Basic Energy Sciences

Program Mission

The mission of the Basic Energy Sciences (BES) program – a multipurpose, scientific research effort – is to foster and support fundamental research in materials sciences and engineering, chemical sciences, biosciences, and geosciences to provide the foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. 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.

The Research Portfolio

The BES program is one of the Nation's largest sponsors of fundamental research. In FY 2000, 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. This investment in academic research has been a constant fraction of the BES research portfolio for more than a decade.

The BES program also supports outstanding scientific user facilities, providing world-class capabilities for imaging and characterizing materials. Experiments at these facilities are conducted on a host of different samples, including ceramics, metals, and alloys; polymers and soft materials; gases and liquids; and fragile biological specimens and crystals. The BES synchrotron radiation light sources, the neutron scattering facilities, and the electron beam characterization centers represent the largest 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. The BES program also supports the vast majority of the federally funded research in the physical sciences at these facilities.

Activities supported by the BES program are a significant part of the national research effort, providing particular strength to the Nation's science enterprise in the physical sciences and in facilities planning, construction, and operation.

DOE's history and mission have played an important role in BES's current position as the Nation's steward and primary user of neutron and x-ray facilities. Historically, neutron sources descended from neutron reactors that were constructed in the early 1940's as part of the U.S. Manhattan Project, an early predecessor of DOE. Similarly, synchrotron facilities stemmed from particle accelerators that were developed for DOE high-energy physics research. Originally constructed for materials sciences research, the BES facilities are now used by a wide variety of scientific disciplines, some far removed from the original vision. Notably about 30% of the users at the synchrotron radiation light sources are structural biologists, a significant increase from only a few percent two decades ago.

Today, spurred by results from the physical sciences and by innovations in accelerator physics, the BES program continues its pioneering role in the development of new instrument concepts and next-generation facilities for "materials science and related disciplines" -- the original motivation for virtually all the BES facilities. A decade or two from now, we expect once again to be surprised by the breadth of disciplines and applications that will thrive at these new facilities.

BES Subprograms

The BES program has four subprograms to address its mission. Research activities within each of the subprograms are strongly coupled to those in the other BES subprograms.

Materials Sciences

The Materials Sciences subprogram supports basic research in condensed matter physics, metal and ceramic sciences, and materials chemistry. 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, 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. This subprogram is the 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.

Chemical Sciences

The Chemical Sciences 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; and heavy element chemistry. 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 the production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. This subprogram provides support equal to that of the National Science Foundation for basic research in chemistry. It provides the Nation's primary support for homogeneous and heterogeneous catalysis, photochemistry, radiation chemistry, gas-phase chemical dynamics, and separations and analysis. It is the Nation's sole support for fundamental research in heavy element chemistry.

Engineering and Geosciences

The geosciences activity in the Engineering and Geosciences subprogram supports basic research to understand the Earth's crust, including 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. This activity provides one third of the total federal support for individual investigator basic research in solid earth sciences. The engineering activity in the Engineering and Geosciences subprogram is integrated with activities in the materials sciences subprogram and focuses on nanotechnology and microsystems, multicomponent fluid dynamics and heat transfer in materials, and nonlinear systems.

Energy Biosciences

The Energy Biosciences subprogram supports basic research in the molecular and cellular mechanisms to understand the capture and conversion of solar energy via natural photosynthesis. The research defines -- at the molecular level -- the structure, synthesis, and assembly of cellular components involved in the light-driven production of chemical energy. Ultimately, this research will aid the development of renewable biomass resources. This subprogram is the prime provider for molecular research on plants not focussed on traditional crop and agricultural interests and a major supporter of research on microbial systems that have broader importance than the model systems used in the biomedical community. This subprogram is one of the Nation’s prime interfaces between bio- and physical sciences, promoting multi- and cross-disciplinary research activities jointly with all of the other BES subprograms.

Program Goal

Maintain U.S. world leadership in areas of materials sciences and engineering, chemical sciences, biosciences, and geosciences relevant to energy efficiency, renewable energy resources, fossil fuels, reduced environmental impacts of energy production and use, science-based stockpile stewardship, and future energy sources.

Program Objectives

- Foster and support world-class, peer-reviewed research in the scientific disciplines encompassed by the BES mission areas, cognizant of DOE needs as well as the needs of the broad national science agenda.
- Provide national and international leadership in select areas of materials sciences and engineering, chemical sciences, biosciences, and geosciences.
- Plan, construct, and operate premier national scientific user facilities for materials research and related disciplines to serve researchers at universities, national laboratories, and industrial laboratories. Operate facilities to the highest standards for scientific productivity, efficiency, user needs, and safety.
- Establish and steward stable, essential research communities and institutions, particularly those for which BES is the Nation's primary or sole support.
- Continue the advanced education and training activities of young scientists to maintain and renew research communities and institutions.
- Manage the operations of the Basic Energy Sciences program to high standards by ensuring that the processes for planning, reviewing, selecting, and managing science projects and programs are sound and based on peer review and merit evaluation.

Evaluation of Objectives

BES evaluates the progress being made toward achieving its scientific and management objectives in a variety of ways. Regular peer review and merit evaluation is conducted for all activities, except those

Congressionally mandated, based on procedures set down in 10 CFR 605 for the extramural grant program and on a similar process for the laboratory programs and scientific user facilities. New projects are selected by peer review and merit evaluation. In addition, BES regularly conducts external reviews of its construction projects to ensure that they are on time and within budget. Beginning in FY 2001, the Basic Energy Sciences Advisory Committee (BESAC) will evaluate the proposal review and selection process and provide advice on subprogram portfolios on a rotating basis, completing the entire BES program portfolio approximately every three to five years. High-level performance measures are given below; specific performances measures are included within the detailed program justification narratives, as appropriate.

- The overall quality of the research in the BES program will be judged excellent and relevant by external evaluation by peers, and through various forms of external recognition.
- Leadership in key BES disciplines that are critical to DOE's mission and the Nation will be measured through external review and other mechanisms.
- At least 80% of all new research projects supported by BES will be peer reviewed and competitively selected, and will undergo regular peer review merit evaluation.
- BES will keep within 10%, on average, of cost and schedule milestones for upgrades and construction of scientific user facilities, including the construction of the Spallation Neutron Source.
- The BES scientific user facilities will be operated and maintained so that unscheduled operational downtime will be less than 10% of total operating time, allowing nearly 8,000 scientists to conduct experiments on an annual basis.
- BES will ensure the safety and health of the workforce and members of the public and the protection of the environment in all its program activities.

Significant Accomplishments and Program Shifts

FY 2000 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 four Nobel Prizes awarded to BES principal investigators during the 1990s. Selected major prizes and awards for FY 2000 include:

- *From ASM International* — the Materials Science Research Silver Medal
- *From the Alexander von Humbolt Foundation* — the Senior Research Award; the Senior Scientist Award
- *From the American Academy of Microbiology* — Procter and Gamble Award in Applied and Environmental Microbiology
- *From the American Ceramic Society* — the George W. Morey Award; the First-in-Class Award for Ceramographic Competition; Norbert J. Kreidl Award for Young Scholars
- *From the American Chemical Society* — the Arthur C. Cope Scholar Award; Award in Inorganic Chemistry; Award in Chemistry of Materials; Award in Colloid or Surface Chemistry; the George

A. Olah Award in Hydrocarbon or Petroleum; F. A. Cotton Medal; Award for Creative Research in Homogeneous or Heterogeneous Catalysis; Distinguished Service Award in Analytical Chemistry

- *From the American Institute of Chemical Engineers* — the Warren K. Lewis Award; the William H. Walker Award for Excellence in Contributions to Chemical Engineering Literature; the Clarence G. Gerhold Award
- *From the American Physical Society* — the Frank Isakson Prize; two recipients of the Herbert P. Broida Prize; the Oliver E. Buckley Prize for Condensed Matter Physics; James C. McGroddy Prize; and the Wheatley Award
- *From the American Society of Plant Physiologists* — Steven Hales Prize
- *From the American Welding Society* — two recipients of the Davis Silver Medal
- *From the Electrochemical Society* — the David C. Graham Award; the Carl Wagner Award
- *From the Institute for Physical and Chemical Research, Tokyo, Japan* — the Eminent Scientist Award
- *From the International Society for Measurement and Control* — the Arnold O. Beckerman Founder Award
- *From the Materials Research Society* — the Gold Award; the Materials Research Society Medal; the MRS Turnbull Award; the Woody Award; the Von Hippel Award
- *From the Minerals, Metals and Materials Society* — the Young Leader Program; the Acta Metallurgica Gold Medal; the John Bardeen Award
- *From the National Institute for Materials Center* — the Center for Excellence Award
- *From R&D Magazine* — R&D 100 Awards for:

  X-ray scanning microprobe, which focuses hard x-rays to a spot size of less than 150 nanometers.

  Differentially deposited x-ray microfocus mirrors, which efficiently focus monochromatic and broad-bandpass x-rays to a submicron spot.

  Combinatorial Synthesis, which permits the acceleration of the discovery of new materials with improved properties.

  ANDE-Advances Nondestructive Evaluation System, which uses ultrasonic interferometry for examining the contents of sealed containers.

- *From the Society of Automotive Engineers* — the Lloyd L. Withrow Distinguished Speaker Award

Three principal investigators were elected to the National Academy of Sciences, and four were elected to the National Academy of Engineering. Two principal investigators were advanced to fellowship in the American Association for the Advancement of Science; two in the American Ceramic Society; seventeen in the American Physical Society; one in the American Welding Society; two in the ASM International; and two in the American Vacuum Society.

Finally, principal investigators served in numerous elected offices including: President-elect, American Ceramic Society; Director, Microbeam Analysis Society; Vice Chair, Division of Materials Physics, American Physical Society; Council, Materials Research Society; Council of Fellow, ASM International; Chair, Materials Research Society; National Program Chair, American Chemical Society; Vice Chair, Fellows Selection Panel of the American Welding Society; Secretary, Vacuum Metallurgy Division, IUVSTA; and Foreign Member, Royal Academy of Engineering.

SELECTED SCIENCE ACCOMPLISHMENTS

Materials Sciences

- **Magnetism at the atomic scale.** When information is written to a computer hard drive, local magnetic moments associated with atoms in a small region of the surface reverse direction like sub-microscopic compass needles. A new theory has helped explain these dynamical processes. This work recently received the Gordon Bell Award for the fastest real supercomputing application and was named to the Computerworld Smithsonian 2000 collection for being the first supercomputing application to surpass one teraflop.
- **Functional nanostructured materials that replicate natural processes.** A newly developed class of nanostructured materials can selectively filter molecules by their size and chemical identity. These remarkable materials are made from a solution of molecular building blocks that spontaneously arrange themselves into a porous solid as the solvent evaporates. This achievement involved creating the self-organizing precursors, controlling the pore size, and employing a novel evaporation process that promotes self-assembly. These materials hold the promise for significant applications. For example, in the future we may wear "breathing" fabrics that block hazardous chemicals while admitting benign species like oxygen.
- **The Library of Congress on a single disk?** The vision that information can be written and erased near the single molecule limit has been realized for the first time. Disordering and re-ordering tiny regions of a thin film show promise for storing a million times more information than with today's computer disks with no increase in space. The film is made of organic material and supported by graphite. It is so thin that 40,000 layers would be only as thick as a sheet of paper. By exposing the film to voltage pulses with a scanning tunneling microscope, nanometer-sized regions can be switched from crystalline to disordered, increasing their ability to conduct electricity by 10,000 times. Each tiny region is one bit of information, not much bigger than a single molecule of the film.
- **Analyses of nanocrystals using coherent (laser-like) synchrotron radiation.** A powerful new x-ray diffraction method for characterizing the structure of nanocrystalline solids has been developed. Tailoring nanocrystalline properties for specific applications depends critically on detailed knowledge of three-dimensional structure. Traditional x-ray diffraction methods are inadequate; however, coherent x-ray diffraction patterns of gold nanocrystals show surface facets, fringes due to interference among facets, nanocrystal lattice distortion, and, ultimately, equilibrium nanocrystal shape.
- **Ion-implantation for strong metal-ceramic bonds**. Ceramics are hard and corrosion resistant but fracture easily. Metals resist fracture but are not as wear or corrosion resistant as ceramics. Coating a metal with a ceramic is a way to improve both. However, current coating technologies can degrade the performance of metals. A new approach has been successfully developed that employs ion-beam intermixing of the coating with the metal from collision cascades, which are microscopic (nanometer-sized) "hot-zones" formed along the ion track. Since the heating in collision cascades is very short and localized, macroscopic heating of the metal does not occur. A patent has been filed using this new approach to improve hip, knee, and dental prosthetic devices. Ion implantation is used to coat the bone mineral (hydroxyapatite) on titanium starting with a high density layer bonded well to the

titanium and changing progressively toward a porous bone mineral outer surface that promotes bone growth and bonding to bone.

