Basic Energy Sciences

Program Mission

The MISSION of the Basic Energy Sciences (BES) program is to foster and support fundamental research in the natural sciences and engineering to provide a basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. As part of its mission, BES plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

The high quality of the research in this program is regularly evaluated through the use of merit based peer review and scientific advisory committees.

Program Goals

- Maintain U.S. world leadership in areas of the natural sciences and engineering that are relevant to energy resources, production, conversion, and efficiency and to the mitigation of the adverse impacts of energy production and use;
- Provide world-class scientific user facilities for the Nation;
- Foster and support the discovery, dissemination, and integration of the results of fundamental, innovative research; and
- Act as a steward of human resources, essential scientific disciplines, institutions, and premier scientific user facilities.

Program Objectives

- *Obtain major new fundamental knowledge.* - Foster and support fundamental, innovative, peer-reviewed research to create new knowledge in areas important to the BES mission, i.e., in materials sciences, chemical sciences, geosciences, plant and microbial biosciences, and engineering sciences.
- *Plan, construct, and operate premier national scientific user facilities* – Provide facilities for materials research and related disciplines to serve researchers at universities, national laboratories, and industrial laboratories, thus enabling the acquisition of new scientific knowledge. These scientific facilities include synchrotron radiation light sources, high-flux neutron sources, electron-beam microcharacterization centers, and specialized facilities such as the Combustion Research Facility. Encourage and facilitate the use of these facilities in areas important to BES activities and also in areas that extend beyond the scope of BES activities, such as structural biology, environmental science, medical imaging, rational drug design, micromachining, and industrial technologies.
- *Support the missions of the Department of Energy (DOE).* - Promote the transfer of the results of basic research to contribute to DOE missions in areas of energy efficiency, renewable energy resources, improved use of fossil fuels, reduced environmental impacts of energy production and use, science-based stockpile stewardship, and future energy sources.

- *Establish and maintain stable, essential research communities and institutions.* - Steward important research communities and institutions in order to respond quickly and appropriately to scientific opportunity and mission need. For example, BES serves as the Nation's primary or sole supporter of such subdisciplines as heavy element chemistry, natural and artificial solar energy conversion, catalysis, organometallic chemistry, combustion-related science including gas-phase kinetics and reaction dynamics, separations science, neutron science, radiation chemistry, and radiation effects in materials. Some of these research activities exist primarily in the DOE laboratories, e.g., heavy element chemistry; others exist both in DOE laboratories and in universities. In all cases, participation by students, postdoctoral research associates, and young faculty and staff is an imperative to ensure continuation and intellectual growth of the research communities.

Performance Measures

BES, which is prototypical of a large, diverse research program existing within a mission agency, measures performance in four ways: (1) peer review; (2) indicators or metrics (i.e., things that can be counted); (3) customer evaluation and stakeholder input; and (4) qualitative assessments, which might include historical retrospectives and annual program highlights. A number of activities that might be considered essential or "foundation" performance measurement activities are already in place in BES. Indeed, some have been ongoing for many years. Paramount among these is peer review of all research activities.

During FY 1998, BES instituted several changes in the way performance measurement is accomplished to better quantify it. First, BES formalized the peer review process for activities at the DOE laboratories. Although research at the laboratories had long been peer reviewed, BES codified that process using a process analogous to that described in 10 CFR 605 for the university grant program. Second, in FY 1999, BES established baselines for all performance indicators for each scientific user facility using a new survey tool. This survey tool, developed in FY 1997 in collaboration with the facility directors and the facility user coordinators, is completed annually by all BES facilities. An integral part of the survey tool is an assessment of user satisfaction. Third, BES began formal peer reviews of its major scientific user facilities to assess, in the aggregate, the scientific output and, to the extent possible, the outcomes of facilities. Recent and forthcoming reviews conducted by the Basic Energy Advisory Committee (BESAC) include: (1) the 1997 review of the four synchrotron radiation light sources, “Synchrotron Radiation Sources and Science,” (2) the 1998 review of the “High-Flux Isotope Reactor Upgrade and User Program,” (3) the 1999 review of R&D requirements for “Novel Coherent Light Sources,” (4) the 1999 review of the four BES electron beam microcharacterization centers, which will be presented to BESAC in February 2000, (5) a forthcoming review of the Advanced Light Source that is planned for February 2000 and which will be presented to BESAC in February 2000, (6) a forthcoming review of the Intense Pulsed Neutron Source and the Manuel Lujan Jr., Neutron Scattering Center that is planned for the summer of 2000, and (7) a review of neutron scattering activities in the context of the permanent closure of the High Flux Beam Reactor, which will be presented to BESAC in February 2000.

Performance measurement helps determine both the distribution of activities supported within the BES program and the individual projects supported within each activity. The funding level for each activity is derived by weighing a number of additional factors including (1) mission need as described by the BES program and the Office of Science (SC) mission statements and the SC strategic plan; (2) scientific opportunity as determined, in part, by proposal pressure and by scientific workshops; (3) the results of international benchmarking activities of entire fields or subfields such as those performed by the National Academy of Sciences; (4) connections with other BES and SC supported work; (5) connections with needs expressed by the DOE technology offices and by energy-intensive industries; (6) program balance including considerations of activities funded by non-BES sources; and (7) budgetary constraints.

In FY 2001, (1) meet the cost and schedule milestones for upgrade and construction of scientific user facilities, including the construction of the Spallation Neutron Source; the cost and schedule will be kept within 10 percent of cost and schedule baselines as reflected by regular external independent reviews of project management cost and schedule; (2) maintain and operate user facilities so that the unscheduled downtime, on average, is less than 10 percent of the total scheduled operating time, as reported to Headquarters by facilities at the end of each fiscal year; (3) all research projects will undergo regular peer review and merit evaluation based on procedures set down in 10 CFR 605 for the extramural grant program and under a similar modified process for the laboratory programs and scientific user facilities; (4) new projects will be selected by peer review and merit evaluation; and (5) research performed by investigators in universities and DOE laboratories will continue to be recognized as outstanding during rigorous peer review and through the awards and accolades of the broader science community and others that use our results as reflected by peer review comments and annual awards data collected by the program.

Prizes, Awards, and Honors

Each fiscal year, principal investigators funded by BES win dozens of major prizes and awards sponsored by professional societies, distinguished foundations, and universities. Paramount among the honors are the four Nobel Prizes awarded to BES principal investigators over the past five years. In FY 1999, many were inducted as members in organizations such as the National Academy of Sciences, the National Academy of Engineering, and other professional societies.

Selected major prizes and awards for FY 1999 include:

From the ASM International (formerly the American Society of Metals) — Materials Science Research Silver Medal

From the American Academy of Microbiology — Proctor & Gamble Award in Applied and Environmental Microbiology

From the American Ceramic Society — the George W. Morey Award; the Richard M. Fulrath Award

From the American Chemical Society — the Priestly Medal; the Arthur C. Cope Scholar Award; Award in Inorganic Chemistry; Buck-Whitney Medal; Charles Holmes Herty Medal; Claude S. Hudson Award in Carbonhydrate Chemistry; George A. Olah Award in Hydrocarbon or Petroleum; James Flack Norris Award in Physical Organic Chemistry; Award for Distinguished Service

From the American Geophysical Union — the Bowen Award

From the American Institute of Chemical Engineers — the Research Achievement Award

From the American Physical Society — the David Adler Lectureship Award; the Davisson-Germer Prize; two James C. McGroddy Prizes; Outstanding Doctoral Thesis Research in Beam Physics; Roger Revelle Medal; the Nottingham Prize

From the U.S. Department of Commerce — the National Medal of Technology

From the Electrochemical Society — the Carl Wagner Memorial Award; the David C. Grahame Award

From the Faraday Society in England — the Bourke Lecturer Award

From the Federal Laboratory Consortium — the Federal Laboratory Consortium Award

From the Geological Society of America — the Arthur L. Day Medal

From the Institute of Liquid Atomization and Spray Systems — the Harold Simmons Award

From the International Society for Measurement and Control — two Arnold O. Beckerman Founder Awards

From the International Society for Optical Engineering — the Harold E. Edgerton Prize

From the International Institute of Welding — U.S. Representation for Study Group on Physics of Welding

From the MacArthur Foundation — the John D. Catherine T. MacArthur Foundation Fellowship

From the Materials Research Society — the Medal for Significant Achievements

From the North American Catalysis Society — the Robert Burwell Lectureship Award; the Paul H. Emmett Award

From R&D Magazine — R&D 100 Awards for:

- Direct Injection High Efficiency Nebulizer, a device for improved introduction of liquid samples into an inductively coupled plasma for subsequent analysis by emission or mass spectrometry
- Acoustic Stirling Cycle Refrigerator, a new heat engine that efficiently converts heat to intense acoustic power in a simple device that comprises only pipes and conventional heat exchangers and has no moving parts
- Gregar Extractor, a more efficient, more reliable, and often faster device for solvent-based chemical extraction from solid samples
- Molecular Sciences Software Suite, the first general-purpose software that allows chemists to easily use high-performance, massively parallel computers for a wide range of applications
- Rolling Assisted Biaxially Textured Substrates, or RABiTS, technology for the manufacture of long lengths of ultra-high-performance superconducting wires necessary for a wide range of high-temperature superconductors.

From the Royal Society of Chemistry — the Centenary Medal

From the Society for Technology Transfer — two Lang Rosen Awards for an Innovative New Approach to R&D Assessment

From the Society of Imaging Science and Technology — the Kosar Memorial Award

One principal investigator received the Presidential Early Career Award for Scientists and Engineers, three were inducted into the National Academy of Sciences, and three were inducted into the National Academy of Engineering. Principal investigators were advanced to fellowship in the following societies and organizations: three in the American Ceramic Society; eleven in the American Physical Society; four in ASM International (formerly the American Society for Metals); two in the Electrochemical Society; four in the Optical Society of America; four in the Japan Society for the Promotion of Science; and one each in the American Academy of Arts and Sciences; the American Association for the Advancement of Science; Institute of Materials of London, Institute of Physics, the American Welding Society, the Metallurgical Society, the International Women's Forum Leadership Program, the American Academy of Arts and Sciences, and the Third World Academy of Sciences.

Finally, principal investigators served in numerous elected offices including: President, International Society of Electrochemistry; President, American Ceramic Society; Vice Chair, Division of Materials Physics, American Physical Society; two Vice Chairs, American Physical Society; Chair, Council of Fellows, ASM International; Director, Photobiology Foundation; Director, Microbeam Analysis Society; and President, Association of Women in Mathematics.

Significant Accomplishments and Program Shifts

The BES program is one of the Nation's major sponsors of fundamental research in broad areas of materials sciences, chemical sciences, geosciences, plant and microbial sciences, and engineering sciences. The program encompasses more than 2,400 researchers in nearly 200 institutions and 16 of the Nation's outstanding user facilities. The BES program funds research at 149 colleges/universities located in 48 states. The inclusion of research activities at this large number of academic institutions is a vital part of the program. These scientists are funded through individual peer-reviewed grants and as members of peer-reviewed research teams involving investigators from both national laboratories and universities. In addition, university-based scientists are among the principal users of the BES user facilities.

The BES program is the premier sponsor of condensed matter and materials physics in the U.S. Furthermore, its chemical sciences program is the U.S. leader in research in homogeneous and heterogeneous catalysis, photchemistry and radiation chemistry, gas-phase chemical dynamics, and separations and analysis. The chemical sciences program is the only program in the U.S. addressing heavy element chemistry, including today's issues of heavy element chemistry in the environment; this aspect of the program traces its roots to the 1940s Manhattan Project. Finally, the stunning portfolio of research and scientific user facilities devoted to visualizing, characterizing, and controlling the nanoworld – from atoms and molecules to bulk materials – makes the BES program unique in the world.

The BES program has taken a leadership role in defining and addressing the 21st century challenges facing the physical and biological sciences – from understanding collective effects in materials to designing new materials atom by atom and, finally, to developing functional materials. Functional materials are those with the ability to self assemble, self repair, sense, respond, and evolve in order to provide functional properties – optical, mechanical, catalytic, electrical, and tribological. Envisioning and creating these materials is the coming challenge for the disciplines of materials sciences, chemistry, physics, and biology.

Presented below are program accomplishments from FY 1999. The selected program highlights are representative of the broad range of studies supported in the BES program. These highlights demonstrate the discovery of new knowledge, the rapidity with which such new knowledge can be incorporated into other scientific disciplines and into the commercial sector, and the great potential of new knowledge for future impacts in energy production and use. Following are discussions of scientific facilities and new program directions for FY 2001.

