Energy savings of tens of billions of dollars per year could be achieved by replacement of household 100-watt light bulbs by white light emitting diodes (LED) made by mixing LEDs emitting primary colors. However, improved LED efficiency is necessary before such replacement becomes feasible. New research has shown that interconnecting hundreds of micro-size LEDs to replace larger conventional LEDs can boost the overall emission efficiency by as much as 60 percent.
- *A New Method for Obtaining Crystal Structures Without Large Crystals.* High-resolution x-ray diffraction using polycrystalline samples ("powders") rather than traditional single-crystal samples has advanced to the point where the structures of complex materials including oxides, zeolites, and small organic structures can be solved. Advantages of powder diffraction are that it is not affected by crystal fracture and polycrystalline samples can be formed over a much wider range of conditions than large single crystals. Recently, powder diffraction was demonstrated for large molecules, such as proteins, that were considered far too complex for powder diffraction experiments. In addition to the many important applications to materials sciences, this technique will also be useful in chemistry and biosciences.
- *NMR and MRI Outside the Magnet.* NMR (nuclear magnetic resonance) imaging and MRI (magnetic resonance imaging) have required large high-field magnets that impose extremely uniform magnetic fields upon the sample. In many circumstances, however, it is impractical or undesirable to place or rotate objects and subjects within the bore of such a large magnet. A new approach for the recovery of highly resolved NMR spectra and MRI images of samples in grossly non-uniform magnetic fields was recently demonstrated. The approach will be useful for the enhanced study of fluids contained in porous materials, such as deep underground oil-well logging studies, and is expected to have dramatic research applications in chemistry, materials sciences, and biomedicine.
- *Terabit Arrays (One trillion bits per square inch).* A 300-fold increase in magnetic storage density has been achieved using a patented technique of self-assembly of block copolymers under the influence of a small voltage. The new technique is simple, robust, and extremely versatile. The key to this discovery lay in directing the orientation of nanoscopic, cylindrical domains in thin films of block copolymers. By coupling this with routine lithographic processes, large area arrays of nanopores can be easily produced. Electrochemical deposition of metals, such as cobalt and iron, produces nanowires that exhibit excellent magnetic properties, key to ultrahigh density magnetic storage. The nanowires are also being used as field emission devices for displays.
- *Observations of Atomic Imperfections.* A new electron beam technique has been developed that has measured atomic displacements to a record accuracy of one-hundredth of the diameter of an atom. Such small imperfections in atomic packing often determine the properties and behavior of materials, particularly in nano-structured devices. This capability has been made possible by a new technique that couples electron diffraction with imaging technology. The result is a greatly enhanced capability to map imperfections and their resulting strain fields in materials ranging from superconductors to multi-layer semiconductor devices.

- *Semiconductor Nanocrystals as "Artificial Leaves."* Recent experiments demonstrated that carbon dioxide could be removed from the atmosphere with semiconductor nanocrystals. These "artificial leaves" could potentially convert carbon dioxide into useful organic molecules with major environmental benefits. However, to be practical, the efficiency must be substantially improved. New theoretical studies have unraveled the detailed mechanisms involved and identified the key factors limiting efficiency. Based on this new understanding, alternative means for improving efficiency were suggested that could lead to effective implementation of artificial leaves to alleviate global warming and the depletion of fossil fuels.
- *"Magic" Values for Nanofilm Thickness.* A key issue for nanotechnology is the structural stability of thin films and the devices made from nanostructures. It was recently demonstrated that nanofilms are significantly more stable at a few specific values of film thickness. The origin of this effect arises from the confinement of electrons within the film leading to electronic states with discrete energy values, much as atomic electrons are bound to the nucleus at discreet energy levels. Calculations demonstrated that increased stability occurred when the number of electrons present in the film completely filled the set of available states, just as filled electronic shells make the mobile gases very stable.
- *Materials Resistant to Damage from Nuclear Waste.* The ability to predict the composition and structure of materials that are resistant to radiation damage, such as in nuclear waste storage, has been formulated on a firm scientific basis. Current nuclear storage materials cannot resist radiation damage for the required thousands of years because radioactive emissions in a storage material jostle atoms out of their carefully ordered arrangements. These materials become unstable and eventually leach into the environment. Computer simulations and experiments revealed that a special class of complex ceramic oxides called fluorites is able to resist this fate. The fundamental principle is rather simple: the configurations of atomic arrangements in these oxides are relatively disordered to begin with allowing them to tolerate displaced atoms caused by radiation.
- *Brilliant X-Rays Shine Light on Welds.* Using high-brightness synchrotron radiation, the details of microstructural changes of welds were mapped and studied for the first time. This advanced capability shows how the welding process alters the structure and changes the properties of metals. Its application is virtually unlimited, since it can investigate dynamic changes in crystal structure near the melting point of any metal. Knowledge gained from this award winning work on titanium and stainless steels is being used to advance and refine theories and numerical models of welding fundamentals. Dramatic savings to the U. S. economy would result from better quality, more reliable welds.
- *Micro Lens for Nano Research.* A silicon lens that is 1/10 the diameter of a human hair has been fabricated and used to image microscopic structures with an efficiency 1,000 times better than existing probes. The combination of high optical efficiency and improved spatial resolution over a broad range of wavelengths has enabled measurement of infrared light absorption in single biological cells. This spectroscopic technique can provide important information on cell chemical composition, structure, and biological activity.
- *Nanofluids.* Nanofluids (tiny, solid nanoparticles suspended in fluid) have been created that conduct heat ten times faster than thought possible, surpassing the fundamental limits of current heat conduction models for solid/liquid suspensions. These nanofluids are a new, innovative class of heat transfer fluids and represent a rapidly emerging field where nanoscale science and thermal engineering meet. This research could lead to a major breakthrough in making new composite (solid and liquid) materials with improved thermal properties for numerous engineering and medical

applications to achieve greater energy efficiency, smaller size and lighter weight, lower operating costs, and a cleaner environment.

Chemical Sciences, Geosciences, and Energy Biosciences

- *Capturing Molecules in Motion with Synchrotron X-Ray Pulses.* Photochemical conversion of solar energy depends on light-driven chemical reactions. Absorption of light ultimately leads to atomic rearrangements necessary to produce photochemical products. The intermediate molecular configurations created by absorption of light are short-lived and their structures are largely unknown. In novel experiments at the Advanced Photon Source, molecular structures of laser-generated reaction intermediates in solutions, having lifetimes as short as 28 billionth of a second, have been obtained. Future experiments are planned that will allow for capture of intermediate structures on even shorter time scales. These studies are providing the fundamental knowledge needed to develop artificial photoconversion devices.
- *Early Precursor Identified in Water Radiolysis.* Radiolytic decomposition of water produces hydrogen gas, which is flammable and potentially explosive. This is of concern in maintenance of water-moderated nuclear reactors, long-term storage of transuranic fissile materials containing adsorbed water, and management of high-level mixed-waste storage tanks. In recent studies on the effects of ionizing radiation on condensed media, a common precursor to essentially all hydrogen from irradiated water has been discovered. This precursor is a solvated electron. External intervention and capture of this precursor can prevent the generation of hydrogen gas from water. The reactivity of the precursor with a large number of scavengers has previously been determined in pulse radiolysis experiments, thus a priori predictions can be made on the efficiency of the intervention and prevention of gas generation.
- *The World's Smallest Laser.* A team of materials scientists and chemists has built the world's smallest laser - a nanowire nanolaser 1,000 times thinner than a human hair. The device, one of the first to arise from the field of nanotechnology, can be tuned from blue to deep ultraviolet wavelengths. Zinc oxide wires only 20 to 150 nanometers in diameter and 10,000 nanometers long were grown, each wire a single nanolaser. Discovering how to excite the nanowires with an external energy source was critical to the success of the project. Ultimately, the goal is to integrate these nanolasers into electronic circuits for use in "lab-on-a-chip" devices that could contain small laser-analysis kits or as a solid-state, ultraviolet laser to allow an increase in the amount of data that can be stored on high-density optical disks.
- *Polymerization to Make Plastics.* The discovery of metallocene catalysts caused major advances in polymer production (e.g., polyethylene, polypropylene), the most widespread of synthetic materials. The ability to control the orientation of each link of a polymer chain allows control of crystallinity, density, softening point, and other important properties. A recent improvement in these catalysts is the synthesis of bimetallic complexes in which two catalytic centers and two cocatalytic centers are held in close proximity in solution or adsorbed on surfaces. By altering the nature of the centers, it is possible to control rate of reactivity, the degree of chain branching, and plastic rigidity.
- *First Ever Chemistry with Hassium, Element 108.* Element 108 - hassium - was discovered in 1984. It does not exist in nature but must be created one atom at a time by fusing lighter nuclei. Recently, the first experiments to examine its chemical properties were performed by an international team (German, Swiss, Russian, Chinese and American scientists) at the Gesellschaft für Schwerionenforschung (GSI) in Darmstadt, Germany using novel techniques developed at the Lawrence Berkeley National Laboratory. Energetic magnesium projectiles bombarded targets of

curium, a rare artificial isotope produced and processed at Oak Ridge National Laboratory. The hassium atoms formed by impacts between beam and target reacted with oxygen to form hassium oxide molecules enabling the study of the properties of this new chemical compound. The chemistry of man-made and heavy elements, particularly chemistry impacting environmental insults, is of major interest, and these experiments are a first step for this element.

- *Improved Materials for Fuel Cells.* Major impediments for the commercialization of fuel cells include the inability to use hydrogen fuel containing traces of carbon monoxide and the necessity of using large amounts of expensive platinum catalysts. A novel ruthenium/platinum catalyst has been produced through a new preparation method involving spontaneous deposition of platinum on metallic ruthenium nanoparticles. The resulting catalyst has a higher carbon monoxide tolerance than commercial catalysts and uses smaller amounts of platinum.
- *Platinum Encrusted Diamond Films.* Research on new catalytic electrodes, e.g., for fuel cells, has shown that synthetic diamond thin films are excellent supports for catalysts because of their corrosion resistance. The challenge to produce an electrode is to incorporate nanometer sized platinum and platinum/ruthenium catalyst particles into the surface structure of the diamond film. Recently, the ability to incorporate 10 to 500 nanometer diameter particles into the bulk structure of the films has been demonstrated. These new surface modified systems may result in significantly improved catalytic activity and stability, and could have even broader applications in chemical synthesis, toxic waste remediation, and chemical and biomedical sensors.
- *Complex Flow in the Subsurface.* Recovery of subsurface fluids, whether oil and gas or contaminants, requires understanding the way fluids flow within porous and fractured rocks and soil. This is particularly complicated when there are multiple fluids (oil-methane-water; water-carbon dioxide). New experiments combined with theory and computational modeling have tracked the simultaneous flow of two fluids in fractured and porous media. Flow paths of both fluids are significantly longer than under single fluid conditions and transport is very sensitive to differences in fluid structure.
- *Complete Plant Genome of the First Model Plant.* The first complete sequencing of a plant genome was completed by an international consortium of researchers from Europe, Japan and the U.S. The DOE was one of the supporters of the U.S. effort. The sequencing of the genome of Arabidopsis will provide the information needed to increase food production in an energy-efficient and environmentally friendly manner, provide increased wood and fiber production, and increase the use of plant materials for energy and the production of petroleum-replacing chemicals.