- **Long-term storage of plutonium.** Worldwide, nuclear energy production and defense programs have created 1,350 metric tons of plutonium. Because plutonium is radiotoxic and has a long half-life (24,500 years), a long-term storage solution must immobilize plutonium in materials that are resistant to radiation damage for millennia. Using heavy-ion irradiation, advanced characterization techniques, and computer simulation methods, researchers have discovered that highly durable gadolinium zirconate can lock plutonium into its structure while remaining resistant to radiation damage for millions of years.
- **Boron doping of silicon semiconductor devices -- faster, lower-power computing.** Boron doping of silicon improves electrical conductivity and other important aspects of silicon device performance. A fifty-fold increase in active boron doping -- far above nature's maximum of 0.01% -- has been achieved using a new process involving atomic hydrogen. Resulting ultra-highly doped silicon layers provide self-aligned "metallic" contacts, improve semiconductor devices, eliminate etching steps in device fabrication, reduce manufacturing costs, and minimize the use of toxic etching gases and chemicals.
- **Seeing electrons.** A novel, quantitative, and highly sensitive method has been developed to image and measure the distribution of valence electrons, which are responsible for chemical bonding and the transport of electrical charge in solids. This new technique, combining imaging and diffraction in the electron microscope, was used to reveal the spatial distribution of valence electrons in complex structures of high-temperature superconductors. The ability to directly observe and measure valence electron distributions with atomic scale resolution will greatly help in the search for better superconductors, ferroelectrics, and semiconductors.
- **Fluctuation microscopy.** Fluctuation microscopy, a new discovery, challenges the common perception that glassy materials have no organization. Fluctuation microscopy relies on the ability of the electron microscope to measure diffraction from tiny volumes (~1000 atoms). It is based on detailed computational simulations coupled with computer-assisted statistical analysis of multiple electron images. It has required development of advanced image-detection methods. In one of the first applications of this method, studies of amorphous silicon and germanium show that both are highly organized over distances of tens of atoms, even though other measurement techniques see these atoms as completely random. This finding is critical to improving the ability of amorphous solar cells.
- **A smart transistor.** A breakthrough in developing the world's smartest transistor has been accomplished. Germanium-based transistors using a new ferroelectric dielectric would be "smart" devices capable of remembering their state. The heart of this new scientific advance is the understanding of the relationship between polarization and microstructure and how to control it. This breakthrough offers enormous potential for energy savings in a myriad of electronic sensors and devices as no power is necessary to maintain a given on/off state. A low-power, gigabyte chip could thus serve as a computer hard drive.
- **Design of semiconductors with prescribed properties**. A theoretical method has been invented by which one can first specify the properties desired in a semiconductor and then work backward to predict the structure of the material that will show those properties. This work was featured in *Fortune Magazine*.

Chemical Sciences

- **Direct measurement of chemical reactions in turbulent flows.** Long known for their dramatic advancements in laser instrumentation for monitoring gas-phase reactions and chemically reacting flows, scientists at the Combustion Research Facility have for the first time monitored multiple flame species directly and simultaneously. These measurements provide a powerful test of combustion models that could lead to improved combustion efficiency.
- **Dynamics of single molecules.** Reactions of single molecules have been observed by monitoring molecular fluorescence using newly developed experimental methods, thus separating the effects of the motion of one molecule from the ensemble motion of the molecule in its environment. The dynamics of a single molecule have been shown to be significantly different from motion in an ensemble, and should lead to the development of new theories for predicting chemical reactivity.
- **Blinking quantum dots.** Quantum dots -- nanometer-size particles in which electrons are confined in a relatively small volume -- have recently been shown to emit light at multiple wavelengths, blinking on and off on a time-scale of seconds. This remarkable behavior, attributed to luminescence from different electronic states, has potential applications for optical logic and photonics and may one day lead to nano-scale computers and/or portable analytical instrumentation.
- **Generation of laser-like x-ray beams.** Combining state-of-the-art ultrafast laser systems with evolutionary computer algorithms has led to a dramatic new demonstration of the controlled generation of coherent x-rays. This represents an important new source of ultrafast, coherent soft x-rays for studies of materials properties and chemical physics.
- **Biomolecular photobatteries.** Voltages have been measured from a single photosynthetic reaction center -- the five nanometer wide molecular structure in green plants that captures solar energy and converts it into electrical energy. The reaction center may be thought of as a tiny photobattery. The reaction center functions as nanometer-sized diodes with possible applications to molecular scale logic devices and computers.
- **Radiation induced chemistry.** Solid particles have been found to enhance the effects of water radiolysis and the resulting production of hydrogen. Furthermore, gas bubbles form on the particles and that impedes the continuous, safe release of hydrogen from the suspension. These results may provide an explanation for the "burps" in storage tanks containing aqueous suspensions and radioactive material.
- **Plutonium chemistry in the environment**. Using newly constructed beamlines at the BES synchrotron radiation light sources, scientists are now able to study small quantities of radioactive materials. X-ray absorption studies on plutonium-containing soils from Rocky Flats revealed that the plutonium is predominantly present as the solid oxide, PuO_2, a form substantially less mobile in soil and ground water than other possible forms. This result demonstrates that the plutonium will remain stable and has led to substantial cleanup cost savings.
- **Actinide supramolecular complexes**. Researchers have for the first time built a supramolecular actinide complex. Supramolecular complexes are molecules that are built from smaller subunits, yet retain their own distinct molecular properties. While there may be future applications in separation science and catalysis, the current worldwide effort in supramolecular chemistry is to understand the principles that govern assembly of such molecules.
- **Molecular theory of liquids**. A molecular theory for the liquid state, which has eluded scientists for years, has now been developed. This provides new opportunities in one of the most important areas

for process engineering and one of its most perplexing problems - the prediction of liquid-gas equilibria based on the well-known properties of molecules.

Engineering and Geosciences

- **Engineering at the nanoscale.** Using nanoscale devices in real-world engineered systems is one of the greatest challenges facing nanoscale research. A portfolio of research activities explores how to engineer at the nanoscale. Recent activities include the development of physics-based models to represent crack initiation as a nanoscale phenomenon; studies of the frictional response of nanochains; electric charge transfer in semiconductor nanostructures; nanoscale quantum-dot self assembly using DNA templates; and the integration of nanoscale biomotors with mechanical devices. In this last activity, researchers constructed integrated nanoscale devices that are powered by biomolecular motors and fueled by light. In one such system, a protein from a photosynthetic bacterium generates an electrochemical gradient across an artificial membrane system. This system is chemically closed, enabling the motors to be continuously supplied with fuel using a total light collection area less than 400 square nanometers.

- **Geosciences imaging from the atomic scale to the kilometer scale.** Advances in geosciences imaging were demonstrated this year at a variety of disparate length scales. At the smallest length scale, the GeoCARS beamline at the Advanced Photon Source was used to examine the interaction of liquid water with alumina as a model for understanding aluminum containing minerals such as clays. Unlike other techniques used to characterize surfaces, the new beamline can study wet crystal surfaces. The result showed a significant change from the experiments using dry surfaces and will help researchers understand water-solid interactions in nature at the atomic level. At an intermediate length scale, researchers are using advanced laser scanning confocal microscopy to image, reconstruct, and characterize fluid flow through pores and cracks. Predicting the magnitudes and directions of flow in earth material is critical in performance assessment of oil and gas reservoirs. Finally, at the largest length scales, researchers are using specially instrumented regions in an earthquake zone to help model and improve geophysical imaging on the kilometer scale.

- **Biogeochemistry.** It is increasingly evident that living processes play a fundamental role in determining the geochemistry of groundwater, near-surface sediments, and deeper rocks. Microbes affect the weathering of rocks and minerals, and microbial metabolism affects the accumulation of heavy metals in soils or their release to groundwater. These and other processes determine how soils, sediments, and ore bodies form and how water quality is affected. Work identifying how microbes affect the fate of zinc released to groundwater percolating through lead-zinc mines and other biogeochemistry work recently led to the award of MacArthur Foundation Fellowship to a BES supported researcher. Biogeochemistry, which links three BES subprograms, is expected to play an increasingly important role in addressing DOE missions.

Energy Biosciences

- **Completion of the gene sequence of *Arabidopsis thaliana*, the first plant genome.** *Arabidopsis thaliana*, a small weed belonging the mustard family, became the world's "model" plant owing to its small physical size, small genome size, low level of junk and repetitive DNA, short life cycle, large number of mutations, and ease in genetic analysis. An international collaboration involving scientists from the U.S., Europe, and Japan announced the completion of the complete sequence of this plant genome in December 2000. The *Arabidopsis* genome is entirely in the public domain, making the results available to scientists worldwide. The Energy Biosciences subprogram has been a partner in this project since its inception; support for research on *Arabidopsis* dates to the early 1980s.

- **Snapshot of a light-driven pump.** Sunlight causes the bacteriorhodopsin protein to change shape, and in the process transport protons across a membrane to provide chemical energy. X-ray crystallographic structure determinations of this light-driven proton pump captured for the first time the molecule frozen mid-stroke of this shape modification. This novel view of the intermediate conformation enables us to see how biological nanostructures capture and transform energy.

SELECTED FACILITY ACCOMPLISHMENTS

The four BES synchrotron radiation light sources and three BES neutron scattering facilities served 6,533 users in FY 2000 by delivering a total of 30,249 operating hours to 218 beam lines at an average of 97.8% reliability (delivered hours/scheduled hours). Statistics for individual facilities are provided below. In two instances, 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 36,750 hours. Most of the BES facilities already operate close to the maximum number of hours possible for their facility. Significant reductions from the maximum in FY 2000 were a result of planned shutdowns for the installation of upgrades.

The first priority for utilizing the facilities optimally is to generate a highly reliable source of beam for the maximum number of operating hours possible. In addition, however, the beamlines and their instruments must be supported and maintained at the state-of-the-art, and the number of beam lines must 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.

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.).

- **The Advanced Light Source (ALS)** served 1,036 users in FY 2000 by delivering 5,367 operating hours to 34 beam lines at 95.0% reliability (delivered hours/scheduled hours). The ALS is supported by the Materials Sciences subprogram.

  New technique for improved storage-ring stability. The electron beam parameters in the storage ring determine x-ray beam lifetime and stability. Using a mathematical technique, accelerator physicists have understood the strength and location of harmful resonances that cause irregular, chaotic electron behavior leading to loss of electrons from the beam.

  Third-harmonic cavities enhance beam lifetime. The electron beam lifetime in a synchrotron-radiation source determines how long users can record data before being interrupted when accelerator operators replenish the train of short bunches that make up the beam. A desirable way to increase the lifetime is to lengthen the bunches. Five new third-harmonic cavities accomplish the bunch lengthening and have increased electron beam lifetime increased by about 50%.

  X-ray science possible at femtosecond speeds. X-ray experiments to study physical, chemical, and biological processes that occur on a time scale of one molecular vibration (typically 100 femtoseconds) are an emerging area of research. Three developments at the ALS brought x-ray science into the femtosecond realm. First, researchers developed a high-speed x-ray detector (a streak camera) with a picosecond time resolution. Second, researchers showed how to use a femtosecond laser to "slice" tiny slivers from the circulating electron bunches in the storage ring and use them to produce pulses of synchrotron radiation lasting just 300 femtoseconds, which is 100 times shorter than the x-ray pulse normally produced. Finally, accelerator physicists devised an arrangement of magnets that allow a narrow-gap undulator optimized for the production of femtosecond x rays to be installed in the storage ring.

Undulator has complete polarization control. The elliptically polarizing undulator (EPU) in the ALS is now in full user operation with a high-resolution beamline to provide state-of-the-art performance. This capability opens up many new experimental possibilities in polymer, biophysics, and magnetism research all without rotation of the sample.

Upgrades improve photoemission electron microscopy. By imaging the photoelectrons emitted from a sample with high spatial resolution, the photoemission electron microscope is an ideal tool for combining spectroscopy with variable polarization microscopy in the study of materials ranging from magnetic materials to polymers. The performance and sample-preparation facility of this instrument have been upgraded, making possible new experiments, such as probing the magnetic roles of the different elements in multilayer structures of the type under development for magnetic memory and data storage.

A facility for sub-micron x-ray diffraction developed. Many properties depend on behavior within individual grains and on the details of grain-to-grain interactions. The ALS has pioneered the technology needed for x-ray micro-diffraction and its application to thin-film stress analysis. The system is capable of measuring structural parameters from grains as small as 0.7 micron. The technique is starting to play a major role in many materials projects, from stress-induced cracking of indented high-strength materials to stress in magnetic thin films.

- **The Advanced Photon Source (APS)** served 1,527 users in FY 2000 by delivering 4,724 operating hours to 34 beam lines at 93.6% reliability (delivered hours/scheduled hours). The APS is supported by the Materials Sciences subprogram.

3-D imaging in real time. A real-time, three-dimensional x-ray microtomography imaging system that can acquire, reconstruct, and interactively display rendered 3-D images of a sample at micrometer-scale resolution within minutes has been developed. This system could bring better understanding of an array of physical processes, ranging from failure in microelectronic devices to growth and depletion processes in medical samples.

Novel x-ray microprobe developed. The magnetic contribution to the cross section for x-ray scattering is of significant interest. A technique has been developed that combines microfocusing x-ray optics with Bragg-diffracting phase retarders to produce a circularly polarized x-ray microprobe. This will enable a wide variety of magnetic scattering experiments in applied fields like magnetic materials and superconducting compounds.

New beam chopper improves time-resolved experiments. A new beam chopper has been developed for time-resolved experiments. The time window of 10 nanoseconds enables time-resolved experiments in condensed-matter physics, atomic physics, and biological science.

Beam-position monitor improvements started. Significant upgrades have been made to the particle beam and x-ray beam position measurement systems. Further progress is expected when these changes are incorporated in all of the beamlines at the APS. This state-of-the-art improvement in beam stability will provide the APS users with more efficient beamlines and the capability of working with smaller samples and increased measurement resolution.