Selected FY 1999 Scientific Highlights/Accomplishments

- In FY 1999, the following performance goal was fully met: Begin Title I design activities, initiate subcontracts and long-lead procurements and continue R&D work necessary to begin construction activities of the Spallation Neutron Source.
- **Serendipitous Applications of Research in the Physical Sciences to the Life Sciences.** It has long been recognized that tools and concepts developed in the physical sciences can revolutionize the life sciences. One need only consider the impact of x-ray synchrotron radiation and MAD (multiple wavelength anomalous diffraction) phasing on macromolecular crystallography; both were developed within the BES program. In FY 1999, many of the annual BES program highlights illustrate the rapidity with which advances in the physical sciences are impacting the life sciences. Two examples are given here. First, new techniques of nuclear magnetic resonance (NMR) are being used to study the molecular structures of solid protein deposits implicated in brain diseases such as Alzheimer's Disease and BSE (Mad Cow Disease); both diseases involve the transformation of normal, soluble proteins in the brain (whose structure is known) into fibers of insoluble plaque (whose structure is largely unknown). Second, a nano-laser device has been shown to have the potential to quickly identify a cell population that has begun the rapid protein synthesis and mitosis characteristic of cancerous cell proliferation. Pathologists currently rely on microscopic examination of cell morphology using century-old staining methods that are labor-intensive, time-consuming, and frequently in error.

Materials Sciences Subprogram

- **Seashell Provides Key to Strong Composites.** Mollusk shells have evolved over millions of years to provide hard, strong, tough shelters for fragile occupants. These outstanding mechanical properties derive from a laminated construction of alternating layers of biopolymer – a biologically produced rubber – and calcium carbonate, commonly known as chalk. It has been recognized for decades that materials with alternating hard and soft layers absorb energy and impede cracking. Unfortunately, it has proven difficult to transcribe seashell-like designs into manufacturable materials. Now, a rapid, efficient self-assembly process has been developed for making “nanocomposite” materials that mimic the construction of seashells. This process can be generalized and should lead to materials with unprecedented mechanical properties.

- **Imaging Fluid Distribution and Flow in Materials.** Dramatic pictures of the distribution and flow of fluids inside intact objects and porous solid materials have been obtained by magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR). The ability to observe such images and spectra results from the use of noble gases, particularly xenon, magnetically polarized by means of a laser. This advance makes possible the observation of MRI pictures and NMR spectra in ultralow magnetic fields. The technique produces brilliant pictures (up to a millionfold increase in brightness) and provides a new capability for noninvasive investigation of flow and transport. The images and spectra allow the characterization of atomic distribution and flow from the smallest scale of nanotubes to the largest scale of macroscopic samples. The flow of fluids through solid materials is a crucial component of many industrial processes from the catalytic conversion of petroleum to the containment of toxic environmental agents. These advances will eliminate the need for high magnetic fields in some applications of MRI and NMR, a welcomed event given the cost, bulk, hazard, and lack of portability of the magnets used in contemporary instrumentation.

- **New Fullerene Species Synthesized - Stickyball, C_{36}.** A new fullerene species, C_{36}, has been synthesized and produced in bulk quantities for the first time. Fullerenes or "buckyballs" are hollow clusters of carbon atoms. They have been studied extensively since the Nobel prize-winning discovery of C_{60} in 1985 (supported by BES). C_{36} is the smallest fullerene discovered to date and is characterized by unusual and potentially very useful properties. For example, in contrast to C_{60} molecules, which interact only very weakly with one another, C_{36} molecules stick together – hence the nickname "stickyballs." The lower fullerenes, such as C_{36} are predicted to have more highly strained carbon bonds, resulting in exciting properties for those molecules such as very high chemical reactivity and high temperature superconductivity. The synthesis of C_{36} is particularly significant, because previously it was believed that any fullerene smaller than C_{60} would be too unstable to isolate in bulk.

- **Seeing Clearly Now.** Using a new imaging technique called Z-contrast imaging, researchers have achieved the highest resolution electron microscope image of a crystal structure ever recorded, resolving adjacent columns of silicon atoms separated by a scant 0.78 angstroms (3 billionths of an inch). Better resolution enables scientists to see and understand important details they had not been able to see before. This technique also offers both high spatial resolution and the ability to distinguish different kinds of atoms. The precise atomic-scale structure of a material controls the performance of materials for semiconductor devices, superconductors, and a host of other applications. Combined with improved electron imaging optics currently under development, this result promises to revolutionize the atomic-scale understanding of materials.

- **New Family of Bulk Ferromagnetic Metallic Glasses for Energy Efficient Motors and Transformers.** New rules for designing alloys have been developed that enable the creation of a family of bulk metallic glass alloys. These alloys exhibit outstanding ferromagnetic behavior with virtually no energy loss. These new alloys are at least 65 percent iron plus contain up to seven other elements. Until now, such alloys could only be produced as thin foils. Commercial transformers based on the thin foil ferromagnetic metallic glasses are in service, but their size and application are limited due to difficulties in thin foil assembly and manufacturing processes. The new bulk glasses can be cast into exact shapes and substituted into the standard assembly processes now in use for traditional crystalline materials. It is expected that the availability of bulk ferromagnetic glasses will decrease the energy losses of transformers by about 2/3 compared to today's transformers made from crystalline ferromagnetic materials. That's good news for electric utility customers, since it is estimated that power-distribution transformer losses cost about $4 billion annually.

- **Universal Magnetic Behavior in High-Temperature Superconductors.** Understanding high temperature superconductors remains one of the most significant research issues in condensed matter physics. The observed properties of two major classes of high temperature superconductors initially appeared to be significantly different from one other, leading scientists to believe that the fundamental interactions responsible for the superconducting behavior were quite different in the two materials. However, recent neutron scattering results have shown that the superconducting behavior of both major classes of superconductors is connected to excitations of the magnetic spin system in each material. The new results offer insight on high-temperature superconductivity including the promise that a single physical mechanism can account for this phenomenon.

Chemical Sciences Subprogram

- **Measuring Chemical Processes in Combustion One Molecule at a Time.** A powerful new experimental instrument just completed at the Combustion Research Facility promises to provide new information about how molecules dissociate when given enough internal energy. Understanding such processes is critically important for combustion, because, at the high temperatures of combustion, dissociation occurs in a variety of ways that are difficult to observe, model, and predict. In the experiment, pulses of laser light a few femtoseconds in duration pump enough energy into a molecule to cause it to dissociate. (One femtosecond is one millionth of a billionth of a second.) A second femtosecond laser pulse ionizes the molecular fragment during the dissociation process. From the simultaneous measurements of the fragments produced by the second laser, the details of the dissociation process can be extracted. These measurements are made one molecule at a time. This new experimental facility promises to be a tool of unrivaled power for the validation of predictive models and theories of chemical reactions.
- **New Designs for Molecular Wires Help Mimic Photosynthesis.** One way to capture and store the sun's energy is to design systems that mimic photosynthesis. In nature, biological systems use charge separation to store energy. This charge separation occurs by transfer of an electron from a photoexcited donor molecule through a bridge molecule to an acceptor molecule. Researchers have recently constructed donor-bridge-acceptor systems in which the bridge – or molecular wire – is a conjugated organic molecule analogous to natural carotenes that transfer charge over long distances. This research may lead to new molecular devices for efficient charge separation and storage.
- **New Insights into Surface Catalysis.** One of the oldest problems in surface-catalyzed reactions is understanding how the molecules actually come together on a metal surface. Researchers studying the hydrogenation of acetylene on crystalline nickel using sophisticated atomic and molecular beam preparations and subsequent thermal desorption spectroscopy demonstrated that this simple reaction proceeds via hydrogen absorbed into the bulk of the metal rather than adsorbed on its surface, as previously thought. This startling discovery has changed the way we think about industrial hydrogenation catalysts such as Raney nickel and palladium, and may have general implications for heterogeneous catalysts presently used in energy-intensive industries such as ammonia production (the Haber Process).
- **First Observation of Relativistic Thomson Scattering – 60 Years After its Prediction.** British physicist J. J. Thomson, who identified the electron in 1897, showed in 1906 that light could cause electrons to oscillate up and down and reemit at the same frequency in a dipole pattern; this phenomenon was subsequently termed Thomson scattering. Nearly a century later, researchers have demonstrated a new phenomena – relativistic Thomson scattering – in which electrons oscillate in a

more complex figure-8 pattern and emit light at both the exciting laser frequency and multiples of that frequency, each emitted in a different direction. The more complex pattern results from the electron interacting simultaneously with both the electric and magnetic fields of the laser light. To observe this phenomena, the research team built a tabletop neodymium-glass laser and compressed its billionth-of-a-second pulses by a factor of about 1,000, boosting their power to 4 trillion watts of very high-quality beam. This experiment is an important milestone in the study of nonlinear optics with electrons unbound to atoms. Furthermore, this work may lead to new laboratory tabletop x-ray sources producing very short x-ray pulses useful, for example, for probing molecular motion during reactions.

Engineering and Geosciences Subprogram

- **Making Waves**. Unfortunately, many facets of nature exhibit chaotic changes, driven by external forces, never settling down to a predictable state. Progress has been made in understanding one kind of chaos in which information travels from one point to another by means of traveling waves. Examples include the ripples on a wind-blown lake, light in a laser, weather patterns, and even the fibrillation of a human heart. In order to understand this kind of chaos, scientists studied the flow patterns in a thin layer of fluid heated from below. In certain fluid mixtures, the patterns move laterally like waves on a pond. The key discovery is that these patterns can be understood in terms of so-called phase defects, which are places where the waves circle around a point in a pinwheel-like motion. Looking at only the defects to understand the entire pattern is much like keeping track of traffic jams and accidents to understand the operation of a freeway system. The next step will be to predict how the patterns change with time. If present ideas are confirmed, they could be useful controlling such important phenomena as heart fibrillation, and controlling lasers used in communications, cutting and welding.
- **Changes in Seismic Properties of Rocks Detects Damage**. Seismology uses the reflection and transmission of elastic waves to locate subsurface features of interest. Various types of rocks respond differently to different kinds and frequencies of waves. The theoretical geophysics program has developed new techniques to study these phenomena. The research examines rock behavior through ultrasonic resonance experiments, which show that rock has both a rapid resonance response and a slow resonance response. The resonance between the vibrational modes gives the rock a memory of the shaking it has been through. The resonance behavior has implications for accurately locating subsurface features, and for understanding strong ground motion damage patterns during earthquakes when the resonant modes of regions of different ground properties couple with those of man-made structures. A similar resonance response is also characteristic of damaged man-made materials such as metals, ceramics and composites. Thus the nonlinear elastic wave studies can contribute to understanding and testing the characteristics of most man-made materials as well as rock or concrete.

Energy Biosciences Subprogram

- **Orienting Molecular Syntheses.** A component of plant cell walls that severely restricts the use of the carbohydrates in plant biomass is lignin. Lignins are aromatic polymers that make up a significant fraction of the earth's renewable carbon resources. Research has provided evidence that the biosynthesis of these large polymers from smaller lignol units does not proceed in a random fashion, as was previously thought. Novel plant genes have been discovered that encode proteins that serve as a scaffold, helping to hold the lignol units in the right orientation as they are joined together by other biosynthetic enzymes. These results have broad implications for the efficient use of plant biomass as well as offering new strategies for enzyme catalysis in an industrial setting.

- **Plant Cell Walls.** The characteristics of plant cell walls – the major energy component of renewable biological resources – vary to meet the structural, metabolic, and developmental needs of different plant cell types. The biosynthesis of the plant cell wall is precisely regulated to conform to these constraints; however, relatively little is known about how such variation is achieved during cell wall formation. Researchers recently identified an enzyme responsible for modifying the xyloglucan polymer backbone, an important factor in determining cell wall strength. This discovery offers the potential to isolate similar enzymes that modify cell wall properties. A better understanding of plant cell wall biosynthesis can eventually improve the properties of wood and other biomass materials through the efficient design of specific complex carbohydrates and other renewable carbon resources.
- **Designer Enzymes.** Research on fatty acid desaturases and hydroxylases has deciphered the mechanism that controls how these two types of enzymes introduce a double bond (desaturase) or a hydroxyl group (hydroxylase) at specific sites along the carbon atom backbone of long-chain fatty acids. This knowledge of the active site of the two enzymes has enabled the modification of the gene that encodes the desaturase for a specific fatty acid to change it into the hydroxylase and vice versa. Both enzymes perform important tasks in altering the melting response of the fatty acid to heat. This pioneering work lays the groundwork for future advances in designing vegetable oils—which have hundreds of potential uses from heart-healthy margarine to lubricants and nylon.

Scientific Facilities Utilization

The BES program request includes $335,593,000 to maintain support of the scientific user facilities. Included within this request is a cost-of-living increase for operations at each of the four BES synchrotron radiation light sources as well as additional funding to address specific recommendations of the 1997 BESAC review “Synchrotron Radiation Sources and Science” for each of the light sources. Also included within this request are funds to address the critical situation in neutron science following the permanent closure of the High Flux Beam Reactor, e.g., additional operating funds are provided to permit increased operations at other neutron sources and additional capital equipment and accelerator improvement funds are provided for new instruments and infrastructure improvements, respectively. The synchrotron radiation light sources and the neutron sources serve a wide variety of research disciplines, and it is important that these facilities be operated effectively, i.e., that they optimize beam availability and that they reliably serve their users. The funds requested will ensure this high level of operation. Research communities that have benefited from the BES supported Scientific User Facilities include materials sciences, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, medical research, and industrial technology development. 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, and engineering. It is anticipated that the facility will be used by 1,000-2,000 scientists and engineers annually and that it will meet the Nation's need for neutron science capabilities well into the next century. When completed in 2006, the SNS will be more than ten times as powerful as the best spallation neutron source now in existence -- ISIS at the Rutherford Laboratory in England.