Selected FY 2001 Facility Accomplishments

The four synchrotron radiation light sources and three BES neutron scattering facilities served 6,982 users in FY 2001 by delivering a total of 26,476 operating hours to 204 beam lines at an average of 96.1% reliability (delivered hours/scheduled hours)[a]. The High Flux Isotope Reactor at Oak Ridge National Laboratory did not operate in FY 2001 due to the installation of upgrades. Statistics for individual facilities are provided below. In one instance, less time was needed for maintenance activities than was scheduled, so more time was delivered to users than planned.

The maximum number of total operating hours for these 7 facilities is estimated to be about 37,100 hours. Most of the BES facilities already operate close to the maximum number of hours possible for their facility. The next priority is to support and maintain beamlines and instruments at the state-of-the art. For the synchrotron radiation light sources and the neutron scattering facilities, the number of beamlines and instruments would need to be increased in order to achieve the full capacity of each of the facilities. Capacity at the light sources could increase by nearly a factor of two if all beamlines were fully instrumented. Capacity at the neutron sources could also increase substantially by upgrading existing instruments and fabricating new ones. These needs are addressed in the current request.

- **The Advanced Light Source (ALS)** served 1,163 users in FY 2001 by delivering 5,261 operating hours to 37 beam lines at 96.2% reliability (delivered hours/scheduled hours). The ALS is supported by the Materials Sciences and Engineering subprogram.

  - *A new beamline for x-ray microscopy of polymers.* Owing to its elemental and chemical specificity, x-ray microscopy is a superior tool for the study of multicomponent polymers. A scanning x-ray microscope that is specifically optimized to the demands of polymer research is being commissioned.

  - *Ambient-pressure photoemission spectroscopy.* The real world of chemistry, biology, and environmental science is a world that is frequently wet, hot, and under atmospheric or higher pressures, whereas experimental measurements are often best done under vacuum with cold samples. One step toward bridging the gap is the development of a new experimental chamber for *in-situ* investigation of samples under ambient conditions.

  - *Interferometer controls scanning x-ray microscope.* In scanning microscopy, it is essential to locate and control the position of the probe over the sample. A control system developed for a scanning x-ray microscope is able to position the x-ray beam with nanometer accuracy, so that features in the sample can be studied at the finest spatial resolution of the instrument.

---

[a] BES defines "users" as researchers who conduct experiments at a facility (e.g., received a badge) or receive primary services from a facility. An individual is counted as one user per year regardless of how often he or she uses a given facility in a year. "Operating hours" are the total number of hours the facility delivers beam time to its users during the Fiscal Year. Facility operating hours are the total number of hours in the year (e.g., 365 days times 24 hour/day = 8,760 hours) minus time for machine research, operator training, accelerator physics, and shutdowns (due to maintenance, lack of budget, faults, safety issues, holidays, etc.).

- ► *Superbend beamlines developed.* To broaden the spectral range of the Advanced Light Source to cover shorter wavelengths, superconducting bend magnets were designed. The first two beamlines will be implemented sequentially over the next year to serve protein crystallographers and to provide much needed harder x-ray sources for ALS diffraction studies.

- **The Advanced Photon Source (APS)** served 1,989 users in FY 2001 by delivering 4,788 operating hours to 37 beam lines at 95.8% reliability (delivered hours/scheduled hours). The APS is supported by the Materials Sciences and Engineering subprogram.

  - ► *Storage ring "top-up operation" becomes routine*. After successful tests with 25% of the scheduled user-beam time dedicated to top-up operation, the APS is scheduling the majority of future operations for top-up mode. During top-up operation, injecting a pulse of electrons once every two minutes holds the stored current constant to 0.2 percent. This operating mode delivers a constant heat load on x-ray optics and various accelerator components, thus improving the x-ray beam stability. It also allows flexibility in operating modes, which are traditionally limited by the short lifetime of the stored beam. Top-up operation has significantly enhanced the research capabilities of the APS.

  - ► *Two undulators on a single straight section deliver two independent x-ray beams to users.* For the first time, a novel concept of spatially separating the beams from two insertion devices placed on single straight section was realized. This was accomplished by placing the undulator axes at a small angle with respect to each other. Successful implementation of this concept enabled 100% efficient utilization of the delivered beam.

  - ► *Low-emittance lattice developed.* Machine studies have successfully established operating conditions for the APS storage ring with the horizontal emittance reduced by approximately a factor of two. This reduces the horizontal source size and divergence of the x-ray beam and results in at least a factor of two improvement in the overall brilliance. Initial user results are encouraging and routine operation with this mode is scheduled for the near future.

- **The National Synchrotron Light Source (NSLS)** served 2,523 users in FY 2001 by delivering 5,556 operating hours to 86 beam lines at 100.0% reliability (delivered hours/scheduled hours). The NSLS is supported by the Materials Sciences and Engineering subprogram.

  - ► *Polarization modulation spectroscopy for magnetism research.* A new high-resolution soft x-ray beamline and a phase sensitive detection system were completed to take advantage of the fast switching capability of the Elliptically Polarized Wiggler. The new system provides high sensitivity and enables magnetic field dependent studies.

  - ► *Focusing of high energy x-rays with asymmetric Laue crystals*. Theoretical prediction and experimental verification of a new concept for focusing of high energy x-rays was demonstrated. This new design results in a more than 100 fold increase in the photon flux delivered to the sample. A new monochromator based on this design was constructed and implemented at the superconducting wiggler beamline for high pressure and materials research.

  - ► *High magnetic field, far-infrared spectroscopy beamline commissioned.* A new high magnetic field, far-infrared beamline was commissioned with a far-infrared spectrometer and 16 Tesla superconducting magnet. Combining this with a high-field magnet system opens up new opportunities for measuring electron spin resonance (ESR), cyclotron resonance, and other magneto-optic effects in solids.

- *X-ray optics for microbeam diffraction, elemental mapping, and high pressure research developed.* A new system for micro-focusing of x-rays was implemented, achieving a focus of 3 microns (vertical) by 9 microns (horizontal). The system has been used in the study of bone diseases, materials under high pressure, and semiconductors.

- *High gain harmonic generation (HGHG) free electron laser (FEL) achieves saturation.* By frequency multiplying and amplifying a seed laser signal, an HGHG FEL imposes the properties of the laser onto the FEL output beam. In a demonstration, light at long wavelength was frequently doubled. Full characterization of the FEL light and its harmonics agreed with theory and demonstrated the utility of an HGHG FEL for producing intense coherent light pulses.

- **The Stanford Synchrotron Radiation Laboratory (SSRL)** served 907 users in FY 2001 by delivering 4,539 operating hours to 25 beam lines at 94.9% reliability (delivered hours/scheduled hours). The SSRL is supported by Materials Sciences and Engineering subprogram.

  - *Stanford-Berkeley synchrotron radiation summer school.* The first Stanford-Berkeley summer school on synchrotron radiation and its applications was held with 36 students from a diverse range of scientific fields. The goal was to introduce young scientists to the fundamental properties of synchrotron radiation and the understanding and use of several techniques, including spectroscopy, scattering, and microscopy.

  - *New actinide facility commissioned.* Synchrotron-based measurements are a crucial part of chemical and materials research programs involving radionuclides and radiologic materials. In order not to limit the scope of experiments that can be performed, a radiologic sample analysis facility has been integrated into a modern synchrotron beamline. This combination insures safe handling of actinide and other radiology materials and also provides state-of-the-art measurement capabilities that have proven extremely useful in remediation efforts.

  - *Materials science small angle x-ray scattering beamline facility completed.* The materials science small and wide-angle x-ray scattering station is now in full user operation. The integrated beamline and experimental equipment facility allows for studies of weakly scattering systems, such as dilute polymer solutions.

  - *Microfocus optics system for X-ray micro-spectroscopy.* An experimental apparatus employing tapered metal capillary optics for conducting X-ray micro-spectroscopy is now in operation. This capability allows X-ray micro-spectroscopy experiments in the materials, biological, and environmental sciences.

  - *Successful 3 GeV injector test.* The SPEAR injector was successfully run at 3 GeV, proving that it is ready to provide at-energy injection for SPEAR3. The 3 GeV test came toward the end of the two-year Injector Upgrade Accelerator Improvement Project, in which power supplies, magnets, and diagnostics were upgraded to insure reliable 3 GeV operation. At-energy injection will improve SPEAR3 performance by providing better fill-to-fill orbit reproducibility and thermal stability.

- ► *RF waveguide dampers improve beam stability and lifetime.* RF waveguide dampers were installed in the two radio frequency (RF) waveguides in the SPEAR storage ring to eliminate high frequency oscillations excited by the electron beam in the RF cavity/waveguide system. The dampers not only eliminated the instabilities but they allowed the use of operations parameters that gave a 20% improvement in the electron beam lifetime.

- **The Intense Pulsed Neutron Source (IPNS)** served 240 users in FY 2001 by delivering 3,968 operating hours to 13 beam lines at 102.6% reliability (delivered hours/scheduled hours). The IPNS is supported by the Materials Sciences and Engineering subprogram.

  - ► *IPNS hosts the national neutron and x-ray scattering school.* In August 2001, Argonne National Laboratory again hosted the two-week National School on Neutron and X-Ray Scattering. The school continues to attract outstanding graduate students and post-doctoral appointees with 179 applications for the 60 available positions.

  - ► *Upgrade of IPNS instruments.* The High Resolution Medium Energy Chopper Spectrometer (HRMECS) instrument was completely upgraded and a chopper was added to the General Purpose Powder Diffractometer (GPPD). The HRMECS upgrade included the complete overhaul of data collection/control software and hardware, addition of position-sensitive detectors at low scattering angles and improved neutron choppers. The T0 chopper on GPPD blocks high energy neutron from entering the diffractometer.

  - ► *Auto-anneal capabilities added to moderator system.* Regular annealing required for IPNS's unique ultra-cold moderator has been accomplished by installing a system that automatically anneals the solid methane moderator every three days. This automation allows for reduced manpower and improved operation of the IPNS target moderator assembly.

- **The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center** LANSCE served 122 users in FY 2001 by delivering 2,364 operating hours to 6 beam lines at 82.0% reliability (delivered hours/scheduled hours). The Lujan Center is supported by the Materials Sciences and Engineering subprogram.

  - ► *HIPPO diffractometer commissioned.* Following three years of design and construction, the recently completed HIPPO (High Pressure, Preferred Orientation) diffractometer took its first neutron-beam-related diffraction pattern on a sample of nickel on July 7, 2001. The scientific thrust of this new state-of-the-art spectrometer is the investigation of dynamic processes in heterogeneous bulk materials in a variety of environments.

  - ► *SMARTS will provide new capabilities in materials research.* SMARTS, a third generation neutron diffractometer for the study of polycrystalline materials, received its load frame and furnace, which were successfully tested onsite during 2001. SMARTS is scheduled to receive first beam in August 2001, followed by commissioning through the remainder of the year.