Storage-ring “top-up” operations developed. The APS is the first facility to implement "top-up" filling of the storage with electrons during normal operations. During 136 hours of top-up operation, the stored current was held constant to about two parts per thousand by injecting a pulse of electrons once every two minutes. This resulted in improvements in x-ray beam stability. Ultimately, top-up filling will be the routine operating mode of the APS.

Record FEL SASE achieved. Using the Low-Energy Undulator Test Line (LEUTL) and the injector linac, an experimental verification was obtained of the self-amplified spontaneous emission (SASE) process for 530 nm light. More recently, saturation of the SASE process at a power level 10,000,000 times higher than the light produced by a single undulator insertion device was verified. These experiments are viewed as necessary experimental milestones for achieving an x-ray free-electron laser.

- **The National Synchrotron Light Source (NSLS)** served 2,551 users in FY 2000 by delivering 5,620 operating hours to 90 beam lines at 112.9% reliability (delivered hours/scheduled hours). The NSLS is supported by the Materials Sciences subprogram and the Chemical Sciences subprogram.

New optical polarizer. A newly developed quadruple-reflector optical polarizer efficiently converts VUV light from linear to either left-circular or right-circular polarization. This polarizer expands the capability the U5UA beamline in the area of ultra-thin magnetic films.

High-resolution photoelectron spectrometer. A new photoelectron spectrometer was installed on the U13UB beamline, and has already produced new physical insights into the electronic structure of high temperature superconductors.

Infrared beamlines revitalized. The 10 year-old infrared microspectrometer at U10B beamline was replaced with a state-of-the-art continuum microscope and advanced Fourier transform infrared spectrometer. The system has been used for the study of interplanetary materials, biological tissues, corrosion, and materials formed at high pressure. Also, the beam delivery optics for the U12IR beamline were rebuilt to provide infrared radiation to a new high-resolution spectrometer. This spectrometer will be used for magnetospectroscopy studies of materials such as $LaMnO_3$.

Fluorescence microscopy. For the first time, an infrared microscope has been modified such that fluorescence sample visualization and infrared microspectroscopic analysis can be performed simultaneously. This unique combination is a valuable analysis tool for probing the chemical composition of materials.

Advanced x-ray detector array enables study of trace elements. X-ray absorption spectroscopy of trace elements in samples poses a serious detection problem. The detector technology developed for high-energy physics applications was used to produce a 100-element energy-resolving detector array for use on an NSLS beamline.

Advanced x-ray detector system developed. One of the ways in which diffraction experiments can be made more efficient is to detect the entire diffraction pattern with high resolution. In order to accomplish this, a novel curved cylindrical detector was developed. In addition, a highly-parallel readout system was developed that is capable of processing events 10 times faster than before.

Low-cost monochromator, low-maintenance spectrometer. A simple device that consists of a monolithic silicon diffracting element is near-zero maintenance and almost adjustment free. It is now used on five NSLS beamlines; several more such detectors will be installed at NSLS and at other facilities. The new device removes need for ultra-fine mechanisms that contribute to most of the cost of such an instrument and makes x-ray monochromators difficult to control.

Digital feedback system improves storage ring stability. Meeting the needs of the large population of NSLS users for high quality photon beams requires an extremely stable electron orbit. To that end, digital orbit feedback systems to replace the original analog ones were designed in both the VUV and the X-ray rings. The main advantage of switching to a digital architecture is the ability to use a higher number of beam position monitors to achieve a better match between disturbances on the beam and corrective action by the feedback system. The digital global orbit feedback system was put into operations in the VUV ring in August 2000. Implementation of the digital orbit feedback system on the X-ray ring is expected in FY 2001.

- **The Stanford Synchrotron Radiation Laboratory (SSRL)** served 895 users in FY 2000 by delivering 4,143 operating hours to 26 beam lines at 96.8% reliability (delivered hours/scheduled hours). The SSRL is supported by Materials Sciences subprogram and the Chemical Sciences subprogram.

Reliability of SPEAR improved. The reliability of the injector was improved by rebuilding the regulation of power supplies in the beam transport line. This contributed to shorter filling times, and, consequently, to longer beam times available to the users.

Quality of the photon beam enhanced. Stable photon beam intensity is one of the requirements for performing demanding synchrotron radiation experiments. Accelerator physics studies determined that one type of beam noise was due to the excitation of high order electro-magnetic modes in the accelerating cavities. To alleviate this problem, waveguide dampers were installed in the radio-frequency accelerating system. As a consequence, SPEAR operates more reliably and the beam stability is improved.

SSRL beam line systems modernized. Six beam line stations were upgraded to the SSRL standard data acquisition system and control software. This greatly increases reliability while reducing user training time, spares requirements, and staff support requirements.

High magnetic field x-ray scattering station commissioned. A new high magnetic field end station incorporating a 13 Tesla superconducting magnet was constructed and commissioned on SSRL's premiere x-ray scattering beam line, BL7-2. This facility is one of the few facilities in the world that enable state-of-the-art x-ray scattering experiments in high field environments. The unique matching of a versatile, high-field magnet with an intense synchrotron x-ray source allows scientists to unravel the properties of these new materials. Eventually, the fundamental understanding that will be derived from this research will lead to higher performance sensors and magnetic storage devices.

Photoemission beamline improved for higher throughput and resolution. The high-resolution angle resolved photoemission beam line station 5-4 has been used to study the fundamental mechanisms of high temperature superconductivity and improvements in FY 2000 have brought the station to new levels of performance. The upgrades include a new primary focusing mirror and an angle mode option to the photoelectron energy analyzer greatly improving throughput.

Molecular environmental science facility commissioned. The importance of molecular based research in the environmental area is increasing in importance due to the emergence problems ranging from environmental remediation at the DOE weapons labs, to long term storage of nuclear waste, to basic questions concerning molecular interactions of pollutants at the surfaces of soils. Beam line station 11-2 has been optimized for x-ray absorption studies of samples in a variety of states and under dilute field conditions. The station also includes capabilities for small spot analysis as well as specialized facilities for the safe handling and analysis of radioactive materials such as soils contaminated with actinides or wastes from nuclear storage sites.

New research and training gateway program initiated. A Gateway pilot program involving SSRL and the University of Texas at El Paso (UTEP) is providing training and research opportunities targeted toward Mexican and Mexican American students. In FY 2000, a group of 16 UTEP students and staff underwent training and carried out experiments on four separate beam lines.

- **The Intense Pulsed Neutron Source (IPNS)** served 230 users in FY 2000 by delivering 3,842 operating hours to 15 beam lines at 101.6% reliability (delivered hours/scheduled hours). The IPNS is supported by the Materials Sciences subprogram.

  Upgrade of QENS instrument. The quasielastic neutron scattering (QENS) instrument was completely upgraded. This instrument is used for measurements that determine the diffusion rates of both molecular rotation and translation on the typical time-scales of simple liquids, adsorbates etc. QENS is also capable of measuring vibrational excitations up to a few hundred meV, providing access to both external and internal vibrational modes for hydrogenous systems.

  IPNS hosts second National Neutron and X-Ray Scattering School. During the two-week period of August 14-26, 2000, Argonne National Laboratory once again hosted the National School on Neutron and X-Ray Scattering. The success of the previous year was so overwhelming that additional funds were provided by BES to increase the size of the school from 48 to 60 graduate students. Funding was also provided by the National Science Foundation. This school fulfills a continuing need for training graduate students in the utilization of national user facilities. The formal program included 32 hours of lectures given by an internationally known group of scientists recruited from universities, national laboratories and industry.

- **The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center** LANSCE served 25 users in FY 2000 by delivering 736 operating hours to 7 beam lines at 78.8% reliability (delivered hours/scheduled hours). LANSCE was down for installation of upgrades and safety shutdowns in FY 2000. The Lujan Center is supported by the Materials Sciences subprogram.

  Neutron flux increased. The Lujan Center is the first spallation neutron source to exploit the increased neutron flux provided by coupled moderators. A new coupled liquid-hydrogen moderator provides an increase of approximately 2.5 times over the previous decoupled moderator. Both the small-angle diffractometer and the Surface Profile Analysis Reflectometer benefit from this increased flux.

- **The High Flux Isotope Reactor (HFIR)** served 269 users in FY 2000 by delivering 5,817 operating hours to 12 beam lines at 92.9% reliability (delivered hours/scheduled hours). The HFIR is supported by the Materials Sciences subprogram and the Chemical Sciences subprogram.

  Cold source progress. Work continues on the development of the nation's highest-intensity cold neutron source. This cold source, which will be comparable in intensity to the world's best at the Institut Laue–Langevin (ILL) in Grenoble, France, will support four neutron guides and instruments. The cold source building and refrigeration plant have been completed, and the guides and cold-source moderator vessel are in fabrication.

- **The Combustion Research Facility (CRF)** is supported by the Chemical Sciences subprogram.

  New capabilities brought on line. The CRF provides a primary interface for the integration of BES programs with those of DOE's Office of Energy Efficiency and Renewable Energy and Office of Fossil Energy related to combustion by collocating basic and applied research at one facility. Phase II of the CRF more than doubled the laboratory floor space to 37,000 square feet, increasing the number of labs to 37. The new wing houses unique instruments, such as picosecond lasers for diagnosing molecular energy transfer. The turbulent flame diagnostics laboratory, which has become an international standard, has been expanded to accommodate two simultaneous and independent experimental stations for visitors. The new laser-imaging laboratory has also been expanded to include several flame geometries with controlled, reproducible flow structures. New staff members have been or are being hired in theoretical chemistry, computer science, and experimental chemical dynamics.

PROGRAM SHIFTS

Materials Sciences

- **Initiation of programs in complex systems, the precursor to activities in nanoscale science, engineering, and technology.** An FY 2000 laboratory solicitation in complex systems began two new programs. The first, at Ames Laboratory, is on extraordinary responsive magnetic rare earth materials and will focus on new materials with enhanced magnetostriction, magnetoresistance, and magnetocaloric effects, i.e., on materials whose properties can change dramatically and reversibly with very small changes in temperature, pressure, or magnetic field. The research will focus on a fundamental understanding of the electronic and structural mechanisms for the changes. There is great potential for future use of these materials to control a variety of devices. The second project, at Argonne National Laboratory, is on laterally confined nanomagnetic materials. The goal is to understand how the physics changes and the ultimate limits of miniaturization and structural perfection are approached. Interactions between nanoscale elements and within the nanoscale elements will be studied. This work will provide the basis for new classes of electronic devices and ultimately, quantum computing.

Chemical Sciences

- **Initiation of programs in complex systems, the precursor to activities in nanoscale science, engineering, and technology.** An FY 2000 laboratory solicitation in complex systems began two new programs. The first, at Lawrence Berkeley National Laboratory, is a collaboration between chemists and bioscientists to understand the molecular origins of photosynthetic light capture and energy conversion mechanisms through the study of time-dependent spectroscopy of genetically modified algae and plants having altered light harvesting molecular complexes and pigment compositions. The second, at Oak Ridge National Laboratory in collaboration with partners at universities and other national laboratories, is a collaboration between chemists and geoscientists to understand the water-oxide interface through the study of specific interfaces and surfaces. This work is fundamental to advancing our knowledge of contaminant migration in the environmental, energy production, energy storage, and catalysis areas.

Scientific Facilities Utilization

The BES program request includes $310,279,000 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 maintained as close to that in FY 2001 as feasible. 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.

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 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 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.

Neutrons enable scientists studying the physical, chemical, and biological properties of materials to determine how atoms and molecules are arranged and how they move -- knowledge needed to understand and "engineer" materials at the atomic level so that they have improved macroscopic properties and perform better in new applications. 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.

Significant progress has been made on the Spallation Neutron Source project. The funding conditions stipulated in the House Report (Report 106-253, pages 113-114) accompanying the FY 2000 Energy and Water Development Appropriations Act were fulfilled, and FY 2000 construction funds were released at the end of February 2000. The Department approved the start of construction in November 1999 and site preparation began at Oak Ridge the following month. Site excavation and grading work has been completed, moving about 1.3 million cubic yards of earth. FY 2001 budget authority has been provided for conducting detailed design and for starting fabrication of the ion source, low-energy beam transport, linac structures and magnet systems, target assemblies, experimental instruments, and global control systems. Construction work will begin on several conventional facilities (buildings and accelerator tunnels).

FY 2002 funding of $291,400,000 (includes construction and other project costs) is requested to complete the ion source and continue component procurements for and fabrication of the linac structures and magnet systems, target assemblies, and the global controls. The assembly and testing of technical components will continue. Installation efforts will begin in the front end and the low energy sections of the linac. Title II design will continue for the target and experimental instruments. Work on conventional facilities will continue; some will reach completion and be turned over for equipment installation, such as the front end building, and portions of the klystron hall and linac tunnel.

Additional information on the SNS Project is provided in the SNS construction project data sheet, project number 99-E-334. The estimated Total Project Cost has remained constant at $1,411,700,000 and the construction schedule calls for project completion by mid-2006.

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 2,900 graduate students and postdoctoral investigators in FY 2000 through grants or contracts; 3,680 graduate students and postdoctoral investigators used the BES science user facilities in FY 2000.