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 the features that make materials of technological significance for many economically important areas. Major research facilities, such as the BES synchrotron and neutron sources, are used to understand and "engineer" materials at the atomic level so that they have improved macroscopic properties and perform better in new applications. The SNS is a next-generation facility for just such research. 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 importance of high neutron flux (i.e., high neutron intensity) cannot be overstated. The relatively low flux of existing neutron sources and the very small fraction of neutrons that get scattered by most materials mean most measurements are limited by the source intensity. However, 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.

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 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 1 giga electron volt (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 to useful levels, 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. There will initially be one instrumented target station with the potential for adding more instruments and a second target station later.

The SNS Project partnership among five 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, Brookhaven National Laboratory in proton storage rings, Argonne National Laboratory in instruments, and Oak Ridge National Laboratory (ORNL) in targets and moderators.

The Department has been diligent in its efforts to meet the conditions stipulated in the House Report (Report 106-253, pages 113-114) accompanying the FY 2000 Energy and Water Development Appropriations Act concerning the release of construction funds for the SNS project, and has regularly communicated its progress to Congress. During the past year, the project has established a revised project management structure with a single Executive Director who has been designated as the primary authority for the project; filled all senior positions with qualified individuals; established cost and schedule baselines that were externally reviewed and determined to be the most cost effective way to complete the project; and established an inter-Laboratory Memorandum of Agreement and incorporated it by reference into the laboratory contracts, thus making it legally binding.

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 funding of $281,000,000 (includes other project costs) is requested for the SNS Project for conducting detailed (Title II) design and starting fabrication of the ion source, low-energy beam transport, linac structure and magnet systems, target assemblies, experimental instruments, and global control systems. Construction will begin on several conventional facilities in preparation for starting installation of major equipment, and construction will start on the front end building, linac tunnel, high-energy beam transport tunnel, ring-service building, ring-to-beam transport tunnel, and the klystron hall. Construction will be completed on roads into the site, site preparation/grading, waste systems, and retention basins. Production of several significant equipment items such as dipole magnets, material for the target transport systems, and klystrons will continue. Project management and integration activities, which are exceptionally important during this phase of the project, will also be conducted. Work will continue on the Safety Assessment Document for all the facility except for the target system, for which a Safety Analysis Report will be prepared. ORNL has subcontracted to a joint venture by Lester B. Knight and Associates, Inc. and Sverdrup Facilities, Inc. for design and construction of the SNS conventional facilities. 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 (TPC) has increased from $1,360,000 to $1,440,000 and the construction schedule has been extended six months to the third quarter of FY 2006 as a result of project restructuring during FY 1999 and the FY 2000 appropriation.

Facility Enhancements

BES will continue to support the following major ongoing enhancements and maintenance activities of existing synchrotron radiation light sources and neutron scattering sources:

(1) Fabrication of instrumentation will continue for the short-pulse spallation source at the Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE). This instrumentation enhancement project was undertaken concurrently with an accelerator enhancement project funded by the Department's Office of Defense Programs. Together, these enhancements will result in a short-pulse spallation source facility equivalent to ISIS in Great Britain, currently the world's best for neutron scattering. This facility meets the requirements set by BESAC for an interim facility to the SNS at least as good as the ISIS facility.

(2) Over the period FY 1999 - FY 2001, a number of improvements are being undertaken at HFIR to improve neutron scattering capabilities. These include larger beam tubes and shutters, a high-performance hydrogen cold source, and neutron scattering instrumentation. The improvements will be undertaken during an extended reactor outage in FY 2000 for the regularly scheduled (approximately every decade) replacement of the beryllium reflector. These improvements require no modification to reactor systems and allow operation at up to 100 MW.

(3) Over the period FY 1999 - FY 2003, the SPEAR 3 upgrade is being undertaken at SSRL to provide major improvements to all existing experimental stations and to significantly benefit the large and growing SSRL user community. The technical goals are to increase injection energy from 2.3 GeV to 3 GeV; decrease beam emittance by a factor of 7; increase operating current from 100 mA to 200 mA; and maintain long beam life time (>25 hr). The increased 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 $58,000,000; DOE and NIH are jointly and equally funding the upgrade. Support from NIH in the amount of $14,000,000 began in FY 1999.

Nanoscale Science, Engineering, and Technology Research

In 1959 Richard Feynman delivered a now famous lecture, *There is Plenty of Room at the Bottom -- An Invitation to Enter a New Field of Physics*. He challenged his audience to envision a time when materials could be manipulated and controlled on the smallest of scales, when new materials could be fabricated and devices could be designed atom by atom. "In the year 2000," he said, "when they look back at this age, they will wonder why it was not until the year 1960 that anybody began seriously to move in this direction." [http://www.zyvex.com/nanotech/feynman.html]

Unfortunately, it took longer than Feynman predicted to arrive at the threshold of such complete control of materials. Now, in the year 2000, controlling and manipulating matter at the atomic and molecular scale -- which is the essence of nanoscale science, engineering, and technology -- has finally become feasible. In the 40 years since Feynman's lecture, instruments have been invented and perfected that enable visualization and control at the nanoscale. Many of these instruments and techniques are contained within the BES collection of scientific user facilities. Theory, modeling, and simulation have also reached the stage at which it is possible to understand and predict phenomena at the nanoscale.

BES has been a leader in the early development of nanoscale science, engineering, and technology since the 1980s, supporting research and sponsoring workshops to help establish the importance of nanostructured materials. Because of the confluence of advances during the past decade, BES is now proposing a major effort in nanoscale science, engineering, and technology to take advantage of opportunities afforded by these advances. This effort has the following broad goals: (1) to attain a fundamental scientific understanding of nanoscale phenomena, particularly collective phenomena; (2) to achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions; (3) to attain a fundamental understanding of the processes by which living organisms create materials and functional complexes to serve as a guide and a benchmark by which to measure our progress in synthetic design and synthesis; and (4) to develop experimental characterization tools and theory/modeling/simulation tools necessary to drive the nanoscale revolution.

(To better understand what is meant by “nanoscale,” ten hydrogen atoms side-by-side span one nanometer, which is one billionth of a meter. A cube one nanometer on a side would contain about one thousand hydrogen atoms. The terms nanoscale science, engineering, and technology generally apply to collections of hundreds to millions of atoms.)

The principal missions of the Department of Energy (DOE) in science, energy, defense, and environment will benefit greatly from developments in these areas. For example, nanoscale synthesis and assembly methods will result in significant improvements in solar energy conversion; more energy-efficient lighting; stronger, lighter materials that will improve efficiency in transportation; greatly improved chemical and biological sensing; use of low-energy chemical pathways to break down toxic substances for environmental remediation and restoration; and better sensors and controls to increase efficiency in manufacturing.

The first goal of this work as noted above is fundamental scientific understanding of structures and interactions at the nanoscale, particularly collective phenomena. It is known that when sample size, grain size, or domain size shrink to the nanoscale, physical properties (such as melting temperature) are strongly affected and may differ dramatically from the corresponding properties in the bulk. Yet, there is remarkably little experience with phenomena at the nanoscale. Because of this limited experience, the physical and chemical properties of nanoscale systems are not understood. In effect, this is a new subject with its own set of physical principles, theoretical descriptions, and experimental techniques. One of the most interesting aspects of materials at the nanoscale involves properties dominated by collective phenomena -- phenomena that emerge from the interactions of the components of the material and whose behavior thus differs significantly from the behavior of those individual components. In some case, collective phenomena can bring about a large response to a small stimulus -- as seen with colossal magnetoresistance, the basis of a new generation of recording memory material. Collective phenomena are also at the core of the mysteries of such materials as the high-temperature superconductors, one of the great outstanding problems in condensed matter physics.

The second goal of this work -- the design and synthesis of materials at the atomic level for desired properties and functions -- is the heart of nanoscale science, engineering, and technology. In the future, design and synthesis of new materials at the atomic level will be accomplished using only the electronic structure of the elements. Furthermore, the properties of new materials will not only be a function of their composition but also of the conditions under which they were synthesized. New synthesis conditions might include nonequilibrium, high pressure, high magnetic field, and high energy density. Also, massively parallel fabrication/characterization combinatorial approaches will be employed. The new field of functional materials would include the design of molecular building blocks, the design of multicomponent structures, and the design of molecular machines.

The third goal of this work is the fundamental understanding of the processes by which living organisms create materials and functional complexes. Nanoscale science, engineering, and technology inexorably links the physical and biological sciences. Nature arranges atoms and molecules precisely into three-dimensional objects of extraordinary complexity to produce objects with required optical, mechanical, electrical, catalytic, and tribological properties. Nature has also learned how to combine materials and structures to build molecular-level machines. Some of these molecular machines serve as pumps, moving material across barriers; others move molecules, structures, or whole cells; others control processes and thus are regulatory systems; and still others produce or convert energy. A major challenge in the physical sciences is to understand how Nature makes these complex objects and molecular machines so that we can develop the tools to design and build materials that function as we want -- materials that have not been envisioned by Mother Nature but use Nature’s self assembly techniques.

By understanding and applying these principles to artificial systems, we can make potentially immense advances in diverse areas including energy conversion; data transmission, processing, and storage; "smart" and adaptable materials; sensors for industrial, environmental, and defense purposes; new catalysts; better drugs; and more efficient waste disposal.

The fourth goal of this work is the development of experimental characterization tools and theory/modeling/simulation tools. The history of science has shown that new tools drive scientific revolutions. They allow the discovery of phenomena not previously seen and the study of known phenomena at shorter time scales, at shorter distances, and with greater sensitivity. The BES program has been a leader in the development of tools for characterization at the nanoscale. For example, one of this year's highlights describes the new imaging technique termed Z-contrast imaging, which has resolved adjacent columns of silicon atoms spaced only 0.78 angstroms apart. BES researchers have also been responsible for the development of numerous tools for visualization and characterization at the nanoscale including x-ray microscopes, magnetic flux imaging instrumentation, spectromicroscopy instrumentation including high-brightness infrared spectromicroscopy photoelectron holography, interfacial force microscopes, and atom probe field ion microscopy instrumentation and techniques. Required new instrumentation will necessarily involve an enhancement of conventional techniques -- scanning-probe microscopies, steady-state and time-resolved spectroscopies, and so forth. However, characterization will also depend heavily on revolutionary experimental tools, including techniques for the active control of growth, for massively parallel analysis, and for small sample volumes. Capabilities will be needed for triggering, isolating, or activating single molecules; for independently addressing multiple molecules in parallel; and for transferring or harvesting energy to or from a single molecule. New generations of theory and computational tools will also be required.

This research involves materials sciences, chemistry, physics, biology, and computation. The BES program has worked with the National Science and Technology Council's Interagency Working Group on Nanotechnology, with BESAC, and with the broad scientific community from academia, industry, and the national laboratories to define and articulate the goals of this research and to determine how best to implement a program of research. Based on recent recommendations from BESAC, the BES program will establish a portfolio of programs balanced in scope and in size, ranging from individual principal investigators to large groups. Proposals will be encouraged from relatively small groups of a few principal investigators at universities and/or national laboratories as well as from larger groups focused on particular problems such as might be appropriate for a university center, a national laboratory, or a user facility. Interactions among scientists with a diverse set of skills in areas such as molecular design, synthesis and assembly, molecular modeling, instrumentation development, theory and modeling, and device engineering will also be encouraged. Involvement of young investigators -- graduate students, postdoctoral research associates, and young faculty and staff -- with appropriate expertise is critical to the success of the science and to the evolving future of this field. Interactions among several institutions, including both academic and national laboratory partners, is expected to occur naturally for each of the major focus areas. It is expected that newly funded work will be approximately equally distributed between academic and DOE laboratory efforts.

In the FY 2001 request, new funding in the amount $36,140,000 is requested for these activities. Funds are distributed within the Materials Sciences, Chemical Sciences, and Engineering and Geosciences subprograms. Specific focus areas within each of the subprograms are described in detail in the subprogram narratives. New activities will be peer reviewed following broad solicitations for proposals.

Microbial Cell Research

The recent elucidation of the complete sequences of the genomes of several bacteria offers the opportunity to fundamentally shift our approach to biology. It is now possible to start with the complete parts list and focus on integrating the various parts into a functional whole organism. In the process of integration, it will be possible to understand all of the functions, structures and complex interactions required to permit life in these simplest of life forms. The understanding of the biochemical, metabolic, physiological, and cellular processes will permit the generation of solutions for today's and tomorrow's challenges in energy production and use, environmental cleanup, medicine, agriculture, and industrial processing.

Microbes have dramatic impacts on energy production and conservation. Adverse effects include the fouling or corrosion of pipelines and other metal components used in energy production, significant reductions in the efficiency of heat exchangers, and the souring of fossil energy reserves. Conversely, microbes play a valuable role in numerous industrial fermentations and other bioprocesses that convert complex biomass into potential biofuels and chemical feedstocks.