  - ► *BES partners on new institutional instruments.* Three institutionally funded instruments, ASTERIX, PHAROS, and IN500 were supported in part under the auspices of BES. ASTERIX produces a highly polarized intense beam of cold neutrons that has a very large cross section and covers a wide wavelength range while minimizing the fraction of the neutron beam that is not used. PHAROS, a high-resolution chopper spectrometer, is designed for low-angle studies.

IN500 is a cold neutron time-of-flight spectrometer, which will offer all the advantageous capabilities of reactor-based instruments.

- *Instrument performance improves with use of new chopper technology.* All of the Lujan Center's new instruments and some of the existing instruments have enjoyed dramatic improvements in chopper technology in FY 2001. These performance improvements in two technical areas, timing reference generators and chopper controls, now enable the accelerator and all neutron choppers to run as slaves of the master timing generator. This success in chopper technology has drawn the attention of several other spallation neutron facilities and has redefined the timing specifications for the Spallation Neutron Source.

- *Upgrades to small-angle scattering instrument.* A new frame-overlap chopper was procured and installed, which enables the small-angle scattering instrument, LQD, to make full use of the higher flux it enjoys from the hydrogen moderator installed over the last two years. Recent additions to LQD also include a gravity-focusing device, which compensates for gravitational drop, especially for slow neutrons.

- *Upgrades to SPEAR improve instrument performance.* SPEAR (Surface Profile Analysis Reflectometer) is used for determining chemical density profiles at solid/solid, solid/liquid, solid/gas, and liquid/gas interfaces. Upgrades to SPEAR during 2001 included the installation of shutter hardware to reduce closure time, and additional automation of flight-path components. For better performance, an evacuated flight path, and two digital chopper controllers were added. In addition, a new collimation system, together with improved software, allowed for the first real-time reflectivity measurements. These upgrades were made to make the instrument user-friendlier.

- **The High Flux Isotope Reactor (HFIR)** served 38 users in FY 2001 by delivering 8 operating hours for materials irradiation and institutes that utilize the transplutonium program and medical isotopes. The reactor was shut down at 8:00 a.m. on October 1, 2000, for the scheduled replacement of the beryllium reflector and installation of upgrades and remained shutdown for the remainder of the year. The HFIR is supported by the Materials Sciences and Engineering subprogram.

  - *Installation of new components enhances scientific capabilities at HFIR.* Many of HFIR's internal components have been replaced with new, upgraded components that will significantly enhance its neutron scattering research capabilities without diminishing its isotope-production or material-testing capabilities. Replaced components include the beryllium reflector, its support structure, and three of the four neutron beam tubes. Beam intensity for some instruments is expected to be three times that of the original design.

  - *Cold Source Project progress.* The moderator vessel has been fabricated and has passed acceptance pressure tests at room and liquid-nitrogen temperatures.

  - *Spectrometers for cold neutron research.* The cold source to be installed at HFIR will provide long wavelength neutron beams that are unsurpassed worldwide. Instrumentation has been designed to make optimum use of the cold neutron beams. Instruments include small angle spectrometers for measurements on large-scale structures, reflectometers for the study of surface phenomena, and triple-axis spectrometers for the determination of low-energy excitations.

- *Spectrometers for thermal neutron research.* The larger beam tubes and new mochromator drums installed at HFIR will permit considerable gains in intensity for the thermal neutron spectrometers, by as much as a factor of five.

- **The Combustion Research Facility (CRF)** is supported by the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

  - *New capabilities.* The CRF provides a primary interface for the integration of BES programs with those of DOE's Offices of Energy Efficiency and Renewable Energy and Fossil Energy related to combustion by collocating basic and applied research at one facility. Three laboratories were completed. The particle diagnostic laboratory can now generate flames with controllable fuel and oxidizer feeds to develop a fundamental understanding of small particle formation from combustion sources. A time-resolved fourier transform spectrometer for chemical kinetics and dynamics studies is now available in the kinetics and mechanisms laboratory. Related to applied research, the investigation of a novel engine combustion concept is being conducted in the new homogeneous-charge, compression-ignition engine laboratory.

Program Shifts

In FY 2003, the engineering activity of the formerly separate Engineering and Geosciences subprogram becomes part of the Materials Sciences and Engineering subprogram. The geosciences activity of the formerly separate Engineering and Geosciences subprogram and the Energy Biosciences subprogram become part of the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. This directly aligns Basic Energy Sciences program management and organizational structures.

Materials Sciences and Engineering

- *Initiation of new activities in nanoscale science, engineering, and technology (NSET).* The FY 2001 NSET laboratory solicitation resulted in six awards including: Lawrence Berkeley National Laboratory in the areas of self assembly of organic/inorganic nanocomposite materials and the design, synthesis, characterization, and applications of functionalized nanotubes; Oak Ridge National Laboratory in the area of self-organized and artificially structured nanoscale materials, with emphasis on neutron scattering; Brookhaven National Laboratory in the area of electron microscopy applied to nanoscale structures; Los Alamos National Laboratory in the area of electronics from nanoscale crystals; and Sandia National Laboratories in the area of nanoelectronics and nanophotonics. The FY 2001 NSET university solicitation resulted in 35 grants.

- *Initiation of new activities in Robotics and Intelligent Machines (RIM).* The FY 2001 RIM university solicitation resulted in four grants for fundamental studies of automated sensing, perception, learning, and action.

Chemical Sciences, Geosciences, and Energy Biosciences

- *Initiation of new activities in nanoscale science, engineering, and technology (NSET).* The FY 2001 NSET laboratory solicitation resulted in six awards including: Argonne National Laboratory in the area of integrating the biomolecule - inorganic interface to build functional materials; Brookhaven National Laboratory in the areas of understanding the chemical reactivity of nanoparticle surfaces and research on electron and photon transfer through molecules connecting nanoparticles; National Renewable National Laboratory in the area of quantum dot communication through proteins and nanotubes; Oak Ridge National Laboratory in the area of research on templated synthesis and reactivity of nanoparticles for energy and environmentally demanding reactions; and Lawrence Berkeley National Laboratory in the area of designing nanoparticle surfaces for controlling reaction selectivity. The FY 2001 NSET university solicitation resulted in 41 grants.

- *Initiation of new research in computational chemistry as part of the Scientific Discovery through Advanced Computing (SciDAC) activities.* The FY 2001 SciDAC laboratory solicitation resulted in awards to Ames Laboratory in the area of advancing multi-reference methods in electronic structure theory; Pacific Northwest National Laboratory and Lawrence Berkeley National Laboratory in the area of advanced methods for electronic structure; Sandia National Laboratory in the area of computation of reacting flows; and Argonne National Laboratory and Sandia National Laboratory for advanced software for the calculation of thermochemistry, kinetics and dynamics. The FY 2001 SciDAC university solicitation for computational chemistry resulted in 10 grants.

Scientific Facilities Utilization

The BES program request includes $313,887,000 to maintain support of 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 2002. 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.

Nanoscale Science Research

In FY 2003, fundamental research to understand the properties of materials at the nanoscale will be increased in three areas: synthesis and processing of materials at the nanoscale; condensed matter physics; and catalysis. In the area of synthesis and processing (Materials Sciences and Engineering subprogram), new activities will develop a fundamental understanding of nanoscale processes involved in deformation and fracture, synthesis of ordered arrays of nanoparticles using patterning techniques, and synthesis of nanoparticles of uniform size and shape. In the area of condensed matter physics (Materials Sciences and Engineering subprogram), new activities will focus on understanding how properties change or can be improved at the nanoscale and how macromolecules reach their equilibrium configuration and self assemble into larger structures. In the area of catalysis (Chemical Sciences, Geosciences, and Energy Biosciences subprogram), new work will focus on fundamental research to understand the role nanoscale properties of materials play in altering and controlling catalytic transformations. In FY 2003, requests for applications in these research areas will be issued to DOE laboratories and to universities. The combination in a single coordinated research program of individual investigators at universities and interdisciplinary groups at the Department's laboratories is a proven excellent mechanism for incorporating advanced basic research, cutting-edge instrumentation, access to facilities, and the needs of energy technologies.

In addition to the increases for research in FY 2003, construction will begin on one Nanoscale Science Research Center (NSRC), and engineering and design will continue on two others. NSRCs are user facilities for the synthesis, processing, fabrication, and analysis of materials at the nanoscale. 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. They involve conventional construction of a simple laboratory building, usually sited adjacent to or near an existing BES synchrotron or neutron scattering facility. 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. Planning for the NSRCs includes substantial participation by the research community through a series of open, widely advertised workshops. Workshops held to date have been heavily attended, attracting up to 300 researchers. Funds are requested for the start of construction of the NSRC located at Oak Ridge National Laboratory and for the continuation of engineering and design for the NSRC located at Lawrence Berkeley National Laboratory and the NSRC at Sandia National Laboratories (Albuquerque) and Los Alamos National Laboratory. These NSRCs were chosen from among those proposed by a peer review process. Additional information on the NSRCs is provided in the construction project data sheet, project number 03-R-312 and in the PED data sheet, project number 02-SC-002.

The research efforts described in the first paragraph above will benefit significantly from these NSRCs. For example, the NSRC at Oak Ridge National Laboratory will provide direct access to sample preparation for neutron scattering, which is ideal for magnetic structures and for soft materials and residual stress in materials; Oak Ridge also has a combination of electron beam microcharacterization instruments that are needed to characterize nanoscale particles and dislocations. The NSRC at Lawrence Berkeley National Laboratory will provide synthesis capabilities to explore the phenomena of macromolecular conformation and assembly and will provided ready access to the Advanced Light Source and other characterization instruments. The NSRC at Sandia/Los Alamos National Laboratories will provide sample preparation capabilities for thin films, electron transport, patterning, and magnetic layered structures. This NSRC will also have an array of characterization instruments for nanoelectronics, thin films, and magnetic structures; in the case of magnetic materials, the NSRC will provide ready access to the National High Magnetic Field Laboratory at Los Alamos.

This research activity will also benefit by new work proposed in FY 2003 in the Advanced Scientific Computing Research (ASCR) program in the area of computational nanoscale science engineering and technology. ASCR will develop the specialized computational tools for nanoscale science.

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.

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. An interagency working group was established under the auspices of the Office of Science and Technology Policy to coordinate the funding neutron scattering instruments at all of the neutron sources in view of the opportunity for new instruments at SNS. In addition to these two instruments, 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.

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.

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.

The SNS project has made progress during FY 2001 and the project continues to meet scheduled milestones and remains within budget. Project-wide, design work is about two-thirds complete, and R&D on technical components is nearing completion. Title II design of conventional facilities is nearly 100% complete. Site preparation has cleared the way for construction of the front end and target buildings, the linac tunnel, and a number of support buildings and utility systems. Procurements for technical components have been awarded with generally favorable cost results, and deliveries of some items to Oak Ridge have begun. Definitive plans have been developed for equipment installation and facility commissioning activities.

FY 2002 budget authority has been provided to continue R&D, design, procurement, and construction activities, and to begin component installation. Essentially all R&D supporting the construction of the SNS will be completed in FY 2002, with instrument R&D continuing throughout the project. Title II design will be completed on the linac, and will continue on the ring, target, and instrument systems. Equipment installation efforts will begin in the front end and the low energy sections of the linac. Other technical components for the linac, ring, target, and instruments will continue to be manufactured. Work on conventional facilities will continue. Some conventional facilities will reach completion and be made available for equipment installation, such as the front end building, and portions of the klystron building and linac tunnel. Construction work will begin on the ring tunnel.