Funding Profile

	(dollars in thousands)				
	FY 2000 Comparable Appropriation	FY 2001 Original Appropriation	FY 2001 Adjustments	FY 2001 Comparable Appropriation	FY 2002 Request
Basic Energy Sciences					
Research					
Materials Sciences	388,602	456,111	-12,869	443,242	434,353
Chemical Sciences	197,940	223,229	-6,703	216,526	218,714
Engineering and Geosciences .	35,639	40,816	-1,050	39,766	38,938
Energy Biosciences	29,850	33,714	-498	33,216	32,400
Subtotal, Research	652,031	753,870	-21,120	732,750	724,405
Construction	100,000	259,500	-571	258,929	280,300
Subtotal, Basic Energy Sciences	752,031 [a]	1,013,370	-21,691	991,679	1,004,705
General Reduction	0	-7,655	7,655	0	0
General Reduction for Safeguards and Security	0	-11,850	11,850	0	0
Omnibus Rescission	0	-2,186	2,186	0	0
Total, Basic Energy Sciences......	752,031 [b c]	991,679	0	991,679	1,004,705

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 $15,083,000 which has been transferred to the SBIR program and $905,000 which has been transferred to the STTR program.

[b] Includes $8,201,000 for Waste Management activities at Ames Laboratory and Argonne National Laboratory that were transferred from the Office of Environmental Management in FY 2001.

[c] Excludes $11,743,000 for Safeguards and Security activities transferred to consolidated Safeguards and Security program in FY 2001.

Funding by Site

	(dollars in thousands)				
	FY 2000	FY 2001	FY 2002	$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory	23,696	22,721	22,927	+206	+0.9%
National Renewable Energy Laboratory ..	5,177	4,873	4,535	-338	-6.9%
Sandia National Laboratories	23,740	22,967	22,843	-124	-0.5%
Total, Albuquerque Operations Office	52,613	50,561	50,305	-256	-0.5%
Chicago Operations Office					
Ames Laboratory	18,105	16,967	16,753	-214	-1.3%
Argonne National Laboratory – East........	151,026	155,902	159,149	+3,247	+2.1%
Brookhaven National Laboratory	73,569	72,005	57,089	-14,916	-20.7%
Chicago Operations Office.....................	93,708	84,792	84,173	-619	-0.7%
Princeton Plasma Physics Laboratory	561	0	0	--	--
Total, Chicago Operations Office...............	336,969	329,666	317,164	-12,502	-3.8%
Idaho Operations Office					
Idaho National Engineering and Environmental Laboratory	2,748	2,220	1,710	-510	-23.0%
Oakland Operations Office					
Lawrence Berkeley National Laboratory ..	65,048	70,760	72,586	+1,826	+2.6%
Lawrence Livermore National Laboratory	5,966	5,316	4,628	-688	-12.9%
Stanford Linear Accelerator Facility (SSRL)..	24,098	33,691	33,991	+300	+0.9%
Oakland Operations Office	37,334	34,693	34,588	-105	-0.3%
Total, Oakland Operations Office	132,446	144,460	145,793	+1,333	+0.9%
Oak Ridge Operations Office					
Oak Ridge Inst. For Science and Education	1,366	866	852	-14	-1.6%
Oak Ridge National Laboratory	212,663	370,312	384,317	+14,005	+3.8%
Total, Oak Ridge Operations Office	214,029	371,178	385,169	+13,991	+3.8%
Richland Operations Office					
Pacific Northwest National Laboratory	12,072	11,846	11,398	-448	-3.8%
Washington Headquarters	1,154	81,748	93,166	+11,418	+14.0%
Total, Basic Energy Sciences....................	752,031[abc]	991,679	1,004,705	+13,026	+1.3%

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[a] Excludes $15,083,000 which has been transferred to the SBIR program and $905,000 which has been transferred to the STTR program.

[b] Includes $8,201,000 for Waste Management activities at Ames Laboratory and Argonne National Laboratory that were transferred from the Office of Environmental Management in FY 2001.

[c] Excludes $11,743,000 for Safeguards and Security activities transferred to consolidated Safeguards and Security program in FY 2001.

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 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 subprogram supports studies of ultrafast spectroscopic techniques to examine energy transfer processes and studies of molecular beams to obtain highly accurate and precise thermochemical information for small molecules and radicals. Ames Laboratory provides leadership in analytical and separations chemistry with strength in catalysis.

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 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, 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 one of the largest BES research efforts, with 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 subprogram supports research in high-temperature superconductivity; polymeric superconductors; thin-film magnetism; surface science; the synthesis, characterization, and atomistic computer simulation of interfaces in advanced ceramic thin-films; the investigation of the effects of neutron, gamma, and ion-irradiation of solids; tribological investigation of the boundary films on aluminum and aluminum alloys; and synthesis and electronic and structural characterization of oxide ceramic materials, including high-temperature superconductors. The Chemical Sciences subprogram supports research in actinide separations; fundamental physical and chemical properties of actinide compounds; structural aspects fundamental to advanced electrochemical energy storage concepts and 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; and atomic, molecular, and optical physics. 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 Notre Dame University. The Engineering and

Geosciences subprogram supports geosciences research in computational microtomography of porous earth materials and in organic geochemistry related to hydrocarbon formation.

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. The CATs, groups of primarily industrial and university researchers, provided approximately $160 million to fund fabrication of the first 40 beamlines at the APS. These instruments attracted 1,527 users in FY 2000 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 APS is considering proposals for the remaining beamline ports, and it is expected that the facility will accommodate over 3,000 users annually when it fully matures. The high-quality, reliable x-ray beams at the APS have already brought about new discoveries in materials structure, encompassing a variety of technological applications including micromachining, lithography, medical insights and even new archaeological information.

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 a tandem accelerator 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 two microscopes permits direct, real-time, in-situ observation of the effects of ion and/or electron 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 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 the structure and composition of grain boundaries and interfaces in high temperature superconductors, in aqueous and galvanic corrosion studies, and in the theory of alloy phases.

The Chemical Sciences 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 an active research effort on studies of the mechanisms of electron transfer related to artificial photosynthesis. Other Chemical Sciences 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, and the formation of atmospheric aerosols and their reactivity.

The Energy Biosciences subprogram supports activities in the plant sciences, which include mechanistic and molecular-based studies on photosynthesis, lipid metabolism, and genetic systems. The studies on lipid biosynthesis may lead to exciting prospects for engineering new pathways for the synthesis of alternative fuels and petroleum-replacing chemicals. The Engineering and Geosciences subprogram supports synchrotron-based studies of rock-fluid interactions, particularly for investigations of diagenetic processes and synchrotron computed microtomography of porosity of reservoir rocks.

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 97% reliability 24 hours a day, seven days a week, with scheduled periods for maintenance and machine studies. In FY 2000, the NSLS served 2,551 researchers from universities, industry, and national laboratories. 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 electronics industry does R&D on semiconductors and develops x-ray lithography processes to produce future generations of computer chips with even smaller features than those presently produced using optical lithographic techniques.

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 Secretary of Energy Bill Richardson 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 will be completed in FY 2001. The permanent shut down of the HFBR has been a significant loss to the scientific community, and it 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 subprogram supports research in the modeling, growth, and properties of functionally gradient materials as an effective means of joining ceramic and metallic materials, on the microstructural evolution of rapidly solidified materials, and on high strength magnetic materials. The Chemical Sciences 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. The Engineering and Geosciences 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, to improve controls of nonlinear systems, and to develop new diagnostic techniques for engineering systems.

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 subprogram supports research in laser spectroscopy, superconductivity, thin films, femtosecond processes, x-ray optics, biopolymers, polymers and composites, surface science, and theory. Research is carried out on the fundamental features of evolving microstructures in solids; alloy-phase stability; structure and properties of transforming interfaces; the structures of magnetic, optical, and electrical thin films and coatings; processing, mechanical fatigue, and high-temperature corrosion of structure ceramics and ceramic coatings; and the synthesis, structure, and properties of advanced semiconductor and semiconductor-metal systems. The Chemical Sciences 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. The Engineering and Geosciences subprogram supports a broad spectrum of experimental and computational geosciences research 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. Engineering research is concerned with the development of modern nonlinear dynamics with applications to problems in engineering sciences. The Energy Biosciences subprogram focuses on the physics of the photosynthetic apparatus and on the genesis 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. The facility is home to the Nation’s highest voltage microscope, one that specializes in high-resolution studies.

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 subprogram supports research in metals and alloys, ceramics, materials for lasers, superplasticity in alloys, and intermetallic metals. The Engineering and Geosciences subprogram supports 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. The Chemical Sciences subprogram supports plasma assisted catalysis for environmental control of pollutants.

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 subprogram supports research on strongly correlated electronic materials; the theory of evolving microstructures; and plasma immersion processes for ion-beam processing of surfaces for improved hardness, corrosion resistance, and wear resistance. The Chemical Sciences 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. The BES Engineering and Geosciences subprogram supports experimental and theoretical geosciences research on rock physics, seismic imaging and the physics of the earth's magnetic field. It also supports fundamental geochemical studies of isotopic equilibrium/disequilibrium and mineral-fluid-microbial interactions in natural and anthropogenically perturbed systems. Engineering research supports work to study the viscosity of mixtures of particles in liquids.

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.

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 subprogram supports basic research efforts that underpin this technological emphasis at the Laboratory, for example on theoretical and experimental studies of properties of advanced semiconductor alloys for prototype solar cells. The Chemical Sciences 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 support for expert panel reviews of major new proposal competitions, external peer review of DOE laboratory programs, technical review of proposals for DOE's EPSCoR program, and EPSCoR site reviews and the evaluation of program needs and impacts. ORISE also assists in the compilation of annual BES subprogram summary books, the administration of topical scientific workshops, and provides support for other activities such as for the reviews of BES construction projects. ORISE manages the **Shared Research Equipment Program** (SHaRE) 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 subprogram supports basic research that underpins technological efforts such as those supported by the energy efficiency program. Research is 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. Research is carried out on the fundamentals of welding and joining and on welding strategies for a new generation of automobiles. 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.

The Chemical Sciences 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.

The Engineering and Geosciences subprogram investigates experimental and analytical geochemistry with innovative technical approaches for understanding low-temperature geochemical processes and rates in mineral-fluid systems. Engineering research provides support for computational nonlinear sciences such as advanced use of neural nets and sensor fusion, stochastic approximations, and global optimization of cooperating autonomous systems such as cooperating, auto-learning robots.

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.

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 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 by the Chemical Sciences subprogram. 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. Theoretical, ab-initio quantum molecular calculations are integrated with modeling and experiment. The Materials Sciences subprogram supports research on stress corrosion cracking of metals and alloys, high temperature corrosion fatigue of ceramic materials, and irradiation effects in ceramic materials relevant to radioactive waste containment. The Engineering and Geosciences program supports research on basic theoretical and experimental geochemical research that underpins technologies important for the Department's environmental missions and research to improve our understanding of the phase change phenomena in microchannels.

Sandia National Laboratories

Sandia National Laboratories (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 subprogram supports projects on the sol-gel processing and properties of ceramics; the development of nanocrystalline materials through the use of inverse micelles; adhesion and wetting of surfaces of metals, glass, and ceramic materials; theoretical and experimental research of defects; and interfaces in metals and alloys. The Engineering and Geosciences subprogram supports geosciences research on fundamental laboratory and theoretical studies 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. Engineering research addresses the viscosity of mixtures of particles in liquids.

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 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.

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 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.

All Other Sites

The BES program funds research at 157 colleges/universities located in 48 states. Also included are funds for research awaiting distribution pending completion of peer review results.

Materials Sciences

Mission Supporting Goals and Objectives

The Materials Sciences subprogram supports basic research in condensed matter physics, metal and ceramic sciences, and materials chemistry. This basic 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 metals, alloys, metallic glasses, ceramics, ceramic matrix composites, semiconductors, superconductors, magnetic materials, catalytic materials, polymers, surface science, neutron and x-ray scattering, chemical and physical properties, corrosion, non-destructive evaluation, 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. These material studies affect developments in numerous areas, such as the efficiency of electric motors and generators; solar energy conversion; batteries and fuel cells; stronger, lighter materials for vehicles; welding and joining of materials; plastics; and petroleum refining.

The Materials Sciences subprogram supports leading institutions and individuals. In particular, the large DOE laboratory programs consistently rank among the top materials sciences institutions worldwide. For example, Argonne National Laboratory, Lawrence Berkeley National Laboratory, University of Illinois (site of the Materials Research Laboratory), and Oak Ridge National Laboratory rank among the top 25 institutions *in the world* in the area of materials sciences based on citations of high-impact papers published (*Science Watch*, 1995). These international studies of high-impact papers from scientific journals typically survey more than 1,000 institutions, including universities, government laboratories, private research institutions, and industries.

Performance will be measured by continuing the new directions in the areas of nanoscale science, engineering, and technology research initiated in FY 2001, and explore concepts and designs for nanoscale science research centers.

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 2000	FY 2001	FY 2002	$ Change	% Change
Materials Sciences Research	175,796	202,977	208,984	+6,007	+3.0%
Waste Management	8,201	8,056	8,056	0	0%
Facilities Operations	204,605	221,963	207,454	-14,509	-6.5%
SBIR/STTR	0	10,246	9,859	-387	-3.8%
Total, Materials Sciences	388,602	443,242	434,353	-8,889	-2.0%

Detailed Program Justification

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Materials Sciences Research	**175,796**	**202,977**	**208,984**
▪ **Structure and Composition of Materials**	**26,092**	**28,236**	**28,236**

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 world-class 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.