The developing DNA transfer strategies that build on ongoing work in microbial biochemistry now permit very precise manipulation of genes to elucidate the complex metabolic and gene regulatory circuitry critical for understanding microbes as integrated functional units. The numerous physiological processes of interest, including metabolic changes in response to environmental signals (e.g., starvation, alternative growth substrates, temperature changes, anaerobiosis), the formation of stable consortia, and cellular development, are approachable using molecular techniques and new analytical and imaging instrumentation. The knowledge of the complex interactions that collectively characterize the life and function of these simplest of life forms will permit the control, modification, and use of microbes for both natural and industrial energy-related applications.

New research activities coordinated with activities in the Biological and Environmental Research program focus on a bacterial cell consisting of a minimal set of genes essential for life. The specific research target will be understanding the biochemical and physiological functions of this set of genes. Additional studies will determine the genes and gene functions required for a particular physiological process.

In the FY 2001 request, funding in the amount $2,440,000 is requested for these activities within the Energy Biosciences subprogram. New activities will be peer reviewed following broad solicitations for proposals.

Climate Change Technology Initiative

The FY 2001 budget contains a continuation of two carbon-related programs, each coordinated among several offices and agencies. The first is the Climate Change Technology Initiative (CCTI). CCTI focuses on the underpinning fundamental science that will enable mitigation of climate change. The second is the U.S. Global Change Research Program (US/GCRP). US/GCRP research focuses on developing the fundamental understanding of the comprehensive climate system and the global and regional manifestations of climate change. The two programs complement one another. For example, “A U.S. Carbon Cycle Science Plan” was undertaken by the US/GCRP and the “Carbon Sequestration Research and Development Report” was developed under the auspices of CCTI.

The component of CCTI conducted by the Office of Science focuses on carbon management science and includes sequestration science, science for efficient technologies, and fundamental science to advance low- and no-carbon energy sources. Research begun in the last two years in the area of low/no carbon energy technologies will provide the knowledge base for advanced technologies to reduce carbon dioxide emissions. This work is coordinated between the Basic Energy Sciences (BES) and Biological and Environmental Research (BER) programs, as well as with DOE's technology programs. These activities are expected to impact the Office of Energy Efficiency and Renewable Energy (EE) and the energy and transportation industry by providing options for increased efficiency and reduced energy consumption in manufacturing with improved sensors, controls, and processes. Other aspects of these research projects impact the Office of Fossil Energy (FE) by providing a foundation for effective and safe underground sequestration. The Office of Fossil Energy was a partner with the Office of Science in the development of the "Carbon Sequestration Research and Development Report." As a result, the two offices have a close connection and are jointly funding integrative systems research.

Ongoing CCTI includes two new efforts for carbon sequestration, the sequencing of the DNA of several microbes critical to biological sequestration, and over 50 single investigator and interdisciplinary projects at universities and national laboratories. Research projects span a broad array of disciplines, including ecological, biological, and geological studies of sequestration science; chemical and biological studies of alternative energy sources; new concepts in light-weight energy efficient materials; and more efficient combustion and conversion processes.

Focus areas within the BES program are those that promise the maximum impact in the area of carbon management and that build on strengths of current BES programs. In the Materials Sciences subprogram, research focuses on three areas: high-temperature materials for more efficient combustion, magnetic materials that reduce energy loss during use, and semiconductor materials for solar-energy conversion. In the Chemical Sciences subprogram, a major component of the research aims at reducing emissions of carbon dioxide through fundamental understanding of the chemistries associated with combustion, catalysis, photochemical energy conversion, electrical energy storage, electrochemical interfaces, and molecular specific separation from complex mixtures. In the Engineering and Geosciences subprogram, research emphasizes areas that will impact carbon dioxide sequestration in subsurface geologic formations. The program includes research to understand mechanical stability of porous and fractured reservoirs/aquifers, multiphase fluid flow within the aquifers, and geochemical reactivity in relevant conditions. Finally, in the Energy Biosciences subprogram, research emphasizes the biological process of photosynthesis, which is central to global carbon cycling.

In FY 2001, resources of $19,504,000 are being requested in BES and $16,257,000 in BER for CCTI activities. For BES, the FY 2001 request is the same as the FY 2000 appropriation. These funds will be used to continue the research projects selected in FY 2000. Specific focus areas within each subprogram are described in the subprogram narratives. All CCTI activities are peer-reviewed fundamental scientific research that expand upon core research activities.

Fundamental Research Relating to Solar and Renewable Energy Resources

Included in this request are funds in the amount of $47,100,000 that potentially impact solar and renewable energy resource production and use in the categories of "biomass," "wind energy," "photovoltaics," "hydrogen," and "other (solar photoconversion)." These funds provide continuing support for multidisciplinary, basic research in the BES Materials Sciences, Chemical Sciences, and Energy Biosciences subprograms.

These multidisciplinary research activities are also relevant to a number of other areas that impact energy. Funding totaling $6,300,000 in this category addresses Climate Change Technology Initiative. Indeed, the nature of most of the BES programs is to provide the results of basic research that impact a wide variety of applications. For example, research in the area of biomass focuses on understanding, at the mechanistic level, the biology of plants, algae, and non-medical microbes. While the majority of fundamental research on plants and non-medical microbes is directly related to biomass or renewables, the research also directly impacts many other disciplines and technologies including agricultural food production, plant-derived pharmaceuticals, textile fibers, wood and wood byproducts, environmental restoration, and fermentation technologies. Similarly, research in solar photoconversion focuses on the detailed nature of how molecules in the photo-excited state transfer electrons (and thus energy); this work impacts numerous technologies in addition to solar and renewable energy programs including sensors, molecular photonics, photodegradation of hazardous wastes, photo-assisted synthesis of chemicals, new analytical techniques (or methodologies), soil science, biological electron transfer, and carbon dioxide photoreduction. As a final example, research in photovoltaics focuses primarily on semiconductor physics and the synthesis of semiconductor materials. These materials are also used in microprocessors, batteries, displays, sensors, electrochromic windows, and semiconductor alloys.

Research activities in biomass, wind energy, photovoltaics, hydrogen, and solar photoconversion are coordinated through Coordinating Committees in the Department, through ad hoc meetings, through workshops, and through joint funding at universities and at the Department's laboratories. BES is a participant in the Department's bioenergy initiative, which is an effort to have a fully integrated research and development program focused on biomass and bioenergy products.

Funding of Contractor Security Clearances

In FY 1999, the Department divided the responsibility for obtaining and maintaining security clearances. The Office of Security Affairs, which was responsible for funding all Federal and contractor employee clearances, now pays only for clearances of Federal employees, both at headquarters and the field. Program organizations are now responsible for contractor clearances, using program funds. This change in policy enables program managers to make the decisions as to how many and what level clearances are necessary for effective program execution. In this way, it is hoped that any backlog of essential clearances which are impeding program success can be cleared up by those managers most directly involved. The Office of Science is estimating contractor clearances in FY 2000 and FY 2001 at $313,000 within this decision unit.

Workforce Development

BES-funded research supports U.S. graduate education to ensure the training of future professionals with scientific and engineering skills in areas important to the missions of BES and the Department, i.e., in materials sciences, chemical sciences, geosciences, plant and microbial biosciences, and engineering sciences. BES provides competitive financial support for doctoral degree candidates and post-doctoral investigators as an integral part of the funding for fundamental scientific research in these disciplines. Furthermore, BES scientific user facilities provide outstanding hands-on research experience to many young scientists. Thousands of students and post-doctoral investigators are among the more than 7,000 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. This program supported 3,000 graduate students and post doctoral investigators in FY 1999 through grants or contracts; 3,100 graduate students and post doctoral investigators used the BES science user facilities in FY 1999.

Funding Profile

	(dollars in thousands)				
	FY 1999 Current Appropriation	FY 2000 Original Appropriation	FY 2000 Adjustments	FY 2000 Current Appropriation	FY 2001 Request
Basic Energy Sciences					
Research					
Materials Sciences	404,885	405,000	-7,815	397,185	456,111
Chemical Sciences	202,157	209,582	-3,028	206,554	223,229
Engineering and Geosciences	41,665	37,545	-436	37,109	40,816
Energy Biosciences	29,078	31,000	-287	30,713	33,714
Subtotal, Research	677,785	683,127	-11,566	671,561	753,870
Construction	105,400	100,000	0	100,000	261,900
Subtotal, Basic Energy Sciences	783,185	783,127	-11,566	771,561	1,015,770
Use of Prior Year Balances	-4,002 [a]	0	0	0	0
General Reduction	0	-5,066	5,066	0	0
Contractor Travel	0	-3,873	3,873	0	0
Omnibus Rescission	0	-2,627	2,627	0	0
Total, Basic Energy Sciences	779,183 [b]	771,561	0	771,561	1,015,770 [c]

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

[a] Share of Science general reduction for use of prior year balances assigned to this program. The total reduction is applied at the appropriation level.

[b] Excludes $15,414,000 which was transferred to the SBIR program and $925,000 which was transferred to the STTR program.

[c] Includes $8,073,000 for Waste Management activities at Ames Laboratory and Argonne National Laboratory that were previously budgeted in FY 1999 and FY 2000 by the Environmental Management program.

Funding by Site

	(dollars in thousands)				
	FY 1999	FY 2000	FY 2001	$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory	24,950	24,427	27,861	+3,434	+14.1%
National Renewable Energy Laboratory	4,492	5,180	5,116	-64	-1.2%
Sandia National Laboratories	27,142	23,075	23,879	+804	+3.5%
Total, Albuquerque Operations Office	56,584	52,682	56,856	+4,174	+7.9%
Chicago Operations Office					
Ames Laboratory	18,838	16,990	16,165	-825	-4.9%
Argonne National Laboratory – East	144,752	140,005	160,726	+20,721	+14.8%
Brookhaven National Laboratory	79,425	75,441	75,769	+328	+0.4%
Princeton Plasma Physics Laboratory	675	0	0	0	0.0%
Chicago Operations Office	101,483	78,506	80,443	+1,937	+2.5%
Total, Chicago Operations Office	345,173	310,942	333,103	+22,161	+7.1%
Idaho Operations Office					
Idaho National Engineering and Environmental Laboratory	3,709	2,674	3,121	+447	+16.7%
Oakland Operations Office					
Lawrence Berkeley National Laboratory	66,080	63,386	68,537	+5,151	+8.1%
Lawrence Livermore National Laboratory	6,618	6,336	6,195	-141	-2.2%
Stanford Linear Accelerator Facility (SSRL)	26,475	23,042	31,592	+8,550	+37.1%
Oakland Operations Office	37,003	32,286	32,553	+267	+0.8%
Total, Oakland Operations Office	136,176	125,050	138,877	+13,827	+11.1%
Oak Ridge Operations Office					
Oak Ridge Inst. For Science and Education	1,881	745	1,114	+369	+49.5%
Oak Ridge National Laboratory	221,267	207,551	372,644	+165,093	+79.5%
Oak Ridge Operations Office	263	245	228	-17	-6.9%
Total, Oak Ridge Operations Office	223,411	208,541	373,986	+165,445	+79.3%
Richland Operations Office					
Pacific Northwest National Laboratory	12,887	12,063	12,295	+232	+1.9%
Richland Operations Office	163	0	0	0	0.0%
Total, Richland Operations Office	13,050	12,063	12,295	+232	+1.9%
Washington Headquarters	5,082	59,609	97,532	+37,923	+63.6%
Subtotal, Basic Energy Sciences	783,185	771,561	1,015,770	+244,209	+31.6%
Use of Prior Year Balances	-4,002[a]	0	0	0	0.0%
Total, Basic Energy Sciences	779,183[b]	771,561	1,015,770[c]	+244,209	+31.6%

[a] Share of Science general reduction for use of prior year balances assigned to this program. The total general reduction is applied at the appropriation level.

[b] Excludes $15,414,000 which was transferred to the SBIR program and $925,000 which was transferred to the STTR program.

[c] Includes $8,073,000 for Waste Management activities at Ames Laboratory and Argonne National Laboratory that were previously budgeted in FY 1999 and FY 2000 by the Environmental Management program.

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 phenomena, 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.

The laboratory is also home to the **Materials Preparation Center** (MPC), a user facility dedicated to the preparation, purification, and characterization of rare-earth, alkaline-earth, and refractory metal materials. Established in 1981, the MPC consolidates and makes available to scientists at university, industry, and government facilities the capabilities related to synthesis, processing, and characterization of advanced materials developed at Ames Laboratory during the course of its 40 years of basic research. Although the MPC is designated a national user facility, its operation differs from that of other such facilities in that the users do not conduct experimental or research activities within the Center; rather, they receive high purity materials or unique characterization services that are not available from commercial suppliers, on a full cost recovery basis. The MPC operates the Materials Referral System and Hotline and provides immeasurable value to the superconductivity community by publishing the bi-monthly High Tc Update.

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, chemical, and geosciences. 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 research on processes controlling the mobility of fluids and metals in the Earth's crust.