FY 2003 funding is requested to continue instrument R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The front end will be commissioned, and low-energy linac component installation and commissioning will commence. Other linac and ring components will begin to be delivered and installed in their respective tunnels. 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.

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. The estimate for annual operating costs has been updated to reflect more recent experience in the operation of major user facilities as well as in design, development, fabrication, maintenance, and user support of modern instruments. Additional information on the SNS Project is provided in the SNS construction project data sheet, project number 99-E-334.

The 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 orders of magnitude (i.e., a factor of 10,000,000,000) 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 orders of magnitude 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 $165,000,000 to $225,000,000. FY 2003 Project Engineering and Design (PED) funding of $6,000,000 is requested for Title I and Title II design work. Additional information on the LCLS Project is provided in the LCLS PED data sheet, project number 03-SC-002.

Research Using X-ray and Neutron Scattering

X-ray and neutron scattering are powerful tools used to investigate the fundamental properties of materials. BES is the major supporter of x-ray and neutron science in the United States and has pioneered the development of virtually all of the instruments and techniques used at these facilities for research in materials sciences, surface science, condensed matter physics, atomic and molecular physics, chemical dynamics, x-ray microscopy, tomography, femtosecond phenomena, interfacial/environmental, and geophysics studies. Within the physical sciences, BES remains the dominant federal supporter of beamline development and instrument fabrication providing as much as 85% of the federal support for these activities.

Major instruments at the synchrotron light sources and the neutron sources have a lifetime of 7-10 years after which the instruments undergo major upgrades or are retired. Thus, after a facility is fully instrumented, about 10-15% of the instruments must be upgraded or replaced each year to keep the facility at the forefront of science. In FY 2003, new funding in the amount of $17,292,000 is requested to support instrument upgrades, instrument replacements, and new instrumentation at the x-ray and neutron scattering facilities. Of these funds, $5,000,000 will be provided for instruments at the Spallation Neutron Source. These funds will be competed among both academic and laboratory institutions, and the resulting instruments and beamlines will be made available to the entire U.S. scientific research community.

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.

This program supported graduate students and postdoctoral investigators in FY 2001 through grants or contracts; 4,046 graduate students and postdoctoral investigators used the BES science user facilities in FY 2001.

Funding Profile

	(dollars in thousands)				
	FY 2001 Comparable Appropriation	FY 2002 Original Appropriation	FY 2002 Adjustments	FY 2002 Comparable Current Appropriation	FY 2003 Request
Basic Energy Sciences					
Research					
Materials Sciences and Engineering	511,608	434,353	+78,169	512,522	547,883
Chemical Sciences, Geosciences, and Energy Biosciences	203,231	218,714	-10,931	207,783	220,146
Engineering and Geosciences	0	38,938	-38,938	0	0
Energy Biosciences	0	32,400	-32,400	0	0
Subtotal, Research	714,839	724,405	-4,100	720,305	768,029
Construction	258,929	279,300	0	279,300	251,571
Total, Basic Energy Sciences	973,768	1,003,705	-4,100	0	0
General Reduction	0	-4,100	4,100	0	0
Total, Basic Energy Sciences	973,768 [a] [b]	999,605	0	999,605	1,019,600

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 $15,962,000 which was transferred to the SBIR program and $958,000 which was transferred to the STTR program.

[b] Excludes $991,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

Funding by Site

	(dollars in thousands)				
	FY 2001	FY 2002	FY 2003	$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory...............	24,205	22,738	23,041	+303	+1.3%
National Renewable Energy Laboratory...	5,876	5,247	4,562	-685	-13.1%
Sandia National Laboratory	24,673	23,349	25,987	+2,638	+11.3%
Total, Albuquerque Operations Office	54,754	51,334	53,590	+2,256	+4.4%
Chicago Operations Office					
Ames Laboratory	17,961	16,114	16,507	+393	+2.4%
Argonne National Laboratory – East	159,028	154,389	152,734	-1,655	-1.1%
Brookhaven National Laboratory	75,942	56,606	57,398	+792	+1.4%
Chicago Operations Office.......................	110,664	88,266	84,204	-4,062	-4.6%
Total, Chicago Operations Office	363,595	315,375	310,843	-4,532	-1.4%
Idaho Operations Office					
Idaho National Engineering and Environmental Laboratory.........................	2,660	1,756	1,494	-262	-14.9%
Oakland Operations Office					
Lawrence Berkeley National Laboratory...	77,896	74,649	78,691	+4,042	+5.4%
Lawrence Livermore National Laboratory..	5,643	4,793	4,676	-117	-2.4%
Stanford Linear Accelerator Center (SSRL).	34,691	31,643	41,716	+10,073	+31.8%
Oakland Operations Office	43,433	36,973	34,497	-2,476	-6.7%
Total, Oakland Operations Office	161,663	148,058	159,580	+11,522	+7.8%
Oak Ridge Operations Office					
Oak Ridge Institute For Science and Education	1,245	440	872	+432	+98.2%
Oak Ridge National Laboratory	374,386	391,333	343,176	-48,157	-12.3%
Oak Ridge Operations Office....................	39	0	0	0	--
Total, Oak Ridge Operations Office	375,670	391,773	344,048	-47,725	-12.2%
Richland Operations Office					
Pacific Northwest National Laboratory	13,024	11,346	11,648	+302	+2.7%
Washington Headquarters	2,402	79,963	138,397	+58,434	+73.1%
Total, Basic Energy Sciences......................	973,768 [a] [b]	999,605	1,019,600	+19,995	+2.0%

[a] Excludes $15,962,000 which was transferred to the SBIR program and $958,000 which was transferred to the STTR program.

[b] Excludes $991,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

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, magnets, 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 hydrocrbon 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, and it is the only one in the Americas. It is a world-class facility. 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 independently controlled beamlines for experimental research. Beamlines are assigned to user groups in Collaborative Access Teams (CATs), whose proposals are reviewed and approved based on their scientific program and the criticality of high-brilliance x-rays to the work. These instruments 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.

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 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 **High Flux Beam Reactor**, commissioned in 1965, was a research reactor designed to produce neutrons for scattering. During its three decades of operation, the HFBR was a premier gathering spot for neutron scientists involved in a broad array of studies, including phonons in rare gases; ferromagnets and antiferromagnets; critical phenomena in magnetic transitions; structure and dynamics of molecules adsorbed on surfaces; direct measure of electron-phonon interaction in 'old' superconductors; structure determination of small sub-unit of ribosomes; critical phenomena in one- and two-dimensional magnets; impurity effects on phase transitions; incommensurate systems in metals and insulators; magnetic correlations in heavy fermions; magnetic superconductors; hydrogen location in amino acids and carbohydrate building blocks; static and dynamic correlations in high temperature superconductors; exotic behavior of one-dimensional magnets; shape memory materials; anomalous correlation lengths in phase transitions; and the structure of ceramics with negative thermal expansion. In December 1996, a plume of tritiated water was discovered emanating from a leak in the HFBR spent fuel pool, which contaminated the groundwater south of the reactor. The facility remained on standby until the Secretary of Energy announced on November 16, 1999, that the reactor would be permanently closed. Activities to place the reactor in a safe state awaiting full decommissioning by DOE's Office of Environmental Management were completed in FY 2001. The permanent shut down of the HFBR increases the importance of the remaining neutron sources in the U.S.

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 geranium 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** 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 and a current PED project, will support research and the operation of a user facility for the design, modeling, synthesis, processing, fabrication and characterization of novel molecules and nanoscale materials. The facility will provide laboratories for materials science, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include a class 100 clean room, 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 macroworlds. 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, the Shared Research Equipment (SHaRE) program, and the Surface Modification and Characterization (SMAC) facility. The SMAC facility is equipped with ion implantation accelerators that can be used to change the physical, electrical, and chemical properties of solids to create unique new materials not possible with conventional processing techniques. Surface modification research has led to important practical applications of materials with improved friction, wear, catalytic, corrosion, and other properties. Engineering research provides support for computational nonlinear sciences.

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 construction project, 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 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.

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, the Office of Fossil Energy, and the Office of 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 macroworlds. 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 orders of magnitude (i.e., a factor of 10,000,000,000) 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 172 colleges/universities located in 49 states. Also included are funds for research awaiting distribution pending completion of peer review results.

Materials Sciences and Engineering

Mission Supporting Goals and Objectives

The Materials Sciences and Engineering subprogram delivers the scientific knowledge and discoveries in the materials sciences and engineering that underpin DOE's missions in science, energy, environmental quality, and national security; extends the frontiers of condensed matter physics, metal and ceramic sciences, and materials chemistry, and materials engineering in order 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; and plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

The Materials Sciences and Engineering subprogram supports basic research in condensed matter physics, metal and ceramic sciences, materials chemistry, and materials engineering. This research seeks 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. **Performance will be measured by** reporting accomplishments on the common performance measures on leadership, excellence, and relevance; quality; and safety and health.

Funding Schedule

	(dollars in thousands)				
	FY 2001	FY 2002	FY 2003	$ Change	% Change
Materials Sciences and Engineering Research	228,141	236,842	261,028	+24,186	+10.2%
Facilities Operations	283,467	263,865	274,118	+10,253	+3.9%
SBIR/STTR	0	11,815	12,737	+922	+7.8%
Total, Materials Sciences and Engineering	511,608	512,522	547,883	+35,361	+6.9%

Detailed Program Justification

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Materials Sciences and Engineering Research	**228,141**	**236,842**	**261,028**
▪ **Structure and Composition of Materials**	**33,767**	**36,070**	**36,697**

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 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 2003, 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. Many of these advanced tools will come from the further development of current microscopies; however, new instruments are needed as well. Additional funding is requested to address one of the major recommendations of BESAC following its FY 2000 review of the electron beam microcharacterization centers for the design of components for an aberration corrected transmission electron microscope. This instrument would advance understanding in many areas related to energy mission needs such as interfaces in solid-state devices, load-bearing

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003

structural composites and protective coatings; deformation behavior that relates to the processing of metals; grain boundary sliding that degrades the strength of structural alloys and ceramics at elevated temperatures; domain walls in ferromagnetic and ferroelectric materials; vortices and flux pinning in superconductors; and long-standing problems of brittle fracture and fracture resistance. Additional funding is also requested to address another BESAC recommendation to enhance the remote telepresence operations at the electron beam microcharacterization centers.

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

	FY 2001	FY 2002	FY 2003
▪ **Mechanical Behavior and Radiation Effects**	**15,286**	**14,530**	**14,530**

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. In an age when economics require life extension of materials and environmental and safety concerns demand reliability, the ability to predict performance from a fundamental basis is a priority. Furthermore, high energy-conversion efficiency requires materials that maintain their structural integrity at high operating temperatures. 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 2003, 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.

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

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
▪ **Physical Behavior of Materials**	**16,449**	**15,735**	**15,735**

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 2003, 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**	**12,801**	**14,690**	**18,595**

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.