In FY 2002, 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. To be at the cutting edge, instruments are needed for the determination of single-atom sensitivity to impurities, 3-dimensional shape with atomic accuracy, functional sites and the origin of the function, and optical absorption and emission from individual elements. Many of these advanced tools will come from the further development of current microscopies including scanning tunneling microscopy, confocal and near-field optical microscopy, atomic resolution transmission and scanning transmission electron microscopy, electron energy loss spectroscopy, cathodeluminescence and electron–beam–induced current imaging. However, new instruments are needed as well to image and characterize buried interfaces with nanoscale resolution; these new instruments must operate over a wide range of temperatures and environments.

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

	FY 2000	FY 2001	FY 2002
▪ **Mechanical Behavior and Radiation Effects**	**16,200**	**14,617**	**14,617**

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 physical 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. 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.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002

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. The scientific results of this program contribute to DOE missions in the areas of fossil energy, fusion energy, and radioactive waste storage.

In FY 2002, 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 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, high-pressure systems, and characterization instrumentation.

	FY 2000	FY 2001	FY 2002
▪ **Physical Behavior of Materials**...	**14,667**	**15,832**	**15,832**

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 2002, 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.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
▪ **Synthesis and Processing Science**	**13,820**	**14,781**	**14,781**

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.

In FY 2002, major activities will include work on thermally unstable systems and large-scale deformation and fracture phenomena. This research will include nanoscale films using epitaxial growth; synthesis of nanoparticles; patterned deposition of nanoparticles and clusters; processing of three-dimensional nanoscale structures and composites; and ion implanted nanostructures. The strength of structural elements and modes of failure also will change as the scale of devices and machines decreases toward the nanoscale. The causes of these changes include different mechanical properties that will modify fracture characteristics; the increased importance of surface tension; and, the enhanced role of diffusion and corrosion at the large surface-to-volume ratios that will occur.

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

	FY 2000	FY 2001	FY 2002
▪ **Neutron and X-ray Scattering**	**22,076**	**31,211**	**36,293**

This activity supports basic research in condensed matter 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 and excitations of materials, and the relationship of these structures and excitations to the physical properties of 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. Also included in this activity is the development of neutron and x-ray instrumentation for next generation sources.

The type of information derived from neutron and x-ray scattering is very diverse with inelastic scattering allowing measurements of elastic, magnetic, and charge excitations (phonons, magnons, crystal field energies) and elastic scattering affording structural information. X-ray scattering allows researchers to "see" where the atoms are since x-ray wavelengths are commensurate with interatomic distances. The dramatic increase in brilliance of synchrotron radiation sources has directly improved the available photon flux to probe a limited sample volume over a small time domain making in-situ experiments on nanoscale samples a reality. Neutron scattering can provide information concerning the positions, motions, and magnetic properties of solids. Neutrons possess unique properties such as sensitivity to light elements which has made the technique invaluable to polymer and biological sciences. Neutrons have magnetic moments and are thus uniquely sensitive probes of magnetic interactions. Taken together, neutron and x-ray scattering cover an enormous range of energies and allow multiple length scales and associated phenomena to be probed.

Included within this request are funds to increase neutron science activities in the U.S. based on three recent BESAC reviews that addressed: (1) 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; (2) the scientific output, the operational effectiveness, and the user programs at the three operating BES neutron scattering facilities; and (3) the impacts resulting from the permanent shutdown of the High Flux Beam Reactor and the strategies to address those impacts. The studies presented several common findings and recommendations, including the importance of establishing a large and well-trained user community by the time the SNS is fully operational in the 2008-2010 timeframe. In FY 2002, funding is increased by $5,802,000 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, including university proposals for instruments at the SNS in the range of $4,000,000 pending review.

	FY 2000	FY 2001	FY 2002
▪ **Experimental Condensed Matter Physics**	**30,785**	**34,326**	**34,326**

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 EE applied and developmental efforts. Research on magnetism and magnetic materials has more emphasis and direction than in other federally supported programs, focussing on hard magnet materials, such as those used for permanent magnets and in motors.

Major efforts in FY 2002 will include continued support for investigations of materials with increasingly complex behavior, composition, and structures. Extremely high quality crystals of transition metal oxides will be grown and subsequent high precision measurements of various physical properties will be made. There will be continued research on ferromagnetism, ferroelectricity, and superconductivity, because these have long been expected to demonstrate substantial changes when structures contain a small number of the relevant particles or when the system size is comparable to the particle size or the coherence length for collective behavior.

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

	FY 2000	FY 2001	FY 2002
▪ **Condensed Matter Theory**	**14,888**	**18,116**	**18,116**

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 though many unanswered questions remain. However, for more complex materials and hybrid structures, even the basic outlines of a theory describing these connections remains to be made. Stochastic simulation methods, as well as computational models incorporating quantum and semiclassical methods, are required to evaluate the performance of nanoscale devices. Consequently, computer simulations -- both electronic-structure-based and atomistic -- 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 those 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 2002, 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, modelling oxidation processes at surfaces and interfaces, and excited state electronic structure and response functions.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002

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

▪ **Materials Chemistry**	**25,353**	**27,823**	**27,823**

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, including research in 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 (NMR), and x-ray and neutron reflectometry. The activity also supports the development of new experimental techniques, such as high-resolution magnetic resonance imaging (MRI) 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 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 2002, the patterning of matter on the nanometer scale will continue to receive support. The controlled positioning of atoms within small molecules is of course routinely achieved by chemical synthesis. Nanometer-size objects are much larger entities, containing thousands or even millions of atoms. There are many powerful new 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 focuses on methods to prepare macroscopic quantities of nanoscale components in complex, designed patterns, using techniques of self-assembly.

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

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
▪ **Experimental Program to Stimulate Competitive Research** ...	**6,815**	**7,685**	**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, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, and the Commonwealth of Puerto Rico. In FY 2002, Hawaii and New Mexico will be included among the DOE EPSCoR states. 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. In FY 2001, an increase was provided to develop scientific manpower in the EPSCoR states through collaborative activities between faculty and students in EPSCoR states and staff in the extensive network of research laboratories and facilities in the Office of Science.

EPSCoR Distribution of Funds by State

	(dollars in thousands)		
	FY 2000	FY 2001 Estimate	FY 2002 Estimate
Alabama	225	425	375
Alaska[a]	0	0	0
Arkansas	90	110	65
Hawaii[b]	0	0	0
Idaho	162	113	60
Kansas	747	710	615
Kentucky	515	468	471
Louisiana	152	130	130
Maine	0	0	0
Mississippi	585	585	535
Montana	125	540	465
Nebraska	300	300	300
Nevada	466	370	325
New Mexico[b]	0	0	0
North Dakota	46	113	55
Oklahoma	100	165	65
Puerto Rico	65	435	435
South Carolina	855	870	120
South Dakota	50	0	0
Vermont	610	585	585
West Virginia	575	525	525
Wyoming	860	60	65
Technical Support	287	400	400
Other	0	781[c]	2,094[c]
Total	6,815	7,685	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 2001 and FY 2002 will be competed among all EPSCoR states.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
▪ **Los Alamos Neutron Science Center (LANSCE) instrumentation enhancement at the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center)**	**3,500**	**0**	**0**

This project is a major item of equipment with a revised total estimated cost of $12,500,000 -- down from the previous TEC of $20,500,000 -- to provide enhanced instrumentation at the Lujan Center. Instrument fabrication was implemented concurrently with an accelerator upgrade funded by the Office of Defense Programs. Two new neutron scattering instruments have been completed and are in different stages of assembly and commissioning. An Office of Science project review of the instrument project concluded that the two new instruments are "best in class." However, the recent BESAC review of the IPNS and the Lujan Center as well as the Office of Science project review of the instrument project concluded that the Lujan Center staff and LANSCE staff are seriously over committed. Based on these reviews, BES and LANL management agreed that the fabrication of the remaining two instruments originally planned for the Lujan Center should be stopped. As a result, the scope of this major item of equipment has been reduced. In order to maintain the communities of scientists who have come together to build these instruments, these instruments will be fabricated and located at the Intense Pulsed Neutron Source or other existing neutron scattering facilities. The Lujan Center remains a critical component of the Nation's neutron scattering capabilities, both in the short term and in the long-term. This change in instrument fabrication strategy does not change the BES or LANL commitment to this facility. Instrument upgrades and new instruments will be incorporated into future plans for this facility.

	FY 2000	FY 2001	FY 2002
▪ **Extension of HB-2 Beam Tube at the High Flux Isotope Reactor**..	**1,600**	**1,150**	**0**

This project is a major item of equipment with a total estimated cost of $5,550,000 that will provide beam access for six thermal neutron scattering instruments. Beam guides and optimized geometry will provide a neutron flux at the instrument positions 2-3 times higher than currently available. Completion of this MIE concludes the improvements that were undertaken at HFIR to improve neutron scattering capabilities during the reactor outage in FY 2000 and FY 2001 for the regularly scheduled (approximately every decade) replacement of the beryllium reflector. These improvements included installation of larger beam tubes and shutters for higher neutron flux on sample and fabrication and installation of a high-performance liquid hydrogen cold source to enable new classes of materials to be studied. **Performance will be measured** by maintaining cost and schedule within 10% of baselines.

	FY 2000	FY 2001	FY 2002
▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor**..	**0**	**0**	**2,000**

Capital equipment funds are provided for new and upgraded instrumentation, such as spectrometers, defractometers, and detectors. **Performance will be measured** by maintaining cost and schedule within 10% of baselines.

	FY 2000	FY 2001	FY 2002
	(dollars in thousands)		
▪ **SPEAR3 Upgrade**	**0**	**8,300**	**8,300**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade 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 is expected to provide $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.

▪ **Advanced Light Source Beamline**	**0**	**900**	**975**

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 Subprogram and the Chemical Sciences Subprogram. **Performance will be measured** by maintaining cost and schedule within 10% of baselines.

Waste Management	**8,201**	**8,056**	**8,056**

These funds will be provided for disposal of wastes from current activities at ANL and Ames. This activity was funded by Environmental Management prior to FY 2001.

Facilities Operations	**204,605**	**221,963**	**207,454**
▪ **Operation of National User Facilities**	**185,727**	**206,622**	**207,454**

The facilities included in Materials Sciences 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 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

	(dollars in thousands)	
FY 2000	FY 2001	FY 2002

reactor facilities that are supported in the Materials Sciences subprogram. Included in the AIP funding are funds for HFIR for the extension of the Neutron Sciences Support Building and for general infrastructure upgrades. 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 subprogram is provided below. Additional funds for facility operations for some of these facilities are included in the Chemical Sciences subprogram of this budget. **Performance will be measured** by maintaining and operating these user facilities so that the unscheduled downtime, on average, is less than 10% of the total scheduled operating time, as reported to Headquarters by facilities at the end of each fiscal year. For the Spallation Neutron Source, **performance will be measured** by maintaining cost and schedule of construction within 10% of baselines as reflected by regular independent reviews of the cost and schedule milestones. **Performance will be measured** by improving U.S. research in neutron science in preparation for the commissioning of the SNS by ensuring that BES neutron facilities are optimally available to the scientific community and by investing in instrumentation for the future.

- **High Flux Beam Reactor (HFBR)**... **18,878** **15,341** **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 2000	FY 2001	FY 2002
Facilities			
Advanced Light Source	30,652	35,605	37,605
Advanced Photon Source	84,783	90,314	90,314
National Synchrotron Light Source	23,174	26,907	26,907
Stanford Synchrotron Radiation Laboratory	3,992	3,858	3,858
High Flux Beam Reactor	18,878	15,341	0
High Flux Isotope Reactor	5,519	8,209	8,400
Intense Pulsed Neutron Source	12,739	13,480	16,080
Manuel Lujan, Jr. Neutron Scattering Center	6,968	9,190	9,190
Spallation Neutron Source	17,900	19,059	15,100
Total, Facilities	204,605	221,963	207,454

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
SBIR/STTR Funding	**0**	**10,246**	**9,859**

In FY 2000, $9,009,000 and $541,000 were transferred to the SBIR and STTR programs, respectively. The FY 2001 and FY 2002 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

Total, Materials Sciences...	**388,602**	**443,242**	**434,353**

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2002 vs. FY 2001 ($000)
Materials Sciences Research	
▪ Increase for neutron and x-ray scattering. This increase results from funds previously used for the support of the operations of the High Flux Beam Reactor. Funding is provided for a number of activities, including increased support for academic scientists to participate in the development of neutron scattering instruments and increased support 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.	+5,082
▪ Decrease in capital equipment funds for the Extension of HB-2 beam tube MIE at HFIR for thermal neutron scattering due to completion of project	-1,150
▪ Increase for neutron scattering instrumentation at HFIR, such as spectrometers, defractometers, and detectors...	+2,000
▪ Increase in capital equipment funds for the ALS Beamline MIE per approved profile	+75
Total, Materials Sciences Research..	+6,007
Facilities Operations	
▪ Increase support for HFIR. Includes a decrease for HFIR operations (-$1,619,000) which is offset by an increase of $1,316,000 for HFIR operations under the Chemical Sciences subprogram. Overall support for HFIR operations decreases by $303,000 due to decreased requirements associated with the tritium release. An increase in AIP for HFIR for extension of the Neutron Sciences Support Building, instrumentation and general infrastructure upgrades (+$2,210,000), and a decrease in GPP for the HFIR due to decreased needs (-$400,000).	+191