The **Advanced Photon Source** is one of only three third-generation, hard x-ray, synchrotron radiation light sources worldwide. Dedicated on May 1, 1996, the project was completed five months ahead of schedule and for $13,000,000 less than the baseline construction budget of $811,000,000. The APS has met or exceeded all technical specifications. The design of the 7 GeV synchrotron is optimized for insertion devices. The synchrotron radiation is produced at 34 bending magnets and 34 insertion devices, so that a capacity of 68 independently controlled beamlines can be made available for experimental research. This high-brilliance light source will be used by as many as 2,000 users annually 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. In addition, the light source will be used for a variety of technological applications, including micromachining and lithography. The first complement of beamlines have been assigned to user groups in Collaborative Access Teams (CATs), whose proposals were reviewed and approved based on their scientific program and the criticality of high-brilliance APS x-rays to their work. The CATs provided approximately $160,000,000 to fund fabrication of the first 40 beamlines at the APS. The facility is now considering proposals for the remaining available beamline ports.

The **Intense Pulsed Neutron Source** is a 30 Hz short-pulsed spallation neutron source using protons from a linac/rapid cycling synchrotron to produce neutrons in a depleted uranium target. Twelve beam lines serve 14 instruments, one of which is a test station for instrument development. IPNS was the first neutron or synchrotron source in the U.S. to operate all instruments in the user mode with time allocated by an external committee. 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. Scientists at IPNS have conceived techniques such as geometric and electronic time focusing, multi-chopper phasing, multiple converging aperture collimation, and neutron reflectometry. 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. 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. Staff at IPNS are taking a leadership role in the design and construction of instrumentation for the Spallation Neutron Source.

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 activities for pulsed radiolysis research at BNL. The innovative short-pulse radiation chemistry facility will contribute significantly to radiation sciences research in the next decade. 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** provides intense focused light from the infrared through the x-ray region of the spectrum by operating two electron storage rings: an X-ray ring and a vacuum ultraviolet (VUV) ring. X-Ray, ultraviolet, visible, and infra-red light from the storage rings is guided into 30 x-ray and 17 VUV beam ports, most of which are split into two to four experimental stations. The NSLS was commissioned in 1982. Annually, 2,300 scientists representing more than 350 institutions, over 50 of them corporations, conduct research at the NSLS in the fields of biology, chemistry, geology, materials science, medicine, metallurgy, and physics. In the basic sciences, researchers investigate the absorption and scattering of light to determine the properties of matter such as crystal structure, bonding energies of molecules, details of chemical and physical phase transformations, electronic structure and magnetic properties. The NSLS also serves as a training ground for future scientists. Between 1988 and 1999, over 600 graduate students used the NSLS in their doctoral thesis research.

The **High Flux Beam Reactor,** commissioned in 1965, is a heavy-water cooled and moderated reactor designed to produce neutrons for scattering. On December 21, 1996, the HFBR was shut down for normal refueling (a routine activity, which occured almost every month). However, before the reactor's scheduled restart, a plume of tritiated water emanating from a leak in the HFBR spent fuel pool was discovered contaminating the groundwater south of the reactor. Since that time, the reactor has been held in standby mode awaiting a decision by the Secretary of Energy on its future. On November 16, 1999, Secretary Richardson announced the permanent closure of the reactor. At that time, activities began that will transition the reactor from standby mode to permanent shut down mode.

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 diagnostics 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. 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, mechnical 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 experimental and computational research on rock physics of porous and fractured rock, subsurface imaging through both seismologic and electromagnetic methods, and hydrologic research on fluid flow through both pores and fractures. Geochemical studies focus on advanced interpretations of low-temperature flow processes, innovations in analytical geochemistry, isotope and trace-element chemistry with mass spectrometric and synchrotron-based analyses. 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 Sourc**e, which began operations in October 1993, is one of the world's brightest sources of ultraviolet light and soft x-rays. Soft x-rays of the ALS are an ideal tool for probing a wide range of electronic structural studies and are particularly useful for x-ray microscopy, surface science, and solid state physics of carbides, actinides and oxides. Such regions of the spectrum also offer special opportunities for research in chemical physics, electron spectroscopy, microscopy, and holography.

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 which 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 some distance 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 research in the mechanisms and kinetics of low-temperature geochemical processes, laboratory research on the source of electromagnetic response in crustal rocks, modeling and laboratory experiments on rock fracturing, and reactive fluid flow and transport within fractures. 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 research on rock physics, seismic imaging, and the physics of the Earth's electromagnetic field. Engineering research supports work to study the viscosity of mixtures of particles in liquids.

The **Los Alamos Neutron Science Center** provides an intense pulse source of neutrons for both national security research and civilian research. LANSCE is comprised of a high-power 800-MeV proton linear accelerator (linac), a Proton Storage Ring (PSR), production targets to the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) and the Weapons Neutron Research (WNR) facility, and a variety of associated experiment areas and spectrometers. Researchers at LANSCE use neutrons to study materials such as polymers, catalysts, and structural composites that are essential for many modern industrial products. 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, theoretical and experimental research on processing and properties of advanced semiconductor alloys and structures provided the basis for the computer-aided design and fabrication of a prototype solar cell; this cell has achieved 30% efficiency in conversion of the solar spectrum into electric energy. 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. There is also basic research in catalysis to better understand the chemistry necessary for carbon dioxide conversion.

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 five-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 which 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 Engineering and Geosciences subprogram investigates experimental and analytical geochemistry with innovative technical approaches for low-temperature geochemical processes in reservoirs and crystal rocks. 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, autolearning robots.

The **High Flux Isotope Reactor** is a light-water cooled and moderated reactor with a design power level of 100 megawatts currently operating at 85 megawatts. HFIR provides state-of-the-art facilities for neutron scattering and materials irradiation and is the world's leading source of elements heavier than plutonium for research, medicine, and industrial applications. HFIR has four horizontal beam tubes, which terminate in the neutron scattering beam room. There are a total of 11 instruments in the beam room and one additional instrument on the upper level. The installation of the new liquid hydrogen cold source will provide beams of cold neutrons for scattering research that are as bright as any in the world. Over the period FY 1999 – FY 2001, a number of improvements will be undertaken at HFIR to improve neutron scattering capabilities. These include the installation of larger beam tubes and shutters, a high-performance hydrogen cold source, and neutron scattering instrumentation. When completed, HFIR will have 14 state-of-the-art neutron scattering instruments on the world's brightest steady-state neutron beams. The improvements will be undertaken during an extended reactor outage in FY 2000 for the regularly scheduled (approximately every decade) replacement of the beryllium reflector.

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 theory and experiments related to the significant environmental clean-up concerns of the Department. Experimental research includes 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.

Princeton Plasma Physics Laboratory

Princeton Plasma Physics Laboratory (PPPL) is a program-dedicated laboratory (Fusion Energy Sciences) located on 72 acres in Princeton, New Jersey. The Basic Energy Sciences (BES) program funded a research program that is part of the Department's participation in the AMTEX Partnership™ to enhance the competitiveness of the U.S. Textile Industry. The program, entitled On-Line Process Control (OPCon), seeks to identify and develop technologies to provide faster transition between products, efficient production of small lots, and improved economics via elimination of off-quality production and off-line testing. The BES supported work is focused on development of instrumentation to measure fiber morphology in real time during synthetic fiber production by analysis of passive and active light scattering to measure birefringence of fibers.

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 Tonapah, Nevada. SNL is home to significant research efforts in materials and chemical sciences with additional programs in engineering and geosciences. SNL 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. Many of the research projects supported by the Materials Sciences subprogram at SNL/NM are relevant to the overall mission of the laboratory. Included among these are 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 leading program on the theory, structure, and dynamics of two-dimensional surface alloys is at SNL/CA.

The BES geophysics research effort at SNL/NM supports fundamental laboratory and imaging studies on rock mechanics, seismologic, and electromagnetic inversion studies, and experimental and theoretical studies on fluid and particulate flow in porous and fractured rock. Geosciences research focuses on theoretical and experimental geochemical investigations of stability and transport within minerals stable in the Earth's crust. 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. Basic research supported by the Chemical Sciences subprogram is often done in close collaboration with applied problems. 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. 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 the intense x-ray beams from the SPEAR storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third-generation synchrotron sources. The facility is now comprised of 29 experimental stations and is used each year by over 700 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 to all of the existing operational experimental stations and be of significant and direct benefit to the large and growing SSRL user community.

All Other Sites

The BES program funds research at 149 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 corrosion, metals, ceramics, alloys, semiconductors, superconductors, polymers, metallic glasses, ceramic matrix composites, catalytic materials, non-destructive evaluation, magnetic materials, surface science, 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. 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.

Research in nanoscale science will focus on the fundamental properties of nanoscale materials including their structural, physical, and chemical properties; on theory of nanoscale structures bridging atomic and molecular properties with bulk properties; and on the synthesis and processing of new nanoscale materials and materials using nanoscale structures. Research will continue on materials that will mitigate climate change effects of energy production and use by increasing efficiency, reducing energy losses, and displacing fossil fuels; focus areas will continue to be improved heat and corrosion resistant alloys to increase the efficiency of power generation, improved magnetic materials to reduce energy losses in motors, and more efficienct photovoltaic cells to displace fossil fuels.

Performance Measures

- Maintain and operate the scientific user facilities so that the unscheduled down time on average is less than 10 percent of the total scheduled operating time.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Materials Sciences Research....................	186,621	184,110	210,587	+26,477	+14.4%
Waste Management	0	0	8,073	+8,073	+100.0%
Facilities Operations................................	218,264	203,596	227,271	+23,675	+11.6%
SBIR/STTR	0[a]	9,479	10,180	+701	+7.4%
Total, Materials Sciences	404,885	397,185	456,111	+58,926	+14.8%

[a] Excludes $9,246,000 which has been transferred to the SBIR program and $555,000 which has been transferred to the STTR program.

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Materials Sciences Research			
■ **Structure of Materials:** This activity supports basic research in the characterization and structure 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 provides world-class scientific facilities to the Nation through the operation of four complementary, network-interfaced electron beam microcharacterization user centers at Oak Ridge National Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, and University of Illinois. These centers contain a variety of highly specialized instruments to characterize localized atomic positions and configurations, chemical gradients, interatomic bonding forces, etc. (FY 2001, $7,428,000) Major activities in FY 2001 will be responsive to the need for advanced instruments with capabilities to characterize and interpret atomic configurations and packing arrangements at the nano-scale with improved resolution and accuracy, including the ability to determine composition, bonding, and physical properties of materials. Needed are: single-atom sensitivity to impurities; 3-dimensional shape determination with atomic accuracy; the ability to find functional sites and determine the origin of the function; and the ability to measure optical absorption and emission from individual elements, preferably with femtosecond time resolution. 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 in a wide range of temperature and environments. Capital equipment is provided for items such as new electron microscopes and improvements to existing instruments.............	24,111	23,841	26,778

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Mechanical Behavior and Radiation Effects:** These activities support basic research in the mechanical behavior of materials including 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. These activities relate 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 also contribute to DOE missions in the areas of fossil energy, fusion energy, and radioactive waste storage. Major activities in FY 2001 will include continued development of experimental techniques and methods for the characterization of 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.	16,267	16,570	16,410
■ **Physical Behavior:** This activity supports basic research in the physical behavior of materials, including aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship to crystal defects and processing parameters to the superconducting current parameters 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. Major efforts in FY 2001 will continue fundamental studies of corrosion resistance and surface degradation, the performance of semiconductors, photovoltaics and 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.	13,496	14,065	13,790

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Engineering Behavior: This activity supports basic research in the engineering behavior of materials. The research includes materials synthesis and processing for 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. 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. The activity includes the operation of the Materials Preparation Center (FY 2001, $910,000) that makes available small quantities of specialized research quality materials for research purposes that are not commercially or otherwise available. Major activities for FY 2001 will include work on thermally unstable systems and large-scale deformation and fracture phenomena. There will be increased research on synthesis and processing of nanoscale materials. 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. .	15,226	15,521	18,218

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Neutron and X-ray Scattering:** This activity supports basic research in condensed matter physics that makes use of neutron and x-ray scattering at major BES-supported user facilities. This research is aimed at a fundamental understanding of the atomic, electronic, and magnetic structure of materials and the effect of structure on the physical properties of materials. In FY 2001, measurements of complex and collective phenomena, particularly in transition metal oxides, using neutron and x-ray scattering will be carried out to achieve greater understanding of how electrons in these materials respond to competing interactions among the charge and spin of electrons and the crystalline lattice. New instruments and techniques to use neutron and x-ray beams will be developed. The level of support for this activity in FY 2001 is determined by balance among all activities in condensed matter physics and by the availability of the neutron and x-ray beams to the scientific community and peer review of proposals. The enhancements of the High Flux Isotope Reactor and the Los Alamos Neutron Science Center, described later, will increase significantly the capacity for neutron scattering. In the long term, the Spallation Neutron Source will make a qualitative difference in the kinds of experiments that can be done. This activity will support increased research in neutron scattering to take advantage of the improved sources and to prepare for the Spallation Neutron Source. Capital equipment is provided for items such as detectors, monochromators, mirrors, and beamline instrumentation.	24,891	23,907	23,441
■ **Experimental Condensed Matter Physics:** This activity supports fundamental experimental research in condensed matter physics. Research includes measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This research is aimed at a fundamental understanding of the behavior of materials which underpins all DOE technologies. The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The measurements include optical and laser spectroscopy, electrical and thermal transport, thermodynamic and phase transition measurements, nuclear magnetic resonance, and scanning-tunneling and atomic-force microscopies. The development of new techniques and			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
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.			
Major efforts in FY 2001 will include continued support for investigations of materials with increasingly complex behavior, composition, and structures. A major new activity will be an enhanced emphasis on the growth of extremely high quality crystals of transition metal oxides and subsequent high precision measurements of various physical properties. The development of a sub-Angstrom resolution, Z-constant electron microscope will be continued as will be the development and operation of a 100 Tesla pulsed field magnet at LANL.			
This activity will provide increased support for nanoscale science including research of the optical, electronic, and transport properties of semiconductors at the nanoscale; charge and energy transport at nanometer length scales; magnets with optimum nanoscale configuration; relationship of nanostructures and thermal transport; photonic band gap materials. There will be increased 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.	32,420	33,313	35,649