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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003

In FY 2003, new funding is requested for new 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, we should be able to make materials that are both strong, tough (resistant to impact fracture) and ductile. The classical law for predicting the dependence of mechanical strength on particle, crystal or grain size appears to break down in the size regime of about 10 to 100 nanometers. A fundamental understanding of both deformation and embrittlement will require new tools, including massively parallel processing computers, techniques for establishing activation energies from atomistic calculations, methods for simplifying computations involving dislocation configurations and networks, electron microscopy, and direct, real-time dislocation studies (densities, types, and patterning). Deformation and fracture are very important to DOE. Embrittlement is a major cause of catastrophic failure in materials. Plastic deformation, which requires ductility, is used for almost all fabrication of structural metals (rolling, spinning, forging, extruding, and drawing); and plastic deformation can also change critical dimensions of materials in energy systems exposed to high temperatures, mechanical loads, or irradiation. Scientific and technological breakthroughs in materials research and development are very often directly coupled to progress in synthesis and processing. A way to control the size, size distribution and assembly of nanoparticles is to use patterns on surfaces. If successful, these assemblies could be used for solar energy conversion, efficient lighting, very sensitive sensors, nanoelectronic devices, improved corrosion and wear resistance and very high-density magnetic information storage. 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**...	**17,352**	**16,480**	**16,480**

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 2003, 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**	**31,682**	**40,611**	**54,377**

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

	(dollars in thousands)	
FY 2001	FY 2002	FY 2003

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.

Included within this request are funds to increase x-ray and neutron science activities in the U.S. based on BES reviews of the synchrotron radiation light sources, on discussions within the OSTP Interagency Working Group on Neutron Science, and on three BESAC reviews that addressed the current status of research activities using neutron scattering in the U.S. and strategies needed to take full advantage of the SNS upon its completion. Funding is increased for new and upgraded instrumentation to take advantage of scientific opportunities in the physical sciences and to leverage the multibillion-dollar investment in these facilities. Funds will be competed among both laboratory and academic institutions for multiyear beamline and instrument development projects in the range $5,000,000-15,000,000 each in such areas as materials sciences, surface science, condensed matter physics, atomic and molecular physics, polymers and soft materials, nanostructured materials, x-ray microscopy, tomography, femtosecond phenomena, interfacial studies, and imaging. Of these funds, $5,000,000 is provided 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. Funding is also increased for academic scientists to participate in the development of neutron scattering instruments and for the neutron science/scattering programs at the host institutions of the BES facilities, where historically the interplay between science programs and instrument design and fabrication has produced advances in instrumentation and seminal scientific results.

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

	FY 2001	FY 2002	FY 2003
▪ **Experimental Condensed Matter Physics**	**35,837**	**34,115**	**38,020**

This activity supports a broad-based experimental program in condensed matter and materials physics with selected 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. Presently, the portfolio includes specific research thrusts in magnetism, semiconductors, superconductivity, materials synthesis and crystal growth, and photoemission spectroscopy. The portfolio addresses well-recognized needs, including understanding magnetism and superconductivity; the control of electrons and photons in solids; understanding materials at reduced dimensionality; the physical properties of large, interacting systems; and the properties of materials under extreme conditions.

The combined projects in superconductivity comprise a concerted and comprehensive energy-related research program. The DOE laboratories anchor the BES multi-disciplinary basic research efforts and maintain integration with the Energy Efficiency (EE) program applied and developmental efforts. 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 Energy Efficiency and Renewable Energy (EE/RW) (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 2003, new funding is requested for increased effort in experimental condensed matter physics to answer very 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. In the case of soft materials, the physics of association and configuration of large molecules is poorly understood. Yet this kind of self assembly, which ubiquitous in nature, will be required for many of the potential applications of nanoscale science. Even the most rudimentary steps, such as how a macromolecule finds its equilibrium shape, are still in controversy. Much less is known about how such molecules can assemble into larger structures with defined shapes. Self-assembled macromolecules can provide very strong, lightweight materials that would decrease the weight in automobiles improving fuel economy.

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

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
▪ **Condensed Matter Theory**	**16,124**	**18,007**	**18,007**

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, the Surface Modification and Characterization Facility at ORNL, and the Center for Synthesis and Processing of Advanced Materials, which consists of collaborating projects at national laboratories, universities, and industry.

In FY 2003, 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**	**30,808**	**27,650**	**29,602**

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.

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

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003

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 2003, 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. An increase is requested for research to understand how the shapes of molecular building blocks affect the spontaneous assembly into fibers, membranes, and other large-scale structures and to understand the effects of pressure, ionic strength, solvents, and external electric and magnetic fields on the shape and properties of the large-scale structures. This work on self-controlling materials lies at the interface of the physical sciences, molecular biology, and materials engineering. Both natural and synthetic molecules in combination can be used to make new molecular species, and the techniques of molecular self-assembly can be used to create new structures with new properties on the nanoscale. This work will focus on the study of simple structures and phenomena and on the emerging arsenal of tools and techniques such as combinatorial chemistry needed to explore the properties and structures of these new materials.

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**.....	**7,685**	**7,679**	**7,685**

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.

EPSCoR Distribution of Funds by State

	(dollars in thousands)		
	FY 2001	FY 2002 Estimate	FY 2003 Estimate
Alabama	350	375	375
Alaska[a]	0	0	0
Arkansas	115	65	65
Hawaii[b]	0	0	0
Idaho	107	60	60
Kansas	933	615	615
Kentucky	468	471	471
Louisiana	130	130	130
Maine	0	0	0
Mississippi	652	535	535
Montana	515	465	465
Nebraska	480	300	300
Nevada	614	325	325
New Mexico[b]	0	0	0
North Dakota	0	55	55
Oklahoma	165	65	65
Puerto Rico	450	435	435
South Carolina	1,201	120	120
South Dakota	0	0	0
Vermont	585	585	585
West Virginia	794	525	525
Wyoming	59	65	65
Technical Support	67	400	400
Other	0	2,088 [c]	2,094 [c]
Total	7,685	7,679	7,685

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

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

[c] Uncommitted funds in FY 2002 and FY 2003 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
▪ **Extension of HB-2 Beam Tube at the High Flux Isotope Reactor**	**1,150**	**0**	**0**

This project is a major item of equipment with a total estimated cost of $5,550,000 that provided beam access for six thermal neutron scattering instruments. The project was completed in FY 2001.

▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**	**0**	**2,000**	**2,000**

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

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

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) is being undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The technical goals are to increase injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decrease beam emittance by a factor of 7 to increase beam brightness; increase operating current from 100 mA to 200 mA to increase beam intensity; and maintain 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 will be replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC is $29,000,000; DOE and NIH are equally funding the upgrade with a total Federal cost of $58,000,000. NIH has provided $14,000,000 in FY 1999, $14,000,000 in FY 2000, and $1,000,000 in FY 2001. The funding profile, but not the TEC, of this MIE has been modified based on an Office of Science construction project review, which recommended that some funds be shifted from later years to early years in order to reduce schedule risk by ensuring that critical components are available for installation when scheduled. That recommendation was accepted and is reflected in the current funding profile.

▪ **Advanced Light Source Beamline**	**900**	**975**	**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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Facilities Operations	**283,467**	**263,865**	**274,118**
▪ **Operation of National User Facilities**	**268,126**	**263,865**	**274,118**

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.

▪ **High Flux Beam Reactor (HFBR)**	**15,341**	**0**	**0**

The HFBR has been closed. Responsibility for the reactor has been transferred from SC to the Office of Environmental Management (EM) for surveillance and decommissioning. Surveillance will continue until the reactor is fully decommissioned and decontaminated by EM.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Facilities			
Advanced Light Source	35,605	37,009	39,561
Advanced Photon Source	90,314	87,380	91,291
National Synchrotron Light Source	34,720	33,671	35,893
Stanford Synchrotron Radiation Laboratory	21,696	21,357	22,673
High Flux Beam Reactor	15,341	0	0
High Flux Isotope Reactor	37,197	37,872	36,854
Radiochemical Engineering Development Center	6,512	6,606	6,712
Intense Pulsed Neutron Source	13,833	15,826	17,015
Manuel Lujan, Jr. Neutron Scattering Center	9,190	9,044	9,678
Spallation Neutron Source	19,059	15,100	14,441
Total, Facilities	283,467	263,865	274,118

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
SBIR/STTR	**0**	**11,815**	**12,737**

In FY 2001, $9,563,000 and $574,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

Total, Materials Sciences and Engineering	**511,608**	**512,522**	**547,883**

Explanation of Funding Changes from FY 2002 to FY 2003

	FY 2003 vs. FY 2002 ($000)
Materials Sciences and Engineering Research	
▪ Increase for structure and composition of materials for the design of components for an aberration corrected transmission electron microscope and to enhance remote operations of the electron beam microcharacterization centers	+627
▪ Increase in the area of synthesis and processing for developing a fundamental understanding of nanoscale processes involved in materials deformation and fracture, synthesis of ordered arrays of nanoparticles using patterns techniques and synthesis of nanoparticles of uniform size and shape	+3,905
▪ Increase for neutron and x-ray scattering for new and upgraded instrumentation fabricated both by university and DOE laboratory researchers and for increased support for academic researchers and students. Within this increase, $5,000,000 is provided for instrumentation for the SNS.	+13,766
▪ Increase in condensed matter physics for understanding how properties change or can be improved at the nanoscale and how macromolecules reach their equilibrium configuration and self assemble into larger structures	+3,905
▪ Increase for materials chemistry for research on self assembly of materials at the atomic/molecular level	+1,952
▪ Increase for the Experimental Program to Stimulate Competitive Research to restore funding to FY 2001 levels	+6
▪ Increase in capital equipment funds for the SPEAR3 MIE per approved profile	+1,000
▪ Decrease in capital equipment funds for the ALS Beamline MIE per approved profile	-975
Total, Materials Sciences and Engineering Research	+24,186

	FY 2003 vs. FY 2002 ($000)
Facilities Operations	
▪ Increase for operations for the Advanced Light Source.	+2,552
▪ Increase for operations for the Advanced Photon Source.	+3,911
▪ Increase for operations for the National Synchrotron Light Source.	+2,222
▪ Increase for operations for the Stanford Synchrotron Radiation Laboratory.	+1,316
▪ Decrease for operations for the High-Flux Isotope Reactor because of completion of Cold Guide Hall Extension ($-2,800,000) and increase for HFIR operations ($+1,782,000)	-1,018
▪ Increase for operations for Radiochemical Engineering Development Center	+106
▪ Increase for operations for the Intense Pulsed Neutron Source.	+1,189
▪ Increase for operations for the Manuel Lujan, Jr. Neutron Scattering Center	+634
▪ Decrease in the Spallation Neutron Source research and development funds per FY 2002 project datasheet	-659
Total, Materials Sciences and Engineering Facilities Operations.	+10,253
SBIR/STTR	
▪ Increase in SBIR/STTR funding because of increase in operating expenses	+922
Total Funding Change, Materials Sciences and Engineering	+35,361

Chemical Sciences, Geosciences, and Energy Biosciences

Mission Supporting Goals and Objectives

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram delivers the scientific knowledge and discoveries in the chemical sciences, geosciences, and biosciences that underpin DOE's missions in science, energy, environmental quality, and national security; extends the frontiers of fundamental chemical interactions and molecular processes in order to expand expand the scientific foundations for the development of such advances as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improves catalysts for cleaner, more efficient, and efficient and cheaper production of fuels and chemicals; and better separations and analytical methods for applications in every DOE mission area; extends the frontiers of energy processes, environmental remediation, and waste management; and geochemistry and geophysics to expand the scientific foundations for contaminant remediation, reservoir definition, and fluid transport to predict repository performance; extends the frontiers of biosciences in order to expand the scientific foundations for the development of renewable biomass resources and the light-driven production of chemical energy via natural photosynthesis; plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports 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. The geosciences activity supports 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. The activity 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. The bioscience activity supports basic research in 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. This subprogram further provides one third of the federal support for individual investigator research in solid earth sciences.