	FY 2002 vs. FY 2001 ($000)
▪ Increase for the Intense Pulsed Neutron Source for operations in response to a BESAC subpanel review recommendation to increase operating hours and user support.	+2,600
▪ Increase for the Advanced Light Source for equipment, such as spectrometers, defractometers, and improvements in insertion devices.	+2,000
▪ Termination of support for the operations of the HFBR. Responsibility has been transferred from SC to the Office of Environmental Management for surveillance and decommissioning.	-15,341
▪ Decrease in the Spallation Neutron Source research and development funds per FY 2002 project datasheet	-3,959
Total, Facilities Operations.	-14,509
SBIR/STTR	
▪ Decrease in SBIR/STTR funding because of decrease in operating expenses	-387
Total Funding Change, Materials Sciences	-8,889

Chemical Sciences

Mission Supporting Goals and Objectives

The Chemical Sciences subprogram supports a major portion of the Nation's fundamental research in the chemical sciences. The research covers a broad spectrum of the chemical sciences including atomic, molecular and optical (AMO) science; chemical physics; photo- and radiation chemistry; physical chemistry; inorganic chemistry; organic chemistry; analytical chemistry; separation science; heavy element chemistry; and aspects of chemical engineering sciences. This research provides a foundation for fundamental understanding of the interactions of atoms, molecules, and ions with photons and electrons; the making and breaking of chemical bonds in gas phase, in solutions, at interfaces, and on surfaces; and understanding the energy transfer processes within and between molecules. This work underpins our fundamental understanding of chemical reactivity. In turn, this enables the production of more efficient combustion systems with reduced emissions of pollutants. It also increases knowledge of solar photoconversion processes resulting in new, improved systems and production methods. This research has resulted in improvements to catalytic systems, new catalysts for the production of fuels and chemicals, and better analytical methods for a wide variety of applications in energy processes. It also provides new knowledge of actinide elements and separations important for environmental remediation and waste management. Finally, it provides better methods for describing turbulent combustion and predicting thermophysical properties of multicomponent systems.

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 2000	FY 2001	FY 2002	$ Change	% Change
Chemical Sciences Research	127,650	145,981	145,793	-188	-0.1%
Facilities Operations	70,290	65,595	67,911	+2,316	+3.5%
SBIR/STTR	0	4,950	5,010	+60	+1.2%
Total, Chemical Sciences	197,940	216,526	218,714	+2,188	+1.0%

Detailed Program Justification

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Chemical Sciences Research	**127,650**	**145,981**	**145,793**
▪ **Atomic, Molecular, and Optical (AMO) Science**	**10,765**	**11,887**	**11,887**

This activity supports theory and experiment 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.

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 2002 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.

▪ **Chemical Physics Research**	**25,019**	**32,647**	**33,488**

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 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 is the Nation's principal supporter of high temperature chemical kinetics and gas phase chemical physics. The Chemical Dynamics Beamline at the Advanced Light Source is run as a national resource. The Combustion Research Facility is home to the foremost fundamental research program on laser-based optical diagnostics for the measurement of chemical and fluid-mechanical parameters.

Work in FY 2002 will emphasize atomic and molecular clusters, which provide a basis for relating detailed, extended structures to the chemistry of molecules and molecular fragments with which they come into contact. Emerging capabilities for locating single molecules on metal surfaces and measuring their properties while on the surface open the way for developing detailed models for surface chemistry. The increased effort reflects a realignment of activities previously funded in chemical energy and chemical engineering that focused on modeling of heat transfer in combustion systems. These activities have developed in directions that incorporate an integrated molecular level focus. Shifting these activities to chemical physics reflects the coordination of theory and modeling that has developed in recent years.

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

	FY 2000	FY 2001	FY 2002
▪ **Photochemistry and Radiation Research**.................................	**23,731**	**26,167**	**26,167**

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, which features cobalt-60 gamma irradiators, a van de Graaff-ESR and resonance Raman, and a linear accelerator for electron pulse radiolysis experiments.

Photochemistry research supports conversion of light energy to electrical or chemical energy, based on light-induced charge separation at semiconductor/liquid interfaces or in molecular biomimetic assemblies. 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. Radiation science research supports fundamental chemical effects produced by the absorption of energy from ionizing radiation. This research provides information on transients in solution and intermediates at liquid/solid interfaces for resolving important issues in solar energy conversion, environmental waste management and remediation; and intermediates relevant to nuclear energy production.

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

For FY 2002 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 2000	FY 2001	FY 2002
▪ **Catalysis and Chemical Transformation**	**23,125**	**24,929**	**24,929**

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. 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. Results from a fundamental, molecular-level understanding of the syntheses of advanced catalytic materials have the potential of providing new chemicals or materials that can be fabricated with greater energy efficiency or function as energy-saving media themselves.

This activity is the Nation's major supporter of catalysis research, and it is the only activity that treats catalysis as a discipline integrating all aspects of homogeneous and heterogeneous catalysis research.

In FY 2002 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 surface catalyzed 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 clusters both in solution as well as dispersed supports. 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 2000	FY 2001	FY 2002
▪ **Separations and Analyses**	**12,255**	**12,747**	**13,047**

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.

Chemical separations are ubiquitous in Department missions and in industry. An analysis is an essential component of every chemical process from manufacture through safety and risk assessment and environmental protection. 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 clean-up mission; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important components of the portfolio.

Increased funding in FY 2002 will emphasize new opportunities in single-molecule detection for the study of molecule-molecule, molecule-membrane, and molecule-surface interactions.

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

	FY 2000	FY 2001	FY 2002
▪ **Heavy Element Chemistry**	**6,753**	**7,410**	**7,685**

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.

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.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002

Approximately twenty undergraduate students chosen from universities and colleges throughout the U.S. are given introductory lectures in actinide and radiochemistry each summer.

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.

Increased funding will enable new opportunities for FY 2002 in the emerging areas of actinide molecular speciation and reactivity and in advanced theoretical and computational methods for prediction of electronic and molecular structure of actinide complexes.

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 2000	FY 2001	FY 2002
▪ **Chemical Energy and Chemical Engineering**	**9,891**	**11,989**	**11,020**

This activity supports research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes. Emphasis is given to improving and/or developing the scientific base for engineering generalizations and their unifying theories. 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

There are strong links with related efforts within the Department and other federal agencies through the Interagency Power Working Group.

For FY 2002, decreased funding reflects the shift of combustion modeling efforts to the chemical physics activity. 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.

	FY 2000	FY 2001	FY 2002
▪ **General Plant Projects (GPP)**	**10,275**	**11,550**	**11,840**

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. The total estimated cost of each GPP project will not exceed $5,000,000.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
▪ **General Purpose Equipment (GPE)**	**5,086**	**4,055**	**4,055**

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**	**0**	**1,700**	**700**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade 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 is expected to provide $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.

▪ **Advanced Light Source Beamline**	**750**	**900**	**975**

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 subprogram and the Chemical Sciences subprogram. **Performance will be measured** by maintaining cost and schedule within 10% of baselines.

Facilities Operations	**70,290**	**65,595**	**67,911**

The facilities included in Chemical Sciences are: National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory, High Flux Isotope Reactor, Radiochemical Engineering Development Center, and Combustion Research Facility. The facility operations budget request, which includes operating funds, capital equipment, general plant projects, and AIP funding under $5,000,000, is

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002

described in a consolidated manner later in this budget. A summary table of the facilities included in this Chemical Sciences subprogram is provided below. Additional funds for facility operations for some of these facilities are included in the Materials Sciences subprogram of this budget. **Performance will be measured** by maintaining and operating these user facilities so that the unscheduled downtime, on average, is less than 10% of the total scheduled operating time, as reported to Headquarters by facilities at the end of each fiscal year.

AIP funding will support additions and modifications to accelerator and reactor facilities, which are supported in the Chemical Sciences 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 for the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front-end components, monochromators, and power supplies.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Facilities			
National Synchrotron Light Source	7,781	7,813	7,813
Stanford Synchrotron Radiation Laboratory	18,749	16,838	17,838
High Flux Isotope Reactor	32,215	28,769	30,085
Radiochemical Engineering Development Center	6,809	6,712	6,712
Combustion Research Facility	4,736	5,463	5,463
Total, Facilities	70,290	65,595	67,911

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
SBIR/STTR Funding	**0**	**4,950**	**5,010**

In FY 2000, $4,435,000 and $266,000 were transferred to the SBIR and STTR programs, respectively. The FY 2001 and FY 2002 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

Total, Chemical Sciences	**197,940**	**216,526**	**218,714**

Explanation of Funding Changes from FY 2001 to FY 2002

	FY 2002 vs. FY 2001 ($000)
Chemical Sciences Research	
▪ Increase in funding for chemical physics reflects a transfer of activities previously funded in chemical energy and chemical engineering that focused on modeling of heat transfer in combustion systems. These efforts are maintained at the FY 2001 level.	+841
▪ Increase in research for separations and analysis to emphasize new opportunities in single-molecule detection for the study of molecule-molecule, molecule-membrane, and molecule-surface interactions.	+300
▪ Increase in research for heavy element chemistry to enable new opportunities in the emerging areas of actinide molecular speciation and reactivity and in advanced theoretical and computational methods for prediction of electronic and molecular structure of actinide complexes.	+275
▪ Decrease in funding for chemical energy and chemical engineering reflects the shift of combustion modeling efforts to the chemical physics activity.	-969
▪ Decrease in capital equipment funding for the SPEAR3 Upgrade MIE per approved funding profile	-1,000
▪ Increase in General Plant Projects	+290
▪ Increase in capital equipment funding for the ALS Beamline MIE per approved funding profile	+75
Total, Chemical Sciences Research	-188
Facilities Operations	
▪ Increase for the Stanford Synchrotron Radiation Laboratory for operations.	+1,000
▪ Increase for the High Flux Isotope Reactor (HFIR) for operations. This increase is offset by a decrease of $1,619,000 for HFIR operations under the Materials Sciences subprogram. Overall support for HFIR operations decreases by $303,000 due to decreased requirements associated with the tritium release	+1,316
Total, Chemical Sciences Facilities	+2,316
SBIR/STTR	
▪ Increase SBIR/STTR funding because of increase in operating expenses.	+60
Total Funding Change, Chemical Sciences	+2,188

Engineering and Geosciences

Mission Supporting Goals and Objectives

Engineering research supports basic research in nanotechnology and microsystems; multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. New capabilities at the nano and micro scale will improve materials processing and quality, increase computing speed, improve sensing and control capabilities; together these lead to higher process efficiency and lower energy consumption. Improving the knowledge base on multi-components fluid dynamics and heat transfer will have a major impact on energy consumption, because these phenomena are an integral part of every industrial process. Advances in non-linear dynamics will lead to improved control and predictive capabilities of complex systems, thus resulting in higher efficiency and lower energy consumption. These activities are closely coordinated with work in the Materials Sciences subprogram, particularly with the Structure and Composition of Materials, Mechanical Behavior and Radiation Effects, Physical Behavior, and Synthesis and Processing activities.

Geosciences research supports basic research in geochemistry and geophysics emphasizing solid earth sciences. The geochemistry research focuses on advanced investigations of mineral-fluid interactions. Work includes studies on rates and mechanisms of reaction, coupled reactive fluid flow, and isotopic tracking of mineral-fluid interactions. The geophysics research focuses on developing an improved understanding of rock, fluid, and fracture physical properties. It includes studies on the surface determination of geologic structures and rock property distributions at depth; improved methods of collection, inversion, analysis of seismic and electromagnetic data; and identification of geophysical signatures of natural and man-made heterogeneities such as fractures, and fluid flow pathways. Also studied are the mechanical stability of geological reservoirs, multi phase flows within aquifers, geochemical reactivity and geophysical imaging; these areas provide fundamental scientific foundations to sequestration science associated with geological formations. The geosciences activity represents one third of the Nation's total federal support for investigator-driven basic research in solid earth sciences. It provides the majority of support in the federal government for basic research related to unique DOE missions, such as high-resolution shallow earth imaging and geochemical processes in the shallow subsurface. As such, it provides the scientific foundation for the multiple earth science-related mission activities in DOE applied programs.

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

Funding Schedule

(dollars in thousands)

	FY 2000	FY 2001	FY 2002	$ Change	% Change
Engineering Research	14,024	17,383	16,577	-806	-4.6%
Geosciences Research	21,615	21,387	21,387	0	0%
SBIR/STTR	0	996	974	-22	-2.2%
Total, Engineering and Geosciences	35,639	39,766	38,938	-828	-2.1%

Detailed Program Justification

(dollars in thousands)

	FY 2000	FY 2001	FY 2002
Engineering Research	**14,024**	**17,383**	**16,577**

This activity focuses on nanotechnology and microsystems; multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. 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; data and engineering analysis; and robotics and intelligent machines.

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. Activities in the control and optimization of robotics and intelligent machines focuses on missions in dynamic, uncertain and extreme environments, sensor fusion and integration for distributive robot systems, collaborative research using remote and virtual systems, intelligent machine controls, and improved remote operation of SC strategic facilities to meet programmatic goals.

In FY 2002, there will be small decreases in research in the areas of fluid dynamics, control systems, sensors, and sensor integration.