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Condensed Matter Theory:** This activity supports basic research in theory, modeling, and simulations. This activity complements much of the experimental work by guiding and stimulating experiments. This activity will provide increased support for theory, modeling and large-scale computer simulation to explore new nanoscale phenomena and the nanoscale regime. The links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not well understood, although for the simplest semiconductor systems, carbon nanotubes, and similar "elementary" systems there has been considerable progress. However, for more complex materials and hybrid structures even the basic outlines of a theory describing these connections remains to be made. In nanoscale systems, thermal energy fluctuations and quantum fluctuations are comparable to the activation energy scale of the materials and devices, so that statistical and thermodynamic methods must include these effects adequately. 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 -- will play a major role in understanding materials at the nanometer scale and in the development "by design" of new nanoscale materials and devices. The greatest challenge and opportunity will be 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 group efforts in which individual scientists from different backgrounds work together to work on common research areas or make use of a common research facility. Capital equipment is provided for items such as computer work stations, beamline instruments, ion implantation and analytical instruments.	15,124	15,767	18,876
■ **Materials Chemistry:** 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. The research is aimed at a			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
fundamental understanding of the behavior of novel materials and structures. This activity includes research in solid state chemistry, surface chemistry, polymer chemistry, crystallography, synthetic chemistry, and colloid chemistry, which underpin technologies such as fuel cells, batteries, membranes, catalysis, electrochemistry, and solar energy conversion. This activity includes investigations of novel materials including 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 double rotation NMR, neutron reflectometry, and atomic force microscopy of liquids. Workshops on self-organized materials, and synchrotron x-ray micro-characterization have stimulated increased emphasis for these areas which will begin in FY 2001.			
The systematic and parallel patterning of matter on the nanometer scale also will receive increased support in FY 2001. The controlled positioning of atoms within small molecules is of course routinely achieved by chemical synthesis of identical molecules. 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 will focus on methods to prepare macroscopic quantities of nanoscale components in complex, designed patterns, using techniques of self assembly.			
Capital equipment is provided for such items as chambers to synthesize and grow new materials, nuclear magnetic resonance and electron spin resonance spectrometers, lasers, neutron reflectometers, x-ray beamlines, and atomic force microscopes. ..	25,938	25,796	27,645

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Experimental Program to Stimulate Competitive Research:** 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. Alaska was added to the group of EPSCoR states in FY 2000 and will be eligible for EPSCoR funding in FY 2001. The DOE EPSCoR program supports research cluster activities at six EPSCoR states through cooperative agreements and has awarded individual investigator grants in nearly all EPSCoR states (only Maine and Nebraska are exceptions) and Puerto Rico. The work supported by the EPSCoR program includes research in organic semiconductors, membranes, photochemistry, synchrotron radiation and ion beams, tribology, thin film optoelectronics, catalysis, high energy particle physics, experimental nuclear physics, human genome research, desert vegetation, characterization of petroleum reservoirs, and wind and electrochemical power sources. In FY 2001, an increase is requested 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. Faculty and student teams from EPSCoR states will engage in research programs that couple academic study with hands-on research experiences in national laboratory settings. Workshops and discussions are ongoing with representative scientists from EPSCoR states to acquaint them with the facilities and personnel at the DOE Laboratories...........	6,815	6,815	9,815

EPSCoR Distribution of Funds by State

(dollars in thousands)

	FY 1999	FY 2000 Estimate	FY 2001 Estimate
Alabama	825	75	25
Alaska	0	0	0
Arkansas	100	100	50
Idaho	100	100	50
Kansas	91	95	85
Kentucky	650	200	0
Louisiana	152	146	0
Maine	750	0	0
Mississippi	50	50	50
Montana	75	75	75
Nevada	855	96	0
North Dakota	47	46	0
Oklahoma	100	100	100
Puerto Rico	800	50	0
South Carolina	800	800	750[a]
South Dakota	50	50	0
Vermont	25	25	0
West Virginia	100	100	0
Wyoming	800	800[a]	0[a]
Other	445[b]	3,907[b]	8,630[b]
Totals	6,815	6,815	9,815

[a] In FY 2000, the funding commitment to the State of Wyoming will expire. The State of South Carolina's funding commitment is scheduled to expire in FY 2001.

[b] Includes technical support for the Experimental Program to Stimulate Coompetitive Research (EPSCoR). Uncommitted funds in FY 2000 and FY 2001 will be competed among all EPSCoR states that do not have active Research Implementation Awards to begin new Research Implementation Awards. All EPSCoR states will be eligible for awards for university-laboratory science education partnerships.

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Los Alamos Neutron Science Center (LANSCE) instrumentation enhancement:** This project is a major item of equipment with a total estimated cost of $20,500,000 that will provide enhanced instrumentation at the LANSCE and will be implemented concurrently with an accelerator upgrade funded by the Office of Defense Programs.	4,500	3,500	4,500
■ **Extension of HB-2 Beam Tube at the High Flux Isotope Reactor:** This project, a major item of equipment with a total estimated cost of $5,550,000, which is lower than the original estimate of $5,900,000, 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.	2,800	1,600	1,150
■ **Replacement of High Flux Isotope Reactor Monochrometer Drums**	1,800	0	0
■ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor:** Capital equipment funds are provided for new and upgraded instrumentation.	0	0	2,000
■ **SPEAR3 Upgrade:** The SPEAR 3 upgrade at SSRL, which is being funded jointly and equally by DOE and NIH, with initial NIH funding in FY 1999, will provide major improvements to all of the existing operational experimental stations. The increased flux from the bending magnet and wiggler beam lines will greatly extend their performance in a variety of applications including, for example: (1) powder and thin film diffraction studies of materials, (2) topographic studies of materials structure, (3) surface microcontamination on Si wafers, (4) x-ray tomographic analysis, (5) x-ray absorption studies of speciation in environmental samples, and (6) 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 physical buildings. The DOE portion of SPEAR 3 is a major item of equipment with a total estimated cost of $29,000,000. The total estimated Federal cost, including NIH funding, is about $58,000,000	0	0	8,000

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Advanced Light Source Beamline:** 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..	1,500	0	900
■ **Climate Change Technology Initiative:** Basic research focuses on three areas: high temperature materials, magnetic materials, and semiconductor materials. A major goal is the derivation of materials that can withstand higher temperatures for more efficient combustion and for improved properties in applications. Research activities include: (1) an atomic-level understanding of bulk metallic glasses, which have the potential to make significant contributions in corrosion and wear resistance, e.g., in fossil fueled power plants, and on structural ceramics, e.g., for use in high temperature applications such as engine components; (2) surface physics and chemistry of oxide layers, which is expected to produce alloys and coatings that have improved corrosion resistance at high temperatures; (3) the microstructure of magnetic materials, which is expected to result in stronger magnets with reduced energy loss during use; (4) new semiconductor materials, in particular innovative nano and mesoscale physics, which could lead to breakthrough advances in the efficiency of conversion of light to electricity; (5) magnetic materials, which are critical to energy efficiency, since electric motors consume about two-thirds of U.S. electric power; and (6) the development of new semiconductor materials for solar energy conversion stressing very innovative studies in nanoscale and mesoscale physics that might lead to breakthrough advances.	1,733	3,415	3,415
Total, Materials Sciences Research	186,621	184,110	210,587
Waste Management			
■ **Waste Management:** 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	0	0	8,073

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Facilities Operations			
■ **Operation of National User Facilities:** The facilities included in Materials Sciences are: National Synchrotron Light Source, Intense Pulsed Neutron Source, Stanford Synchrotron Radiation Laboratory, Manuel Lujan, Jr. Neutron Scattering Center, High Flux Isotope Reactor, Advanced Light Source, and the Advanced Photon Source. Research and development in support of the construction of the Spallation Neutron Source is also included. The facility operations budget request includes operating funds, capital equipment, and Accelerator and Reactor Improvements (AIP) funding under $5,000,000 that are presented in a consolidated manner later in this budget. AIP funding will support additions and modifications to accelerator and reactor facilities that are supported in the Materials Sciences subprogram. Included in the AIP funding are funds for HFIR extended cold guides, extension of the Neutron Sciences Support Building, and general infrastructure upgrades. Capital equipment is needed at the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front end components, monochromotors, 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....	195,496	184,014	209,750
■ **High Flux Beam Reactor (HFBR):** Funding in FY 2001 is provided to complete the process of placing the Reactor in a safe shutdown condition and for surveillance. Disposition of the scientific instruments is included within this funding. As long as the reactor contains activated components, surveillance activities will continue. Surveillance will continue until the reactor is fully decommissioned and decontaminated.................	22,768	19,582	17,521
Total, Facilities Operations	218,264	203,596	227,271

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Facilities			
Advanced Light Source	31,206	31,039	35,445
Advanced Photon Source	86,226	85,625	94,677
National Synchrotron Light Source	24,094	24,038	28,293
Stanford Synchrotron Radiation Laboratory	4,046	3,942	4,015
High Flux Beam Reactor	22,768	19,582	17,521
High Flux Isotope Reactor	700	2,400	4,600
Intense Pulsed Neutron Source	12,102	11,699	13,642
Manuel Lujan, Jr. Neutron Scattering Center	7,397	7,371	9,978
Spallation Neutron Source	28,600	17,900	19,100
Partial Offset to Science General Reduction Applied to BES	1,125	0	0
Total, Facilities	218,264	203,596	227,271

SBIR/STTR Funding

■ In FY 1999, $9,246,000 and $555,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	9,479	10,180
Total, Materials Sciences	404,885	397,185	456,111

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Materials Sciences Research	
■ Decrease in research for structure of materials ($-468,000); increase in research in the area of nanoscale science, engineering, and technology for structure of materials ($+3,405,000).	+2,937
■ Decrease in research for mechanical behavior and radiation effects.	-160
■ Decrease in research in physical behavior.	-275
■ Decrease in research for engineering behavior ($-303,000); increase in research in the area of nanoscale science, engineering, and technology for engineering behavior ($+3,000,000).	+2,697

	FY 2001 vs. FY 2000 ($000)
■ Decrease in research for neutron and x-ray scattering.	-466
■ Decrease in research for experimental condensed matter physics ($-654,000); increase in research in the area of nanoscale science, engineering, and technology for experimental condensed matter physics ($+2,990,000).	+2,336
■ Decrease in research for condensed matter theory ($-308,000); increase in research in the area of nanoscale science, engineering, and technology for condensed matter theory, modeling and simulation at the nanoscale ($+3,417,000).	+3,109
■ Decrease in research for materials chemistry ($-503,000); increase in research in the area of nanoscale science, engineering, and technology for experimental condensed matter physics ($+2,352,000).	+1,849
■ Increase in support for the Experimental Program to Stimulate Competitive Research to facilitate student training and university/laboratory science education partnerships.	+3,000
■ Increase in capital equipment for ALS beamline	+900
■ Increase in capital equipment for LANSCE instruments.	+1,000
■ Decrease in capital equipment funds for extension of HB-2 beam tube at HFIR for thermal neutron scattering because of completion of scheduled activities.	-450
■ Increase for SPEAR 3 upgrade	+8,000
■ Increase for the High Flux Isotope Reactor for capital equipment for new and upgraded instrumentation.	+2,000
Total, Materials Sciences Research	+26,477
Waste Management	
■ Increase for Waste Management activities at ANL and Ames	+8,073
Facilities Operations	
■ Increase for the Advanced Light Source for operations, increased support for users, capital equipment, and infrastructure improvements	+4,406
■ Increase for the Advanced Photon Source for operations, increased support for users, capital equipment, fabrication of front ends and insertion devices, and other infrastructure improvements	+9,052
■ Increase for the National Synchrotron Light Source for operations, capital equipment, and infrastructure improvements	+4,255
■ Increase for the Stanford Synchrotron Radiation Laboratory for operations	+73
■ Decrease for the High Flux Beam Reactor operations because of shutdown	-2,061

	FY 2001 vs. FY 2000 ($000)
■ Increase for the High Flux Isotope Reactor for cold guide extensions, an extension of the Neutron Sciences Support Building, and infrastructure improvements.........	+2,200
■ Increase for the Intense Pulsed Neutron Source for operations..............................	+1,943
■ Increase for the Manuel Lujan, Jr. Neutron Scattering Center for the operations....	+2,607
■ Increase in the Spallation Neutron Source research and development funds	+1,200
Total, Facilities Operations.	+23,675
SBIR/STTR	
■ Increase in SBIR/STTR funding because of increase in operating expenses	+701
Total Funding Change, Materials Sciences	+58,926

Chemical Sciences

Mission Supporting Goals and Objectives

The Chemical Sciences subprogram has two major components. One major component is comprised of photo- and radiation chemistry; chemical physics; and atomic, molecular and optical (AMO) science. This research provides a foundation for understanding fundamental interactions of atoms, molecules, and ions with photons and electrons. This work also underpins our fundamental understanding of chemical reactivity. This, in turn, 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. The other major component of the research program is comprised of physical chemistry, inorganic chemistry, organic chemistry, analytical chemistry, separation science, heavy element chemistry, and aspects of chemical engineering sciences. The research supported provides a better molecular level understanding of homogeneous and heterogeneous reactions occurring at surfaces, interfaces, and in bulk media. This has resulted in improvements to known heterogeneous and homogeneous catalytic systems, new catalysts for the production of fuels and chemicals, and better analytical methods in a wide variety of applications in energy processes. It has also provides new knowledge of actinide elements and separations important for environmental remediation and waste management, and better methods for describing turbulent combustion and predicting thermophysical properties of multicomponent systems.