Performance will be measured by reporting accomplishments on the common performance measures on leadership, excellence and relevance; quality; and safety and health.

Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	$ Change	% Change
Chemical Sciences, Geosciences, and Energy Biosciences Research	197,768	197,636	209,319	+11,683	+5.9%
Facilities Operations	5,463	5,377	5,805	+428	+8.0%
SBIR/STTR	0	4,770	5,022	+252	+5.3%
Total, Chemical Sciences, Geosciences, and Energy Biosciences	203,231	207,783	220,146	+12,363	+5.9%

Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
Chemical Sciences, Geosciences, and Energy Biosciences Research	**197,768**	**197,636**	**209,319**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**11,428**	**11,815**	**11,815**

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 experimental and theoretical 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.

	(dollars in thousands)	
FY 2001	FY 2002	FY 2003

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.

Research priorities for FY 2003 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; and the development and application of novel x-ray light sources based on table-top lasers and new utilization of third generation synchrotrons in advance of next-generation BES light sources.

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.

	FY 2001	FY 2002	FY 2003
▪ **Chemical Physics Research**..	**27,875**	**33,285**	**33,285**

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 at energies characteristic of combustion with the aim of developing validated theories and computational tools for predicting chemical reaction rates 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 the Office of Fossil Energy, the Office of 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. The chemical physics program supports the development of theories and computational algorithms to predict the rates of chemical reactions at temperatures characteristic of combustion. It supports the development and application of experimental techniques for characterizing gas phase reactions in sufficient detail to develop, test, and validate predictive models of chemical reaction rates. 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. New catalysts are few; improvements come principally from modification of known catalytic materials. There is no body of organized knowledge such as exists for the field of organic chemistry that can be used to find new catalysts for new or existing processes. The knowledge gained from this research program will guide in the development of a predictive capability for surface chemistry.

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

	FY 2001	FY 2002	FY 2003
▪ **Photochemistry and Radiation Research**	**26,298**	**26,064**	**29,163**

This activity supports fundamental molecular level research on the capture and conversion of energy in the condensed phase. Fundamental research in solar photochemical energy conversion supports organic and inorganic photochemistry, photoinduced electron and energy transfer in the condensed phase, photoelectrochemistry, biophysical aspects of photosynthesis, and biomimetic assemblies for artificial photosynthesis. Fundamental research in radiation chemistry supports chemical effects produced by the absorption of energy from ionizing radiation. The radiation chemistry research encompasses heavy ion radiolysis, models for track structure and radiation damage, characterization of reactive intermediates, radiation yields, and radiation-induced chemistry at interfaces. Accelerator-based electron pulse radiolysis methods are employed in studies of highly reactive transient intermediates, and kinetics and mechanisms of chemical reactions in the liquid phase and at liquid/solid interfaces. This activity supports the Notre Dame Radiation Laboratory, a BES collaborative research center, emphasizing research in radiation chemistry.

Solar photochemical energy conversion is a long-range option for meeting the world's 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.

	(dollars in thousands)	
FY 2001	FY 2002	FY 2003

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 NERI and EMSP projects.

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

An increase is requested in FY 2003 for photochemistry and radiation research for studies of nanoscale structures important to photochemical energy conversion. New opportunities offered by nanoscale science, engineering and technology have enabled studies of artificial and biological self- assembled membranes to isolate and optimally configure chromophores to act as electron-donors and acceptors for efficient charge separation that will allow the desired reaction pathways to be controlled. In addition, studies of quantum dots having unique spectral and electrical properties have the potential to revolutionize direct solar to electrical energy conversion. For FY 2003 research will continue 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; biophysical studies of 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 2001	FY 2002	FY 2003
▪ **Molecular Mechanisms of Natural Solar Energy Conversion**	**12,345**	**12,150**	**12,150**

This activity, part of the formerly separate Energy Biosciences subprogram, 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.

	FY 2001	FY 2002	FY 2003
▪ **Metabolic Regulation of Energy Production**...........................	**19,508**	**19,224**	**19,224**

This activity, part of the formerly separate Energy Biosciences subprogram, 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

(dollars in thousands)		
FY 2001	FY 2002	FY 2003

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 2003, 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.

	FY 2001	FY 2002	FY 2003
▪ **Catalysis and Chemical Transformation**	**25,464**	**24,779**	**31,333**

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. While the "art" of catalysis is widely practiced in industry, the fundamental scientific principles that enable predictability are lacking. 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. This is becoming more and more important as petroleum supplies diminish and demands for cleaner burning fuels increase. Also, the production of virtually every chemical-based consumer product requires catalysts at some point. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added chemicals. Catalysts are also indispensable for processing and manufacturing fuels that are a primary means of energy storage. 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.

Included within this request are funds to increase x-ray and neutron science activities in the U.S. based on BES reviews of the synchrotron radiation light sources, on discussions within the OSTP Interagency Working Group on Neutron Science, and on three BESAC reviews that addressed the current status of research activities using neutron scattering in the U.S. and strategies needed to take full advantage of the SNS upon its completion. Funding is increased for new and upgraded instrumentation to take advantage of scientific opportunities in the physical sciences and to leverage the multibillion-dollar investment in these facilities. Funds will be competed among both laboratory and academic institutions for multiyear beamline and instrument development projects in the range $5,000,000-15,000,000 each in both homogeneous and heterogeneous catalysis

In FY 2003 research will continue to focus on understanding the unique catalytic properties of metal, as well as mixed metal and oxide particles and their role in catalyzing reactions enabled by nanoscience engineering and technology. Increased emphasis will also be placed on the properties of reactions within nanoscale cavities. Key to these efforts will be studies on the structure, function, and reactivity of metal containing structures both in solution as well as on supports or isolated within three dimensional structures, all within the nanoscale size regime. These activities will focus on understanding the role of nanoscale properties of catalytic materials in controlling chemical reactivity through control of transitions states. Other activities will include the synthesis of discrete nanomaterials created from a controlled assembly of molecular building blocks. 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 2001	FY 2002	FY 2003
▪ **Separations and Analyses**..	**14,393**	**12,967**	**14,407**

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 and for the Environmental Management clean-up mission; 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

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003

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.

Studies in at the nanoscale address molecular transport in nanoscale structures as well as the formation of macroscopic separation systems via self-assembly of nanoscale precursors. Increased funding in FY 2003 is requested for separations and analysis research to address fundamental questions of how individual molecules move on membrane surfaces and within the pores resulting in molecular separations and transformations. This work will build on recent advances in imaging single-molecule interactions and reactions and will expand our knowledge of how molecules interact with pore walls, with one another, and with other molecules to effect separation between molecules.

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

▪ **Heavy Element Chemistry**	**8,154**	**7,637**	**8,637**

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.

Increased funding in FY 2003 is requested for research in the chemistry of transuranic elements, particularly the role of f-orbital electrons in the coordination chemistry of neptunium, plutonium, americium, and curium. The involvement of the f-orbital electrons in chemical bonding occurs most frequently in the actinide elements and particularly those elements most uniquely associated with the Department of Energy's defense and environmental missions. Experiment combined with theory and modeling will lead to new understanding of chemical bonding in these elements. Experimental studies will include aqueous and non-aqueous high-pressure chemistry and surface chemistry of these elements. In addition, new beamlines at synchrotron light sources capable of handling samples of these heavy elements will permit detailed spectroscopic studies of specimens under a variety of conditions. The study of the bonding in these heavy elements may also provide new insights into organometallic chemistry, beyond that learned from "standard" organometallic chemistry based on transition metals with d-orbital bonding.

Capital equipment is provided for items used to characterize actinide materials (spectrometers, ion chambers, calorimeters, etc.) and equipment for synchrotron light source experiments to safely handle the actinides.

	FY 2001	FY 2002	FY 2003
▪ **Geosciences Research**	**21,419**	**21,262**	**21,262**

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. Research also seeks to understand the fundamental geological processes that impact concepts for sequestration of carbon dioxide in subsurface reservoirs. 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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
▪ **Chemical Energy and Chemical Engineering**	**12,679**	**10,953**	**10,953**

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

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

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

For FY 2003, there will be continued emphasis on 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.

▪ **General Plant Projects (GPP)**	**11,524**	**12,170**	**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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
▪ **General Purpose Equipment (GPE)**..	**4,081**	**3,655**	**4,180**

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.

▪ **SPEAR3 Upgrade**	**1,700**	**700**	**700**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) is being undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The technical goals are to increase injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decrease beam emittance by a factor of 7 to increase beam brightness; increase operating current from 100 mA to 200 mA to increase beam intensity; and maintain 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 will be replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC is $29,000,000; DOE and NIH are equally funding the upgrade with a total Federal cost of $58,000,000. NIH has provided $14,000,000 in FY 1999, $14,000,000 in FY 2000, and $1,000,000 in FY 2001. The funding profile, but not the TEC, of this MIE has been modified based on an Office of Science construction project review, which recommended that some funds be shifted from later years to early years in order to reduce schedule risk by ensuring that critical components are available for installation when scheduled. That recommendation was accepted and is reflected in the current funding profile. **Performance will be measured** by continuing upgrades on the major components of the SPEAR3, maintaining cost and schedule within 10% of baselines. The increased brightness for all experimental stations at SSRL will greatly improve performance in a variety of applications and scientific studies. This subprogram funds the Combustion Research Facility. The x-ray and neutron scattering facility operations, formerly funded in Chemical Sciences, are now funded in the Materials Sciences and Engineering subprogram.