	FY 2000	FY 2001	FY 2002
Geosciences Research	**21,615**	**21,387**	**21,387**

The Geosciences subprogram supports long term basic research in geochemistry and geophysics. Geochemical research focuses on fundamental understanding of and the ability to predict subsurface solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. The range of geochemical knowledge needed to impact energy and environmental technologies ranges from the molecular levels to the field scale.

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 research enables the advancement in remote imaging of subsurface properties. These studies provide the fundamental science base for new

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002

capabilities to locate and monitor oil and gas reservoirs, contaminant migration and for characterizing disposal sites for energy related wastes. Improved understanding of earth processes is required to quantitatively predict the response of earth systems to natural and man-made perturbations. Research also seeks to understand the fundamental geological processes that impact concepts for sequestration of carbon dioxide in subsurface reservoirs.

	FY 2000	FY 2001	FY 2002
SBIR/STTR Funding	**0**	**996**	**974**

In FY 2000, $885,000 and $53,000 were transferred to the SBIR and STTR programs, respectively. The FY 2001 and FY 2002 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

	FY 2000	FY 2001	FY 2002
Total, Engineering and Geosciences	**35,639**	**39,766**	**38,938**

Explanation of Funding Changes from FY 2001 to FY 2002

	FY 2002 vs. FY 2001 ($000)
Engineering Research	
▪ Decrease in engineering research in areas of fluid dynamics, control systems, sensors, and sensor integration.	-806
SBIR/STTR	
▪ Decrease in SBIR/STTR funding because of decrease in operating expenses.	-22
Total Funding Change, Engineering and Geosciences	-828

Energy Biosciences

Mission Supporting Goals and Objectives

The Energy Biosciences subprogram supports fundamental research in the plant and microbial sciences to create the science base to develop future energy-related biotechnologies. The program supports research in a number of topic areas. These include fundamental molecular level understanding of solar energy capture by plants and microbes through photosynthesis; the genetic regulation of carbon fixation and carbon/energy storage; metabolic pathways for biological synthesis, degradation and molecular inter-conversions of energy-rich organic compounds and polymers; the regulation of plant growth and development. The subprogram also provides a fundamental biological research base to interface with traditional disciplines in the physical sciences. There are connections with research activities in each of the other BES subprograms, including, for example, materials sciences and engineering at the nanoscale; materials chemistry; photochemistry; biomaterials synthesis; and biogeochemistry.

Plant genome research will continue developing knowledge gained from sequencing efforts to characterize gene sets involved in specific metabolic and intermediary pathways and networks, providing a foundation for future control and manipulation of plant genetic resources. Research on the microbial cell will focus on understanding the complete physiological and biochemical roles of the genes required for growth and specific bioprocesses. This information will enable the control, modification, and use of microbes for both natural and industrial energy-related applications.

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

Funding Schedule

(dollars in thousands)

	FY 2000	FY 2001	FY 2002	$ Change	% Change
Energy Biosciences	29,850	32,353	31,559	-794	-2.5%
SBIR/STTR	0	863	841	-22	-2.5%
Total, Energy Biosciences	29,850	33,216	32,400	-816	-2.5%

Detailed Program Justification

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Energy Biosciences Research	**29,850**	**32,353**	**31,559**
▪ **Molecular Mechanisms of Energy Conversion**	**12.760**	**12,554**	**12,221**

This activity supports fundamental research to characterize the molecular mechanisms involved in the conversion of solar energy to biomass, biofuels, bioproducts, and other renewable energy resources. Research supported includes the characterization of the energy transfer processes occurring during photosynthesis, the kinetic and catalytic mechanisms of enzymes involved in the synthesis of methane, the biochemical mechanisms involved in the synthesis and degradation of lignocellulosics, and the mechanisms of plant oil production. The approaches used include biophysical, biochemical, and molecular genetic analyses. The goal is to enable the future biotechnological exploitation of these processes and, also, to provide insights and strategies into the design of non-biological processes. This activity also encourages fundamental research in the biological sciences that interfaces with other traditional disciplines in the physical sciences. In FY 2002, funding decreases reduce support for fundamental kinetic studies of enzyme catalyzed reactions.

▪ **Metabolic Regulation of Energy Production**	**17,090**	**17,391**	**16,930**

This activity supports fundamental research in regulation of metabolic pathways and the integration of multiple pathways that constitute cellular function in plants and microbes. Plants and microorganism have the capacity to synthesize an almost limitless variety of energy-rich organic compounds and polymers. Research supported includes the identification of genes and gene families in relation mechanisms of enzyme activity and the control of metabolic and signaling pathways of energy related pathways in plants. The goal is to understand entire gene expression profiles in response to developmental, environmental and metabolic requirements. Knowledge gained from plant and microbial gene sequencing, functional genomics and traditional molecular genetic, biochemical and biophysical studies will be integrated to address these goals. Plants and microbes are important commercial sources of materials such as cellulose (paper and wood), starch, sugars, oils, waxes, a variety of biopolymers, and many other biofuels and energy rich biomaterials. Thus, a basic understanding of plant and microbe cellular function has great ramifications for efficient energy utilization and renewal. In FY 2002, decreased funding will reduce support for studies on gene expression in response to environmental factors.

Major activities in FY 2002 will include functional genomic analysis of the *Arabidopsis* genome and continued use of *Arabidopsis* as a model system for the study of other plant systems with broader utility. Microbial research will include the molecular genetic, physiological, and biochemical characterization of the regulation and synthesis of components underlying energy relevant processes.

	FY 2000	FY 2001	FY 2002
(dollars in thousands)			
▪ **Microbial Cell Research**	**0**	**2,408**	**2,408**

This activity supports fundamental research to understand reactions, pathways, and regulatory networks involved in bioprocesses relevant to the DOE mission, such as cellulose degradation; carbon sequestration; the production, conversion, or conservation of energy (e.g. fuels, chemicals, and chemical feedstocks); and the bioremediation of metals and radionuclides from contaminated sites. Research areas of particular interest include biochemical and physiological characterization of components involved in energy-related bioprocesses; intracellular localization of proteins and metabolites; microbial cell modeling; and functional analysis of the microbial proteome. Research will focus on such physiological processes as extracellular polymer degradation, photoautotrophy, cell movement, syntrophic or synergistic interactions with other bacterial, and responses to external physical stresses. Of particular scientific interest is understanding how individual genes (or gene families) and their encoded bioprocesses interact at the molecular level to permit control and stability in the entire microbial cell. This activity combines the strengths of the Energy Biosciences subprogram in biochemistry and physiology with the strengths of the Biological and Environmental Research program in genomics, structural biology and computational biology in a coordinated activity.

	FY 2000	FY 2001	FY 2002
SBIR/STTR Funding	**0**	**863**	**841**

Amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

	FY 2000	FY 2001	FY 2002
Total, Energy Biosciences	**29,850**	**33,216**	**32,400**

Explanation of Funding Changes from FY 2001 to FY 2002

	FY 2002 vs. FY 2001 ($000)
Energy Biosciences Research	
▪ Decrease in molecular mechanisms reduces support for fundamental kinetic studies of enzyme catalyzed reactions.	-333
▪ Decrease in metabolic regulation reduces support for studies on gene expression in response to environmental factors.	-461
▪ Decrease in SBIR/STTR because of decrease in operating expenses.	-22
Total Funding Change, Energy Biosciences	-816

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 2000	FY 2001	FY 2002	$ Change	% Change
Construction, SNS	100,000	258,929	276,300	+17,371	+6.7%
Project Engineering Design	0	0	4,000	+4,000	+100.0%
Total, Construction	100,000	258,929	280,300	+21,371	+8.3%

Detailed Program Justification

(dollars in thousands)

	FY 2000	FY 2001	FY 2002
Construction	**100,000**	**258,929**	**280,300**
Spallation Neutron Source	**100,000**	**258,929**	**276,300**

FY 2002 budget authority is requested to complete the ion source and continue component procurements for and fabrication of the linac structures and magnet systems, target assemblies, and the global controls. The assembly and testing of technical components will continue. Installation efforts will begin in the front end and the low energy sections of the linac. Title II design will continue for the target and experimental instruments. Work on conventional facilities will continue; some will reach completion and be turned over for equipment installation, such as the front end building, and portions of the klystron hall and linac tunnel. **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.

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Project Engineering Design...	**0**	**0**	**4,000**

FY 2002 budget authority is requested to provide Title I and Title II design-only funding for Nanoscale Science Research Centers (NSRCs) 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.

Explanation of Funding Changes from FY 2001 to FY 2002

	FY 2002 vs. FY 2001 ($000)
Construction	
▪ The increase in funding for the Spallation Neutron Source represents the scheduled ramp up of activities.	+17,371
▪ Increase in funding for Project Engineering Design related to design-only activities for Nanoscale Science Research Centers.	+4,000
Total Funding Change, Construction...	+21,371

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 Chemical Sciences subprograms.

	(dollars in thousands)				
	FY 2000	FY 2001	FY 2002	$ Change	% Change
Advanced Light Source	30,652	35,605	37,605	+2,000	+5.6%
Advanced Photon Source	84,783	90,314	90,314	0	0%
National Synchrotron Light Source	30,955	34,720	34,720	0	0%
Stanford Synchrotron Radiation Laboratory	22,741	20,696	21,696	+1,000	+4.8%
High Flux Beam Reactor	18,878	15,341	0	-15,341	-100.0%
High Flux Isotope Reactor	37,734	36,978	38,485	+1,507	+4.1%
Radiochemical Engineering Development Center	6,809	6,712	6,712	0	0%
Intense Pulsed Neutron Source	12,739	13,480	16,080	+2,600	+19.3%
Manuel Lujan, Jr. Neutron Scattering Center	6,968	9,190	9,190	0	0%
Spallation Neutron Source	17,900	19,059	15,100	-3,959	-20.8%
Combustion Research Facility	4,736	5,463	5,463	0	0%
Total, Major User Facilities	274,895	287,558	275,365	-12,193	-4.2%

Detailed Program Justification

	(dollars in thousands)		
	FY 2000	FY 2001	FY 2002
Major User Facilities	**274,895**	**287,558**	**275,365**
▪ Advanced Light Source at Lawrence Berkeley National Laboratory.	**30,652**	**35,605**	**37,605**
▪ Advanced Photon Source at Argonne National Laboratory.	**84,783**	**90,314**	**90,314**
▪ National Synchrotron Light Source at Brookhaven National Laboratory.	**30,955**	**34,720**	**34,720**
▪ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.	**22,741**	**20,696**	**21,696**
▪ 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.	**18,878**	**15,341**	**0**
▪ High Flux Isotope Reactor at Oak Ridge National Laboratory.	**37,734**	**36,978**	**38,485**
▪ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	**6,809**	**6,712**	**6,712**
▪ Intense Pulsed Neutron Source at Argonne National Laboratory.	**12,739**	**13,480**	**16,080**
▪ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	**6,968**	**9,190**	**9,190**
▪ Spallation Neutron Source at Oak Ridge National Laboratory.	**17,900**	**19,059**	**15,100**
▪ Combustion Research Facility at Sandia National Laboratories/California.	**4,736**	**5,463**	**5,463**
Total, Major User Facilities	**274,895**	**287,558**	**275,365**

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 2000	FY 2001	FY 2002	$ Change	% Change
General Plant Projects	10,622	12,300	12,190	-110	-0.9%
Accelerator Improvement Projects	11,816	9,435	11,645	+2,210	+23.4%
Capital Equipment	47,416	59,340	62,940	+3,600	+6.1%
Total, Capital Operating Expenses	69,854	81,075	86,775	+5,700	+7.0%

Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2000	FY 2001	FY 2002	Unapprop-riated Balances
99-E-334 Spallation Neutron Source, ORNL	1,192,700	101,400	100,000	258,929	276,300	456,071
02-SC-002 PED, Nanoscale Science Research Centers	14,000 [a]	0	0	0	4,000	10,000
Total, Construction		101,400	100,000	258,929	280,300	466,071

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

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 2000	FY 2001	FY 2002 Request	Accept-ance Date
Short Pulse Spallation Upgrade at LANSCE – LANL	12,500	9,000	3,500	0	0	FY 2002
HB-2 Beam Tube Extension at HFIR - ORNL	5,550	2,800	1,600	1,150	0	FY 2001
SPEAR3 Upgrade	29,000 [b]	0	0	10,000	9,000	FY 2003
ALS Beamline	6,000	1,500	750	1,800	1,950	FY 2003
Total, Major Items of Equipment		13,300	5,850	12,950	10,950	

[a] The full Total Estimated Cost (design and construction) ranges between $220,000,000 and $330,000,000. This estimate is based on conceptual data and should not be construed as a project baseline.

[b] 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 2001 Congressional Budget Request are denoted with a vertical line in the left margin.)

1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost ($000)	Total Project Cost ($000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 1999 Budget Request (*Preliminary Estimate)*	1Q 1999	4Q 2003	3Q 2000	4Q 2005	1,138,800	1,332,800
FY 2000 Budget Request	1Q 1999	4Q 2003	3Q 2000	1Q 2006	1,159,500	1,360,000
FY 2001 Budget Request	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,220,000	1,440,000
FY 2001 Budget Request (*Amended*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2002 Budget Request (*Current Estimate*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700

2. Financial Schedule

(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	228,506
2002	276,300	276,300	285,600
2003	210,571	210,571	231,600
2004	124,600	124,600	143,000
2005	79,800	79,800	94,800
2006	41,100	41,100	66,512

3. Project Description, Justification and Scope

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.