The Climate Change Technology Initiative (CCTI) effort, begun two years ago will continue in FY 2001 at a constant level of effort. New research in nanoscience and computational chemistry will expand the base programs in areas that support the DOE and BES missions. The compelling new science these expanded research efforts promise include understanding the preparation and structure/function relationship of large molecules and molecular assemblies with applications in catalysis, membranes, electochemistry, and chemically reacting flow. Nanoscale systems represent the smallest assemblies of atoms and molecules that demonstrate the collective behavior of macroscopic systems whose properties can be modeled and predicted using modern computational tools based on fundamental quantum theories and which exhibit, in themselves, unique and novel properties as exemplified by buckyballs and nanotubes. The study of chemistry at the nanoscale is crucial for understanding how molecules recognize one another and self-assemble and how chemistry is controlled by and within self-contained nanostructures. Nanoscale chemistry suggests unique control of chemical reactions with a specificity and degree of cooperativity that heretofore has been seen only in the self-replicating chemistry of biological systems. Coupled with computational chemistry, nanoscale research affords an opportunity of unparalleled complexity and imagination. It bridges the gap in chemical understanding between the molecular scale and the laboratory scale of our macroscopic world.

Performance Measures

- Maintain and operate the scientific user facilities so that the unscheduled downtime on average is less than 10 percent of the total scheduled operating time.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Chemical Sciences Research	132,109	131,681	148,893	+17,212	+13.1%
Facilities Operations	69,561	70,173	69,243	-930	-1.3%
SBIR/STTR	0[a]	4,700	5,093	+393	+8.4%
Congressional Direction	487	0	0	0	0.0%
Total, Chemical Sciences	202,157	206,554	223,229	+16,675	+8.1%

Detailed Program Justification

(dollars in thousands)

FY 1999	FY 2000	FY 2001

Chemical Sciences Research

- **Photochemistry and Radiation Research:** The photochemistry and radiation science research program focuses on fundamental molecular level understanding of the capture and conversion of energy. Photochemistry research is centered on understanding capture of energy from light (solar energy) and conversion of that energy into other forms, like electrical or chemical. Among the important chemical issues are the light-induced charge separation needed for chemical reactions to proceed from excited states. Radiation science research focuses on similar processes at the molecular level but associated with 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. For FY 2001 the focus will include improved theoretical models of heterogeneous electron transfer; studies of the photophysics and chemistry of excited states; early processes in capture of high energy electrons derived from radiation sources and improved understanding of natural photosynthesis.

[a] Excludes $4,425,000 which has been transferred to the SBIR program and $265,000 which has been transferred to the STTR program.

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
New opportunities offered by nanoscale science, engineering and technology will enable studies of artificial and biological self assembled membranes to isolate and optimally configure chromophores to act as electron-donors and acceptors for efficient charge separation that will allow the desired reaction pathways to be controlled. In addition, studies of quantum dots having unique spectral and electrical properties will be pursued, which have the potential to revolutionize direct solar to electrical energy conversion.			
Capital equipment is provided for such items as lasers, microscope scanners, liquid chromatographs, and temperature controllers.	23,871	23,351	25,842

- **Chemical Physics Research:** This program investigates -- at the molecular level -- chemical reactions in the gas phase, at surfaces, and at interfaces and the relationship between molecular scale phenomena and bulk phenomena. Research activities involve closely-coupled experimental and theoretical efforts. Experimental projects include studies of molecular dynamics, chemical kinetics, spectroscopy, clusters, and surface science. The surface science and clusters research is aimed at providing predictive capability for surface mediated catalysis through provision of explanatory theories relating surface structure to surface mediated chemistry. One of the goals of the chemical physics program is to provide data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models for predicting the efficiency and emission characteristics of combustion devices and for optimization and control of combustion devices.

  In FY 2001, nanoscience engineering and technology research will expand chemistry of clusters focusing on understanding the relationship between unique electronic properties of nanoscale clusters and their chemical and catalytic properties.

  Another expanded activity in FY 2001 will be theory, modeling, and computational chemistry both at the nanoscale and at the macroscopic scale. Chemistry at the nanoscale is taken to mean the chemistry that occurs between individual molecules, between molecules and small agglomerations or clusters of molecules, and between molecules and surfaces. The behavior of such processes as catalysis, chemical vapor deposition, and combustion is the result of a very large number of individual

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
processes occurring at the nanoscale. Theory and modeling at the nanoscale is concerned with solving the fundamental quantum mechanical equations that describe the chemistry of individual molecules with one another and with extended structures such as clusters and surfaces. Great progress has been made in the past half century in bringing molecular theory and modeling from a purely qualitative aid to an exact predictive tool for three and four atom systems. Moving to the scale of chemistry at the nanoscale, which may involve molecules with tens to hundreds of atoms interacting with themselves and with extended structures, requires new computational tools of greater complexity than are available today. Chemistry at the macroscopic scale involves the processes that relate the microscopic to the macroscopic. Of particular importance is the interaction of chemistry with fluid dynamics. Fluid dynamics is responsible for the mixing of reactants and the removal of products. The energy release in chemical reactions directly affects the fluid dynamics of the reacting system whether it is gas phase, liquid phase, or chemistry at interfaces. Computational chemistry methods based on the tools and theories from statistical mechanics and thermodynamics will be developed and applied with the end of accurate prediction of macroscopic scale chemistry for a range of energy relevant applications. Approximately $2,050,000 is requested for theory, modeling, and simulation of chemistry at the nanoscale; and $1,952,000 is requested for theory, modeling, and simulation of chemistry at the macroscopic scale.			
Capital equipment is provided for such items as pico- and femtosecond lasers, high speed detectors, spectrometers and computational resources..	27,460	26,188	32,784
■ **Atomic, Molecular, and Optical (AMO) Science:** This program supports theory and experiment to understand the interactions among atoms, molecules, ions, electrons, photons, and electromagnetic fields. This work provides the most basic underpinning of a broad spectrum of BES research activities including chemical reactivity, chemical physics, analytical techniques, materials sciences, and new instrumentation. It is this program that contributes knowledge at the most fundamental level necessary for science-based optimization of current energy sources and development of new ones.			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Furthermore, this program has produced our most detailed understanding of the interactions of particles with matter, which enables us to understand the phenomena observed at the BES-supported synchrotron radiation light sources, the electron beam microcharacterization centers, and the neutron scattering facilities. Furthermore, work in AMO science has resulted in new measurement techniques and instrumentation that are widely used by other scientific disciplines and by industry and medical sciences. A continuing series of workshops have helped define areas of priority for BES for FY 2001 and beyond. These areas include studies of novel materials such as nanostructured materials, quantum dots, and artificial atoms; and heavy-ion and highly-charged ion collisions.			
New funding for nanoscience engineering and technology will enable expanded efforts to understand the most fundamental aspects of collective phenomena that are the basis for the unique properties of nanoscale materials.			
Capital equipment is provided for such items as pulse processing electronics, laser upgrades, position sensitive and solid state (SiLi) detectors..	11,018	11,092	12,123
■ **Catalysis and Chemical Transformation:** This activity supports basic research related to chemical transformations and conversions that are fundamental to new or existing concepts for improving energy efficiency, production and storage. The emphasis is on understanding the fundamental chemical principles underlying new and developing technologies. Of particular interest are research activities with the objectives of understanding the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources; and the chemistry of precursors to 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 products. The creation of new organometallic precursors has the potential of providing materials that are synthesized by less-energy-intensive processes than older materials they replace or which function as energy-saving media themselves. New opportunities identified for FY 2001 include understanding how the structural changes induced by molecular substrates alter the catalytic activity of surfaces, and understanding chemistry at the interface between water and catalytic oxides.			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
New research enabled by nanoscience engineering and technology will focus on understanding the unique catalytic properties of metal, mixed metal and oxide particles on surface catalyzed reactions, the properties of reactions within nanoscale cavities, and the structure/function and reactivity of nanoscale rafts dispersed on active and inactive supports. Other activities will include the synthesis of discrete nanomaterials derived from molecular building blocks.			
Capital equipment is provided for such items as ultrahigh vacuum equipment, Fourier-transform infrared instrumentation, and high-field, solid-state Nuclear Magnetic Resonance (NMR) spectrometers..	22,304	21,857	24,952
■ **Separations and Analyses:** Chemical separations are ubiquitous in Department missions and in industry, and analysis is an essential component of every chemical process, from manufacture through safety and risk assessment. This research addresses the fundamental molecular level questions that underpin chemical separations and analytical methods. The program covers a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. The effort continues to improve the sensitivity, reliability, and productivity of analytical determinations, as well as enable entirely new approaches to analysis. The program focus is to obtain a thorough understanding of the basic chemistry of separations systems and analytical tools so that their utility can be realized. For FY 2001 new opportunities identified are to more fully understand the responses of molecular systems to changes driven by small energy differences and developing the understanding necessary to enable scaling from the molecular to meso- and finally to macoscale.			
New studies at the nanoscale will address molecular transport in nanoscale structures as well as the formation of macroscopic separation systems via self-assembly of nanoscale precursors. Analytical research will explore monitoring of chemical processes in individual cells along with single-molecule detection in nanoscale volumes.			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Capital equipment is provided for such items as computational workstations and inductively-coupled plasma torch spectrometers for atomic emission determination.	13,463	12,617	14,617
■ **Heavy Element Chemistry:** This program is the principal source of support in fundamental chemistry of the actinide elements for the Nation. The Department has stewardship responsibilities for providing the Nation with basic knowledge of the chemistry of these elements because of their importance to nuclear technology and to the Department's efforts to remediate its former weapons production sites. There are strong links between this activity and the actinide chemistry efforts in the Environmental Management Science Program.			
New opportunities for FY 2001 are in the emerging areas of solid-state speciation and reactivity, and advanced theoretical methods for prediction electronic and molecular structure and reactivity.			
New activities at the nanoscale will focus the role of actinides as probes to understand nanoscale disorder on the chemistry of materials and the chemistry and properties of nanostructures for actinide encapsulation relevant to remediation and drug delivery systems.			
Capital equipment is provided for such items as an x-ray diffractometer and equipment for synchrotron light sources to safely handle the actinides.	6,642	6,720	7,376
■ **Chemical Energy and Chemical Engineering:** This activity addresses energy aspects of chemically related engineering sciences, including thermodynamics, turbulence related to combustion, and physical and chemical rate processes. Particular attention is given to experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena, and to the physics of gas phase turbulence. Also included are fundamental studies of thermophysical and thermochemical properties. 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 non-automotive electrochemical energy storage systems. The			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
program covers a broad spectrum of research including fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces.			
There are strong links with related efforts within the Department and other federal agencies through the Combustion Coordinating Committee and the federal interagency battery consortium.			
For FY 2001 new opportunities highlight the need to couple the current emphasis of the program in molecular simulations with molecular level theory.			
New nanoscience engineering and technology activities will include the controlled chemical modification and construction of nanoscale carbon structures to enable improved molecular electronic devices and electrochemical energy storage and conversion systems.			
Capital equipment is provided for such items as computer work stations and electrochemical apparatus.	9,207	9,009	9,975
■ **Climate Change Technology Initiative:** Basic research in carbon management emphasizes atomic and molecular level understanding of chemical processes to enable predictive capability. Examples of these activities are: understanding charge separation and electron transfer processes critical to photochemical reduction of carbon dioxide with water or hydrogen to hydrocarbons; understanding the interactions and dynamics between molecules and catalysts that result in new catalysts for carbon dioxide insertion into chemicals and understanding the complex relationship between chemical reaction dynamics and turbulence that are critical to improving the efficiency of fossil fuel combustion processes.	2,214	4,394	4,394
■ **General Plant Projects (GPP):** 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 landlord responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. Additional			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
GPP funding is included in the Facilities Operations justification. The total estimated cost of each GPP project will not exceed $5,000,000	10,844	10,153	10,275
■ **General Purpose Equipment (GPE):** GPE funding is provided for Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the Basic Energy Sciences responsibilities for these laboratories for general purpose equipment that supports multipurpose research.	5,086	5,550	5,655
■ **Advanced Light Source Beamline:** 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	0	750	900
Total, Chemical Sciences Research	132,109	131,681	148,893