▪ **Advanced Light Source Beamline**	**900**	**975**	**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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Facility Operations	**5,463**	**5,377**	**5,805**

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 2001	FY 2002	FY 2003
Facilities			
Combustion Research Facility	5,463	5,377	5,805
Total, Facilities	5,463	5,377	5,805

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
SBIR/STTR	**0**	**4,770**	**5,022**

In FY 2001, $4,646,000 and $279,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

Total, Chemical Sciences, Geosciences, and Energy Biosciences	**203,231**	**207,783**	**220,146**

Explanation of Funding Changes from FY 2002 to FY 2003

	FY 2003 vs. FY 2002 ($000)
Chemical Sciences, Geosciences, and Energy Biosciences Research	
▪ Increase in photochemistry and radiation research for studies of nanoscale structures important to photochemical energy conversion....	+3,099
▪ Increase in catalysis research to understand the role nanoscale properties play in altering and controlling catalytic transformations.	+6,554

	FY 2003 vs. FY 2002 ($000)
▪ Increase for chemical separations and analysis research on how individual molecules move on membrane surfaces and within the pores resulting in molecular separations and transformations.	+1,440
▪ Increase in heavy element chemistry research in the chemistry of transuranic elements, particularly the role of f-orbital electrons in the coordination chemistry of neptunium, plutonium, americium, and curium	+1,000
▪ Increase in General Plant Projects	+40
▪ Increase in General Purpose Equipment	+525
▪ Decrease in capital equipment funding for the ALS Beamline MIE per approved funding profile	-975
Total, Chemical Sciences, Geosciences, and Energy Biosciences Research	+11,683
Facilities Operations	
▪ Increase for operations of the Combustion Research Facility.	+428
Total, Chemical Sciences, Geosciences, and Energy Biosciences Facilities Operations	+428
SBIR/STTR	
▪ Increase SBIR/STTR funding because of increase in operating expenses.	+252
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences	+12,363

Construction

Mission Supporting Goals and Objectives

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 2001	FY 2002	FY 2003	$ Change	% Change
SNS	258,929	276,300	210,571	-65,729	-23.8%
Project Engineering Design, NSRCs	0	3,000	11,000	+8,000	+266.7%
Project Engineering Design, LCLS	0	0	6,000	+6,000	--
Center for Nanophase Materials Science (ORNL)	0	0	24,000	+24,000	--
Total, Construction	258,929	279,300	251,571	-27,729	-9.9%

Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
Construction	**258,929**	**279,300**	**251,571**
Spallation Neutron Source	**258,929**	**276,300**	**210,571**

FY 2003 funding is requested to continue instrument R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The front end will be commissioned, and low-energy linac component installation and commissioning will commence. Other linac and ring components will begin to be delivered and installed in their respective tunnels. 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. **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.

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Project Engineering and Design, Nanoscale Science Research Centers......................	**0**	**3,000**	**11,000**

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 Laboratory to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. NSRCs will 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.

Project Engineering and Design, Linac Coherent Light Source.	**0**	**0**	**6,000**

FY 2003 budget authority is requested to provide Title I and Title II design-only funding for the Linac Coherent Light Source (LCLS) at SLAC to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. The LCLS will provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) greater in peak power and peak brightness than any existing coherent x-ray light source. Additional information follows later in PED data sheet 03-SC-002.

Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL..	**0**	**0**	**24,000**

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. **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.

Total, Construction..	**258,929**	**279,300**	**251,571**

Explanation of Funding Changes from FY 2002 to FY 2003

	FY 2003 vs. FY 2002 ($000)
Construction	
▪ The decrease in funding for the Spallation Neutron Source represents the scheduled ramp down of activities.	-65,729
▪ Increase in Project Engineering and Design for Nanoscale Science Research Centers at ORNL, LBNL, and SNL	+8,000
▪ Increase in funding for the start of construction of the Center for Nanophase Materials Science to be located at ORNL	+24,000
▪ Increase in funding for Project Engineering Design related to design-only activities for the Linac Coherent Light Source (LCLS).	+6,000
Total Funding Change, Construction	-27,729

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 2001	FY 2002	FY 2003	$ Change	% Change
Advanced Light Source	35,605	37,009	39,561	+2,552	+6.9%
Advanced Photon Source	90,314	87,380	91,291	+3,911	+4.5%
National Synchrotron Light Source	34,720	33,671	35,893	+2,222	+6.6%
Stanford Synchrotron Radiation Laboratory	21,696	21,357	22,673	+1,316	+6.2%
High Flux Beam Reactor	15,341	0	0	0	--
High Flux Isotope Reactor	37,197	37,872	36,854	-1,018	-2.7%
Radiochemical Engineering Development Center	6,512	6,606	6,712	+106	+1.6%
Intense Pulsed Neutron Source	13,833	15,826	17,015	+1,189	+7.5%
Manuel Lujan, Jr. Neutron Scattering Center	9,190	9,044	9,678	+634	+7.0%
Spallation Neutron Source	19,059	15,100	14,441	-659	-4.4%
Combustion Research Facility	5,463	5,377	5,805	+428	+8.0%
Total, Major User Facilities	288,930	269,242	279,923	+10,681	+4.0%

Detailed Program Justification

	(dollars in thousands)		
	FY 2001	FY 2002	FY 2003
Major User Facilities	**288,930**	**269,242**	**279,923**
▪ Advanced Light Source at Lawrence Berkeley National Laboratory.	35,605	37,009	39,561
▪ Advanced Photon Source at Argonne National Laboratory.	90,314	87,380	91,291
▪ National Synchrotron Light Source at Brookhaven National Laboratory.	34,720	33,671	35,893
▪ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.	21,696	21,357	22,673
▪ High Flux Beam Reactor at Brookhaven National Laboratory. On November 16, 1999, Secretary Richardson announced the permanent closure of the reactor. Responsibility has been transferred from SC to the Office of Environmental Management for surveillance and decommissioning.	15,341	0	0
▪ High Flux Isotope Reactor at Oak Ridge National Laboratory.	37,197	37,872	36,854
▪ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	6,512	6,606	6,712
▪ Intense Pulsed Neutron Source at Argonne National Laboratory.	13,833	15,826	17,015
▪ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	9,190	9,044	9,678
▪ Spallation Neutron Source at Oak Ridge National Laboratory.	19,059	15,100	14,441
▪ Combustion Research Facility at Sandia National Laboratories/California.	5,463	5,377	5,805
Total, Major User Facilities	288,930	269,242	279,923

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

	(dollars in thousands)				
	FY 2001	FY 2002	FY 2003	$ Change	% Change
General Plant Projects	11,874	12,518	12,570	+52	+0.4%
Accelerator Improvement Projects	11,935	11,577	9,067	-2,510	-21.7%
Capital Equipment	62,165	62,235	76,249	+14,014	+22.5%
Total, Capital Operating Expenses	85,974	86,330	97,886	+11,556	+13.4%

Construction Projects

	(dollars in thousands)					
	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2001	FY 2002	FY 2003	Unapprop-riated Balances
99-E-334 Spallation Neutron Source, ORNL	1,192,700	201,400	258,929	276,300	210,571	245,500
02-SC-002 PED, Nanoscale Science Research Centers	15,000 [a]	0	0	3,000	11,000	1,000
03-SC-002, PED, Stanford Linear Accelerator Center	33,500 [b]	0	0	0	6,000	27,500
03-R-312, ORNL, Center for Nanophase Material Sciences	64,250	0	0	0	24,000	40,250
Total, Construction		201,400	258,929	279,300	251,571	314,250

[a] The full Total Estimated Cost (design and construction) ranges between $160,000,000 and $235,000,000. 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 $165,000,000 and $225,000,000. This is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

Major Items of Equipment (TEC $2 million or greater)

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2001	FY 2002	FY 2003 Request	Accept-ance Date
HB-2 Beam Tube Extension at HFIR - ORNL	5,550	4,400	1,150	0	0	FY 2001
SPEAR3 Upgrade..	29,000[a]	0	10,000	9,000	10,000	FY 2003
ALS Beamline..	6,000	2,250	1,800	1,950	0	FY 2003
Total, Major Items of Equipment		6,650	12,950	10,950	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 2002 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

Clarifying language has been added to Sections 2 and 3 with respect to scientific instruments that are related to, but not a part of, the SNS Project.

Estimate of related Annual Funding Requirements has been updated in Section 7.

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	3Q 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 (*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	287,732
2003	210,571	210,571	301,304
2004	124,600	124,600	159,752
2005	79,800	79,800	83,146
2006	41,100	41,100	47,631

[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.

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.

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 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, biological, and medical 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 in full 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. Neutrons enable scientists studying the physical, chemical, and biological properties of materials to determine how atoms and molecules are arranged and how they move. This is the microscopic basis for understanding and developing materials of technological significance to support information technology, transportation, pharmaceuticals, magnetic, and many other economically important areas.

The importance of neutron science for fundamental discoveries and technological development is universally acknowledged. The scientific justification and need for a new neutron source and instrumentation in the U.S. have been thoroughly 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.

Neutrons are a unique and increasingly indispensable scientific tool. Over the past decade, they have 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. In addition to creating the new scientific knowledge upon which unforeseen breakthroughs will be based, neutron science is at the core of many technologies that currently improve the health of our citizenry and the safety and effectiveness of our industrial materials.

The information that neutrons provide 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.

[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.

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

The importance of high power, and consequently high neutron flux (i.e., 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 flux enables studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions. Put most simply, high flux enables studies of complex materials in real time and in all disciplines--physics, chemistry, materials science, geosciences, and biological and medical sciences. Oak Ridge National Laboratory has extensive research efforts in all of these areas.

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 (GeV) 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. Thus 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. Many of these future instruments will be provided by other entities, such as the National Science Foundation, other countries, as well as other DOE programs.

The SNS project made significant progress in FY 2001 towards scheduled milestones. R&D supporting technical component design is now over 90% complete. Project-wide, design work is about 70% complete, with conventional facility Title II design nearly 100% complete. Site preparation was completed, and construction began on the front end and target buildings, the linac tunnel, as well as a number of support buildings and utility systems. A number of procurements for materials and technical components were awarded, with generally favorable cost results, and delivery of some items to Oak Ridge began. Definitive plans for equipment delivery and installation and for handoff of technical systems to Oak Ridge for commissioning activities were developed.

FY 2002 budget authority will be used to continue R&D, design, procurement, and construction activities, and to begin component installation. Essentially all R&D supporting construction of the SNS will be completed, with instrument R&D continuing. Title II design will be completed on the linac, and will continue on the ring, target, and instrument systems. The completed front end ion source and portions of the drift tube linac will be delivered to the site to begin their installation. Other system components for the accelerator, ring, target, and instruments will continue to be manufactured. Work on conventional facilities will continue, 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 will begin 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 front end 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.

4. Details of Cost Estimate

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 22% of construction costs	159,500	179,400
Construction management at approximately 2% of construction costs	14,000	20,400
Project management at approximately 14% of construction costs	104,700	121,800
Land and land rights	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	31,500	28,300
Buildings	181,600	173,600
Utilities (electrical, water, steam, and sewer lines)	20,900	25,100
Technical Components	505,500	441,400
Standard Equipment	17,500	1,900
Major computer items	5,500	5,300
Design and project liaison, testing, checkout and acceptance	31,000	16,600
Subtotal	1,071,700	1,013,800
Contingencies at approximately 11% of above costs[1]	121,000	178,900
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 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 - Front End; 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 2001	FY 2002	FY 2003	Outyears	Total
Project Cost						
Facility Cost [1]						
Line Item TEC	142,682	170,453	287,732	301,304	290,529	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	142,682	170,453	287,732	301,304	290,529	1,192,700
Other project costs						
R&D necessary to complete project [2]	60,356	13,019	4,323	2,328	4,526	84,552
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	0	0	0	0	1,948
Other project-related costs [5]	3,824	6,707	11,421	12,553	82,495	117,000
Capital equipment not related construction [6]	664	183	100	100	56	1,103
Total, Other project costs	81,189	19,909	15,844	14,981	87,077	219,000
Total project cost (TPC)	223,871	190,362	303,576	316,285	377,606	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 $84,552,000 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] Estimated costs of $1,948,000 are included to complete the Environmental Impact Statement.