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 means 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.

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 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. In order to keep pace with the current state-of-the-art in scientific instruments, the average cost per instrument has roughly doubled in recent years. Although this translates into fewer than the ten instruments originally envisioned in the TEC, there will be no sacrifice in scientific capability. 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.

The FY 2000 budget authority provided for completing most preliminary (Title I) design activities and starting detailed (Title II) design, construction site preparation, long-lead hardware procurement, and continued critical research and development work necessary to reduce technical and schedule risks.

FY 2001 budget authority is being used for conducting detailed design and starting fabrication of the ion source, low-energy beam transport, linac structures and magnet systems, target assemblies, experimental instruments and global control systems. Construction work will include site preparation, the beginning of several conventional facilities, and the completion of roads into the site.

FY 2002 budget authority is being requested to complete the ion source and continue component procurements for and fabrication of the linac structures and magnet systems, target assemblies, and the global controls. The assembly and testing of technical components will continue and installation efforts will begin in the front end, and the low energy sections of the linac. Title II design will continue for the target and experimental instruments. Several conventional facilities will be turned over for equipment installation: such as the front end building, portions of the klystron hall, and the linac tunnel.

The House Report (Report 106-253, pages 113-114) accompanying the FY 2000 Energy and Water Development Appropriations Act stipulated prerequisites to commitment of appropriated funds for the SNS project, and established a requirement for an annual status report for the project which is incorporated into this project data sheet. All conditions for commitment of funds were satisfied, and FY 2000 construction funds were released at the end of February 2000. The SNS Project has made significant progress. Site excavation began at Oak Ridge in April. At the end of FY 2000, the project was 14 percent complete (15 percent planned); had expended $225,000,000 ($221,000,000 planned); and was on schedule and budget for completion in June 2006 at a Total Project Cost of $1,411,700,000. Site preparation was well underway with 1.1 of 1.3 million cubic yards of earth moved, one access road complete and the second being prepared for paving. Title I design was nearly complete, and prototype equipment was being assembled for the ion source, linac, ring, target, and instruments. Preliminary safety documents for the facility had been prepared, and site construction was proceeding without a reportable injury. FY 2001 budget authority has been provided for 1) conducting detailed design; 2) beginning fabrication of the ion source, low-energy beam transport, linac structures and magnet systems, target assemblies, experimental instruments, and global control systems; and 3) beginning construction on several conventional facilities (buildings and accelerator tunnels). The project remains on-track for completion consistent with the baseline; Total Project Cost of $1,411,700,000 completion by June 2006, and with the capability of providing at least 1 MW of proton beam power on target.

4. Details of Cost Estimate.

(dollars in thousands)

	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 27% of construction costs	179,400	127,100
Construction management at approximately 3% of construction costs	20,400	15,400
Project management at approximately 18% of construction costs	121,800	135,000
Land and land rights	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	28,300	26,200
Buildings	173,600	144,800
Other structures	0	600
Utilities (electrical, water, steam, and sewer lines)	25,100	24,400
Technical Components	441,400	415,700
Standard Equipment	1,900	2,700
Major computer items	5,300	7,300
Removal cost less salvage	0	0
Design and project liaison, testing, checkout and acceptance	16,600	5,200
Subtotal	1,013,800	904,400
Contingencies at approximately 18 percent of above costs	178,900	288,300
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

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, RF Systems and overall linac physics design; TJNAF – Superconducting Linac; Oak Ridge - Target. Project execution is the responsibility of the SNS Project Executive 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 Executive 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 which 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 2000	FY 2001	FY 2002	Outyears	Total
Project Cost (budget outlays)						
Facility Cost.[a]						
Line Item TEC	37,140	105,542	228,506	285,600	535,912	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	37,140	105,542	228,506	285,600	535,912	1,192,700
Other project costs						
R&D necessary to complete project.[b]	42,378	17,978	12,199	5,673	7,524	85,752
Conceptual design cost.[c]	14,397	0	0	0	0	14,397
Decontamination & Decommissioning (D&D)	0	0	0	0	0	0
NEPA Documentation costs.[d]	1,916	32	0	0	0	1,948
Other project-related costs.[e]	1,150	2,674	6,880	9,580	95,516	115,800
Capital equipment not related construction.[f]	210	454	100	100	239	1,103
Total, Other project costs	60,051	21,138	19,179	15,353	103,279	219,000
Total project cost (TPC)	97,191	126,680	247,685	300,953	639,191	1,411,700

a Construction line item costs included in this budget request are for providing Title I and II design, inspection, procurement, and construction of the SNS facility for an estimated cost of $1,192,700,000.

b A research and development program at an estimated cost of $85,752,000 is needed to confirm several design bases related primarily to the accelerator systems, the target systems, safety analyses, cold moderator designs, and neutron guides, beam tubes, and instruments. Several of these development tasks require long time durations and the timely coupling of development results into the design is a major factor in detailed task planning.

c Costs of $14,397,000 are included for conceptual design and for preparation of the conceptual design documentation prior to the start of Title I design in FY 1999.

d Costs of $1,948,000 are included for completion of the Environmental Impact Statement.

e Estimated costs of $115,800,000 are included to cover pre-operations costs.

f Estimated costs of $1,103,000 to provide test facilities and other capital equipment to support the R&D program.

7. Related Annual Funding Requirements.

	(FY 2006 dollars in thousands)	
	Current Estimate	Previous Estimate
Facility operating costs	21,300	N/A
Facility maintenance and repair costs	25,300	N/A
Programmatic operating expenses directly related to the facility	22,500	N/A
Capital equipment not related to construction but related to the programmatic effort in the facility	2,100	N/A
GPP or other construction related to the programmatic effort in the facility	1,000	N/A
Utility costs	30,400	N/A
Accelerator Improvement Modifications (AIMs)	4,100	N/A
Total related annual funding (4Q FY 2006 will begin operations)	106,700	N/A

During FY 2001, more detailed planning for the SNS operating program will be conducted. Based on that planning, an updated estimate of the annual funding requirements will be submitted with the FY 2003 data sheet.

8. Design and Construction of Federal Facilities

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

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

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	2Q 2002	3Q 2004	N/A	N/A	14,000 [a]

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	4,000	4,000	4,000
2003	8,000	8,000	8,000
2004	2,000	2,000	2,000

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.

FY 2002 PED design projects are described below. Some changes may occur due to continuing conceptual design studies or developments prior to enactment of an appropriation. These changes will be reflected in subsequent years. Construction funding will be separately requested after completion of preliminary (Title I) design work.

<u>Nanoscale Science Research Centers (NSRCs)</u>

To support research in nanoscale science, engineering, and technology, the U.S. has constructed outstanding

[a] The full Total Estimated Cost (design and construction) ranges between $220,000,000 - $330,000,000. This estimate is based on conceptual data and should not be construed as a project baseline.

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, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, and a consortium of Los Alamos National Laboratory, Sandia National Laboratory and the University of New Mexico. PED funding will be provided to four of these centers in FY 2002. PED funding for the fifth center would begin in FY 2003. Construction funding, which will be contingent upon the results of the design studies and on scientific peer review of the proposal, would be staggered in the out years depending upon which centers actually receive final approval.

FY 2002 Proposed Design Projects

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

Fiscal Quarter				Total Estimated Cost (Design Only) ($000)	Full Total Estimated Cost Projection [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	1,000	1,000	1,000
2003	1,000	1,000	1,000

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.

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	3,000	55,000-75,000

Fiscal Year	Appropriations	Obligations	Costs
2002	1,000	1,000	1,000
2003	2,000	2,000	2,000

[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.

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 beamlines at the ALS, not part of this PED activity, will support efforts at the Molecular Foundry.

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	1,000	1,000	1,000
2003	2,000	2,000	2,000

The Center for Functional Nanomaterials will include class 10 clean rooms, general laboratories, wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be 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

[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.

exchange of ideas essential to creative research processes.

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 2003	3Q 2004	4Q 2004	N/A	3,000	45,000-65,000

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	0	0	0
2003	1,000	1,000	1,000
2004	2,000	2,000	2,000

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. The CNMS will play a critical role in integrating the growing neutron scattering community with the emerging research in nanoscale science by encouraging the use of neutrons in this premier scientific area. Progress in nanoscale science and engineering requires determining the atomic-scale structure of nanomaterials, developing a detailed understanding of the synthesis and assembly processes of complex nanomaterials systems, and understanding collective (cooperative) phenomena that emerge on the nanoscale. 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 facility will consist of a multistory, mutipurpose building located east of the SNS complex. It will house the core support facilities, offices, and laboratories necessary to ensure the mission of the CNMS. The location and synergy off the functions for the facility will provide the required support and services for broad R&D collaborations in nanoscience among researchers from ORNL, other national laboratories, universities, and industries. The completed design will enable construction of a new two-story Laboratory/Office building of approximately 100,000 square feet. The facility will include two state-of-the-art clean rooms, (one class 100 and the other class 10), general laboratories, wet and dry laboratories for sample preparation, fabrication and analysis. Included will be equipment necessary to synthesize, manipulate, and characterize nanoscale materials and structures. Also included are individual offices, cubicles, visitor and viewing lobby, two conference rooms, a loading dock, and a common computer design and operations room.

[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.

02-05: Synthesis and Characterization Laboratory – Los Alamos 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	1,500	15,000-30,000

Fiscal Year	Appropriations	Obligations	Costs
2002	500	500	500
2003	1,000	1,000	1,000

The Center for Integrated Nanotechnologies (CINT), a distributed Center operated by the Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL) and the University of New Mexico (UNM), 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. The CINT brings together the strengths of the three institutions to generate the knowledge needed to integrate nanoscale electronic materials into micro and macro scale assemblies and devices needed for the DOE defense, energy, and environmental mission areas. The CINT will focus on nanophotonics, nanoelectronics, nanomechnics, and functional nanomaterials. The Center will make use of a wide range of specialized facilities at the three institutions, including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL; the Miccroelectronics Development Laboratory and the Compound Semiconductor Research Laboratory at SNL; and the Center for High Technology Materials and the Center for Micro-Engineered Materials at University of New Mexico. Specialized nanoscale science laboratories are needed at Albuquerque and Los Alamos to take advantage of these existing facilities at each site. In Los Alamos, the Synthesis and Characterization Laboratory will focus on theory, synthesis, and characterization of nanoscale materials. In Albuquerque, the Nanofabrication and Integration Laboratory will focus on fabrication and integration of nanoscale materials.

The LANL role in CINT requires the construction in Los Alamos of an approximately 40,000 gross sq ft Synthesis and Characterization Laboratory with an integrated theory, modeling, and simulation module. The laboratory will house state-of-the-art equipment, CINT research, collaborators from Sandia and UNM, visiting research collaborators, students and postdocs, appropriate additional complementary funded research, and central high-speed communications between the Sandia and UNM sites. It will be located to meet the CINT's mission of ease of access and collaboration as well as access to complementary Los Alamos research capabilities. In addition, the existing Los Alamos Electron Microscopy Laboratory and Ion Beam Materials Laboratory will be part of the CINT program and will be upgraded to further nanoscale research. Los Alamos will seek a DOE waiver for open and unrestricted access, similar to that for several existing buildings, to support this mission.

[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.

02-06: Nanofabrication and Integration Laboratory – 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	1,500	15,000-30,000

Fiscal Year	Appropriations	Obligations	Costs
2002	500	500	500
2003	1,000	1,000	1,000

The Center for Integrated Nanotechnologies (CINT), a distributed Center operated by the Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL) and the University of New Mexico (UNM), 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. The CINT brings together the strengths of the three institutions to generate the knowledge needed to integrate nanoscale electronic materials into micro and macro scale assemblies and devices needed for the DOE defense, energy, and environmental mission areas. The CINT will focus on nanophotonics, nanoelectronics, nanomechnics, and functional nanomaterials. The Center will make use of a wide range of specialized facilities at the three institutions, including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL; the Miccroelectronics Development Laboratory and the Compound Semiconductor Research Laboratory at SNL; and the Center for High Technology Materials and the Center for Micro-Engineered Materials at University of New Mexico. Specialized nanoscale science laboratories are needed at Albuquerque and Los Alamos to take advantage of these existing facilities at each site. In Los Alamos, the Synthesis and Characterization Laboratory will focus on theory, synthesis, and characterization of nanoscale materials. In Albuquerque, the Nanofabrication and Integration Laboratory will focus on fabrication and integration of nanoscale materials.

The SNL role in CINT requires the construction in Albuquerque of the Nanofabrication and Integration Laboratory in 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 and electronics labs and offices for Center staff and collaborators. The complex will require 5,500 sq ft of class 1,000 clean room space for nanofabrication and characterization equipment and an additional 500 sq ft of 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,

[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.

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)	10,500	N/A
Design Management costs (15% of TEC)	2,100	N/A
Project Management costs (10% of TEC)	1,400	N/A
Total Design Costs (100% of TEC)	14,000	N/A
Total, Line Item Costs (TEC)	14,000	N/A

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 2000	FY 2001	FY 2002	Outyears	Total
Facility Cost						
PED	0	0	0	4,000	10,000	14,000
Other project costs						
Conceptual design cost	0	0	1,155	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	0	1,155	0	0	1,155
	0	0	1,155	4,000	10,000	15,155

[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.