[5] Estimated costs of $117,000,000 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)[1]	
	Current Estimate	Previous Estimate
Facility operating costs	45,700	21,300
Facility maintenance and repair costs	24,800	25,300
Programmatic operating expenses directly related to the facility	40,000	22,500
Capital equipment not related to construction but related to the programmatic effort in the facility	11,800	2,100
GPP or other construction related to the programmatic effort in the facility	1,000	1,000
Utility costs	19,400	30,400
Accelerator Improvement Modifications (AIMs)	7,300	4,100
Total related annual funding (4Q FY 2006 will begin operations)	150,000	106,700

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.

[1] The previous estimate was in FY 2006 dollars.

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

(Changes from the FY 2002 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 (Current Estimate)	2Q 2002	3Q 2003	N/A	N/A	15,000 [a]

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	3,000	3,000	3,000
2003	11,000	11,000	11,000
2004	1,000	1,000	1,000

3. Project Description, Justification and Scope

This PED request provides for Title I and Title II Architect-Engineering (A-E) services for Basic Energy Sciences (BES) 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.

Updated FY 2003 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 one of the FY 2002 subprojects is also separately requested in FY 2003.

[a] The full Total Estimated Cost (design and construction) ranges between $239,000,000 - $329,000,000. 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 changed to $15,000,000. The full Total Estimated Cost for one project, subproject 02-04, currently proposed for construction is identified in the FY 2003 construction datasheet.

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 is being provided in FY 2002 and requested in FY 2003 for LBNL, ORNL, and LANL/SNL. Construction funding is also requested for ORNL in FY 2003.

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 [a] ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	2Q 2003	3Q 2003	N/A	2,000	45,000-65,000

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

The Center for Nanoscale Materials (CNM) at ANL will consist of conventional facilities, fabrication facilities, characterization instruments, computational capabilities, and beamlines 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. Most specifications of the conventional facilities design for CNM will be intimately connected to the specifications of the technical systems. Towards this end, effort will be dedicated to optimizing both the conventional facilities and the technical facilities, looking for value engineering opportunities. The Center at Argonne will require approximately 10,000 square feet of class 1,000 clean room space for nanofabrication and characterization equipment. This facility will also require general purpose chemistry/biology laboratories (7,000 square feet) and electronic and physical measurement laboratories (3,000 square feet). To house the CNM staff, university collaborators (post docs, visiting students and faculty), and industry collaborators, approximately 16,000 square feet for offices and meeting rooms will be provided. The CNM is being coordinated with a State of Illinois effort. Based on the results of the FY 2001 peer review of the CNM, PED funding is not planned for FY 2002 or requested for this effort in FY 2003.

[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 funding of $1,000,000 in FY 2002 and FY 2003 for this project. Based on results of peer review, funding is not planned for FY 2002 or requested for this project in FY 2003.

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

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection [a] ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	3Q 2003	4Q 2003	N/A	8,300	55,000 – 75,000

Fiscal Year	Appropriations	Obligations	Costs
2002	500[b]	500[b]	500[b]
2003	6,800[b]	6,800[b]	6,800[b]
2004	1,000	1,000	1,000

The Molecular Foundry will be a two to four story high structure adjacent to the Advanced Light Source, with a total gross area of approximately 90,000 square feet and net usable area of approximately 53,000 square feet. Space in the new facility will support studies in nanostructures by providing offices and laboratories for materials science, physics, chemistry, biology, molecular biology and engineering, as well as approximately 6,000 square feet of high bay area. The building will be a state-of-the art facility for the design, modeling, synthesis, processing, and fabrication of novel molecules and nanoscale materials and their characterization. State-of-the-art equipment will support this research; e.g.: cleanroom, class 10-100; controlled environment rooms; scanning tunneling microscopes; atomic force microscopes; transmission electron microscope; fluorescence microscopes; mass spectrometers; DNA synthesizer, 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. 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 2002 Request included $1,000,000 for FY 2002 and $2,000,000 for FY 2003. Based on the results of peer review, current funding plan is $500,000 for FY 2002, $6,800,000 for FY 2003, and $1,000,000 for FY 2004.

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

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection [a] ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	3Q 2003	4Q 2003	N/A	3,000	45,000-65,000

(dollars in thousands)

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

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 the equipment necessary to explore, manipulate, and fabricate nanoscale materials and structures. Also included are individual offices and landscape office areas, seminar area, transient user space for visiting collaborators with access to computer terminals, conference areas on both floors, and vending/lounge areas. In addition it will include circulation/ancillary space, including mechanical equipment area, toilet rooms, corridors, 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 is not planned for FY 2002 or requested for this project in FY 2003.

[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 is not planned for FY 2002 or requested for this project in FY 2003.

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

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection [a] ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002 [b]	3Q 2003 [b]	4Q 2003 [b]	N/A	2,500 [b]	64,000

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	1,500 [b]	1,500 [b]	1,500 [b]
2003	1,000 [b]	1,000 [b]	1,000 [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 will occupy an 80,000 sq.ft. building containing 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 review, this project is now proposed for construction funding in FY 2003.

[a] 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).

[b] Funding of $1,000,000 in FY 2003 and $2,000,000 in FY 2004 was identified in the FY 2002 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.

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

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection [a] ($000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
1Q 2002	3Q 2003	4Q 2003	N/A	4,200	30,000 – 60,000

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

The Center for Integrated Nanotechnologies (CINT), a Center jointly managed by the Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL), 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 main research facility to be located in an unrestricted area just outside the restricted area at Sandia National Laboratory (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 main research facility and the gateways will be managed as one integrated facility by a single management structure. 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 main CINT building 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 equipment for nanolithography, atomic layer deposition, and materials characterization along with general purpose chemistry

[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 identifies 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 FY 2003.

and electronics labs and offices for Center staff and collaborators.

The complex will require class 1,000 clean room space for nanofabrication and characterization equipment and an additional class 100 clean room space for lithography activities. This facility will also require general purpose chemistry/biology laboratories and electronic and physical measurement laboratories. To house the Center staff, collaborators, Center-sponsored post docs, visiting students and faculty, and industry collaborators, offices and meeting rooms will be provided.

4. Details of Cost Estimate [a]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	11,250	10,500
Design Management costs (15% of TEC)	2,250	2,100
Project Management costs (10% of TEC)	1,500	1,400
Total Design Costs (100% of TEC)	15,000	14,000
Total, Line Item Costs (TEC)	15,000	14,000

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 2001	FY 2002	FY 2003	Outyears	Total
Facility Cost.						
PED	0	0	3,000	11,000	1,000	15,000
Other project costs						

[a] This cost estimate is based on direct field inspection and historical cost estimate data, coupled with parametric cost data and completed conceptual studies and designs when available. The cost estimate includes design phase activities only. Construction activities will be requested as individual line items on completion of Title I design. The annual escalation rates assumed in the FY 2002 estimate for FY 2002 and FY 2003 are 3.3 and 3.4 percent, respectively.

(dollars in thousands)

	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	Total
Conceptual design cost........................	0	1,155	0	0	0	1,155
NEPA documentation costs..................	0	0	0	0	0	0
Other project related costs	0	0	0	0	0	0
Total, Other Project Costs	0	1,155	0	0	0	1,155

03-SC-002, Project Engineering Design (PED), Stanford Linear Accelerator Center

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost[1] ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Project Complete	
FY 2003 Budget Request (Preliminary Estimate)	1Q FY2003	2Q FY2005	1Q FY2004	4Q FY2006	$33,500

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2003	6,000	6,000	5,500
2004	15,000	15,000	15,500
2005	10,000	10,000	10,000
2006	2,500	2,500	2,500

3. Project Description, Justification and Scope

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.

The FY 2003 Request is for the Linac Coherent Light Source (LCLS) Project to be located at the Stanford Linear Accelerator Center (SLAC).

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) 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

[1] The full TEC Projection (design and construction) ranges between $165,000,000 and $225,000,000. This is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray free-electron-laser (FEL) in the 1.5 – 15 A 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 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 orders of magnitude 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 makes 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 whole 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.

4. Details of Cost Estimate[1]

(dollars in thousands)

	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design costs (Design Drawings and Specifications)	25,125	N/A
Design Management costs (15% of TEC)	5,025	N/A
Project Management costs (10% of TEC)	3,350	N/A
Total Design Costs (100% of TEC)	33,500	N/A
Total, Line Item Costs (TEC)	33,500	N/A

5. Method of Performance

A Conceptual Design Report (CDR) for the project will be completed and reviewed prior to beginning this work. 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).

[1] This cost estimate includes design phase activities only. Construction activities will be requested to be funded in FY 2004.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	Total
Facility Cost						
PED	0	0	0	5,500	28,000	33,500
Other project costs						
Conceptual design cost	0	0	1,500	0	0	1,500
NEPA documentation costs	0	0	0	0	0	0
Other project related costs	0	0	0	0	0	0
Total, Other Project Costs	0	0	1,500	0	0	1,500
Total Project Cost (TPC)	0	0	1,500	5,500	28,000	35,000

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

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

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Project Engineering & Design (PED)			
2002	1,500[a]	1,500[a]	1,500[a]
2003	1,000[a]	1,000[a]	1,000[a]
Construction			
2003	24,000[a]	24,000[a]	14,000[a]
2004	20,000	20,000	20,000
2005	17,500	17,500	21,500
2006	0	0	6,000

[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 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, bringing together four areas where the United States has clear national research needs. 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, collocated 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 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	N/A
Design and Project Management Costs	300	N/A
Total, Design Costs	2,000	N/A
Construction Phase		
Improvements to Land	500	N/A
New Building and Additions	19,700	N/A
Special Equipment[2]	26,000	N/A
Utilities	500	N/A
Inspection, design and project liaison, testing, checkout and Acceptance	1,800	N/A
Construction and Project Management	1,700	N/A
Total, Construction Costs	50,200	N/A
Contingency (23.5% of Construction Costs)[3]	11,800	N/A
Total, Line Item Costs	64,000	N/A
Less: Non-Agency Contribution	0	N/A
Total, Line Item Costs (TEC)	64,000	N/A

[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.

[3] Percent of TEC includes contingency for special equipment in the calculation.

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.

6. Schedule of Project Funding

	Prior Years	FY 2002	FY 2003	FY 2004	FY 2005	FY 2006	Total
Project Cost							
Facility Cost							
Design	0	1,500	1,000	0	0	0	2,500
Construction	0	0	14,000	20,000	21,500	6,000	61,500
Total, Line item TEC	0	1,500	15,000	20,000	21,500	6,000	64,000
Other project costs							
Conceptual design costs	150	0	0	0	0	0	150
NEPA documentation Costs	5	0	0	0	0	0	5
Other project related Costs [1]	0	220	100	250	175	100	845
Total, Other Project Costs	155	220	100	250	175	100	1,000
Total Project Cost	155	1,720	15,100	20,250	21,675	6,100	65,000
Less: Non-Agency Contribution	0	0	0	0	0	0	0
Total, Project Cost (TPC)	155	1,720	15,100	20,250	21,675	6,100	65,000

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

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	TBD	N/A
Total operating costs (operating from FY 2006 through FY 2055)	TBD	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 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.