Facilities Operations

	FY 1999	FY 2000	FY 2001
■ **Facilities Operations:** The facilities included in Chemical Sciences are: National Synchrotron Light Source, High Flux Isotope Reactor, Radiochemical Engineering Development Center, Stanford Synchrotron Radiation Laboratory, 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 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. 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	69,561	70,173	69,243

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Facilities			
National Synchrotron Light Source	8,082	8,071	8,207
Stanford Synchrotron Radiation Laboratory	19,373	17,982	18,459
High Flux Isotope Reactor	29,659	32,132	29,601
Radiochemical Engineering Development Center	7,027	6,985	7,145
Combustion Research Facility	5,024	5,003	5,831
Partial Offset to Science General Reduction Applied to BES	396	0	0
Total, Facilities	69,561	70,173	69,243

SBIR/STTR Funding			
■ In FY 1999, $4,425,000 and $265,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	4,700	5,093
Congressional Direction			
■ Funds research related to identification of trace element isotopes in environmental samples at the University of Nevada – Las Vegas (per Congressional Direction).	487	0	0
Total, Chemical Sciences	202,157	206,554	223,229

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Chemical Sciences Research	
■ Increase in research for photochemistry and radiation research ($+591,000); and increase in research in the area of nanoscale science engineering, and technology for photochemistry and radiation research ($+1,900,000).	+2,491
■ Increase in research for chemical physics ($+664,000); increase in research in the area of nanoscale science engineering, and technology for chemical physics ($+3,980,000); and increase in research for theory, modeling, and simulation in nanoscale chemistry and in computational chemistry ($+1,952,000).	+6,596
■ Increase in research for atomic, molecular and optical sciences ($+281,000); and increase in research in the area of nanoscale science engineering, and technology for atomic, molecular and optical sciences ($+750,000).	+1,031
■ Increase in research for catalysis and chemical transformation ($+555,000); and increase in research in the area of nanoscale science engineering, and technology for catalysis and chemical transformations ($+2,540,000).	+3,095
■ Increase in research for separations and analysis ($+320,000); and increase in research in the area of nanoscale science engineering, and technology for separations and analysis ($+1,680,000).	+2,000
■ Increase in research for heavy element chemistry ($+170,000); and increase in the area of nanoscale science engineering, and technology for heavy element chemistry ($+486,000).	+656
■ Increase in research for chemical energy and chemical engineering ($+231,000); and increase in research in the area of nanoscale science engineering, and technology for chemical energy and chemical engineering ($+735,000).	+966
■ Increase in research for ALS Beamline	+150
■ Increase in GPE.	+105
■ Increase in GPP.	+122
Total, Chemical Sciences Research	+17,212
Facilities Operations	
■ Increase for the National Synchrotron Light Source for operations	+136
■ Increase for the Stanford Synchrotron Radiation Laboratory for operations	+477

	FY 2001 vs. FY 2000 ($000)
■ Increase for the High Flux Isotope Reactor for operations and to provide increased support for users	+3,448
■ Decrease funding for the High Flux Isotope Reactor in accordance with completion of the Be reflector	-5,979
■ Increase for Radiochemical Engineering Development Center	+160
■ Increase for the Combustion Research Facility for operations	+828
Total, Chemical Sciences Facilities	-930
SBIR/STTR	
■ Increase SBIR/STTR funding because of increase in operating expenses	+393
Total Funding Change, Chemical Sciences	+16,675

Engineering and Geosciences

Mission Supporting Goals and Objectives

The Engineering and Geosciences subprogram conducts research in two disciplinary areas, engineering and geosciences. In Engineering Research, the goals are to extend the body of knowledge underlying current engineering practice to create new options for improving energy efficiency and to broaden the technical and conceptual knowledge base for solving the engineering problems of energy technologies. In Geosciences Research, the goal is on fundamental knowledge of the processes that transport, concentrate, emplace, and modify the energy and mineral resources and the byproducts of energy production. The research supports existing energy technologies and strengthens the foundation for the development of future energy technologies. Ultimately the research impacts control of industrial processes to improve efficiency and reduce pollution, to increase energy supplies, and to lower cost and increase the effectiveness of environmental remediation of polluted sites.

Engineering Research will have increased emphasis on fundamental engineering principles that are needed to exploit advances in nanoscale science, including thermal and mechanical properties at the nanoscale; control methods for nanosystems; reliable packaging, assembling, powering, and actuating of nano-devices; and instrumentation for on-line diagnostics and control of nanodevices. In addition, a new, university-based research effort in Robotics and Intelligent Machines will focus on sensors and sensor integration, remote operation and data acquisition, and controls. Geosciences Research will continue activities in Climate Change Technology research to gain the scientific understanding for improving the characterization of subsurface formations and their host potential for carbon dioxide sequestration.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Engineering Research	17,476	14,352	17,767	+3,415	+23.8%
Geosciences Research	24,189	21,819	22,027	+208	+1.0%
SBIR/STTR	0[a]	938	1,022	+84	+9.0%
Total, Engineering and Geosciences	41,665	37,109	40,816	+3,707	+10.0%

[a] Excludes $1,013,000 which has been transferred to the SBIR program and $61,000 which has been transferred to the STTR program.

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Engineering Research			
■ **Engineering Research:** The Engineering Research activity supports work in mechanical systems including fluid mechanics, heat transfer, and solid mechanics; systems sciences including process control, instrumentation, and intelligent machines and systems; and engineering analysis including nonlinear dynamics, data bases for thermophysical properties, models of combustion processes for engineering applications and foundation of bioprocessing of fuels, and energy related waste and materials. In FY 2001, a program will be established in nanoscale science, engineering, and technology with emphasis on fundamental engineering principles that are needed to exploit advances in nanoscale science, including thermal and mechanical properties at the nanoscale; control methods for nanosystems; reliable packaging, assembling, powering, and actuating of nano-devices; and instrumentation for on-line diagnostics and control of nanodevices. In addition, in FY 2001, a new, university-based research effort in Robotics and Intelligent Machines will focus on sensors and sensor integration, remote operation and data acquisition, and controls. ($1,947,000).	17,476	14,352	17,767
Geosciences Research			
■ **Geosciences Research:** The Geosciences subprogram supports basic research in geochemistry and geophysics. The objective is to advance our understanding of fundamental geological processes so we can make wise choices among current and emerging energy and environmental technologies. Geochemical research focuses on fundamental understanding of subsurface solution chemistry, mineral-fluid interactions, mineral thermodynamics and natural isotopic systems. These studies provide a critical foundation for understanding oil, gas, and geothermal resource recovery and control of contaminants in groundwater flow. Geophysical research focuses on understanding the physical properties of fluids, rocks and minerals and developing improved methods to image these properties. Geophysical imaging is the key for non-invasive discovery and monitoring subsurface reservoirs, fluid pathways,			

	FY 1999	FY 2000	FY 2001
and physical property distributions in the earth. These studies provide the fundamental science base for new capabilities to locate and monitor oil and gas reservoirs, contaminant migration and for characterizing disposal sites for energy related wastes. Improved understanding of earth processes is required to quantitatively predict the response of earth systems to natural and man-made perturbations	22,792	14,997	15,205
■ **Climate Change Technology Initiative:** Geosciences research will continue to emphasize improved understanding of fundamental geological processes that impact concepts for sequestration of carbon dioxide in subsurface reservoirs. The research will continue with its focus on four areas: (1) improved understanding of the mechanical stability of porous and fractured reservoirs/aquifers over injection periods required for sequestration; (2) improved understanding of multiphase fluid flow within aquifers; (3) improved understanding of the geochemical reactivity within and among fluids, and between fluids and rock material within reservoirs/aquifers; (4) improving the resolution of geophysical imaging to monitor the injection and storage integrity during the lifetime of the sequestration site..	1,397	6,822	6,822
Total, Geosciences Research	24,189	21,819	22,027
SBIR/STTR Funding			
■ In FY 1999, $1,013,000 and $61,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	938	1,022
Total, Engineering and Geosciences	41,665	37,109	40,816

(dollars in thousands)

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Engineering Research	
■ Decrease in core engineering research ($-293,000); and increase in research in the area of nanoscale science, engineering, and technology ($+1,761,000).	+1,468
■ Increase for new, university-based research effort in Robotics and Intelligent Machines.	+1,947
Total, Engineering Research	+3,415
Geosciences Research	
■ Increase in research	+208
SBIR/STTR Funding	
■ Increase SBIR/STTR funding because of increase in operating expenses	+84
Total Funding Change, Engineering and Geosciences	+3,707

Energy Biosciences

Mission Supporting Goals and Objectives

The Energy Biosciences subprogram supports fundamental research related to a molecular level understanding of the formation, storage, and interconversion of energy by plants and microorganisms. Plants and microbes serve as renewable resources for fuel and other fossil resource substitutes, as agents to restore previously disrupted environmental sites, and as potential components of industrial processes to produce new products and chemicals in an environmentally benign manner. The program supports research in a number of topics related to these areas. These include research in photosynthesis and bioenergetics; the biosynthesis, structure and function of plant cell walls (the major component of plant biomass); the bioproduction and bioconversion of methane; the biodegradation of lignocellulose; the biosynthesis of starch and lipids (plant energy storage compounds); plant secondary metabolism; microbial fermentations; microbial thermophily; and processes that offer unique possibilities for research at the interface of biology and the physical, earth, and engineering sciences.

Research will continue on activities that impact climate change, including investigations of plants, algae, and microbes and their role in the capture and release of atmospheric carbon dioxide. The biological processes of carbon dioxide fixation offer numerous possibilities leading to the reduction of atmospheric carbon dioxide levels by replacing fossil-derived fuels with renewable resources or providing fixed carbon for long-term sequestration. New research in 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.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Energy Biosciences	29,078	29,914	32,839	+2,925	+9.8%
SBIR/STTR	0[a]	799	875	+76	+9.5%
Total, Energy Biosciences	29,078	30,713	33,714	+3,001	+9.8%

[a] Excludes $730,000 which has been transferred to the SBIR program and $44,000 which has been transferred to the STTR program.

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Energy Biosciences Research			
■ **Photosynthesis:** Photosynthesis is the capture of solar energy by plants and photosynthetic microbes. A broad range of research activities is supported to understand the detailed mechanisms of this fundamental process. The approaches used to dissect the photosynthetic machinery range from biophysical studies to traditional biochemical and molecular genetic analyses. The work interfaces with the photochemistry activities supported in the Chemical Sciences subprogram to provide a complete analysis from the physical to the biological level. A prominent area of interest is the examination of the mechanisms used to transfer energy from numerous accessory pigments into the reactive center where oxygen evolution and energy transduction occur. The approach of using molecular genetics to modify a single amino acid (the fundamental component of proteins) followed by biophysical analysis of the effects on energy transfer is providing a detailed picture of the function of the various proteins and cofactors involved in this processes. A number of studies provide indications that evolution has attempted to optimize the photosynthesis process to assure that the organisms have sufficient energy to survive in as many environmental situations as possible, particularly under conditions of very low light. It is likely that, through fundamental understanding, it may be able to modify this process to have much higher efficiencies under high light conditions.	4,315	4,055	4,039

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Biological Synthesis:** Plants and microorganisms are important commercial sources of materials such as cellulose (paper and wood), starch, sugars, oils, waxes, and many biopolymers. These renewable, energy-rich biomaterials can also comprise a biomass resource for energy production and conservation. When all plants and microorganism are considered, their collective genetic capacity to synthesize different energy-rich organic compounds and polymers is almost limitless. Genomics, including research on genetic mechanisms controlling growth, metabolism, and cellular functions in plants and microbes, is already yielding biotechnological tools and promising opportunities to specify the type of starch and oil produced, and has even been used to move microbial genes into plants for the synthesis of thermal plastics. Plant and microbial genomics is experiencing tremendous expansion. An example is the large scale sequence of the entire Arabidopsis genome a project jointly funded with the NSF and USDA, which is expected to be completed at the close of the year 2000. Arabidopsis is a model for all plants and knowledge of its genome is being used to locate and study genetic traits in other plants ranging from corn to poplar trees. The great challenge and exciting opportunity ahead is to place this genomic complement within a functional context. For the first time, enormous possibilities are developing for defining entire gene expression profiles in response to developmental, environmental, or metabolic requirements. The functional genomics of energy-related processes in plants is a critical component of the interagency National Plant Genome research. The comprehensive ramifications for efficient energy utilization and renewal are particularly great as genomic information is integrated with existing biochemical and biophysical information in living systems.	15,089	14,185	14,712
■ **Metabolic Interconversion:** Research in this area includes the conversion of minerals or simple organic molecules to biologically useful energy-rich compounds; the degradation and recycling of biomass in the form of plant lignins or celluloses by fungi or bacteria; the syntrophic or symbiotic relationship between different plant and microbial species to facilitate the utilization and interconversion of biological macromolecules; the microbial production of biofuels such as hydrogen or methane through respiration and fermentation; the development			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
of strategies to convert toxic substances into benign or beneficial biological molecules; and the use of natural biological processes and molecules to synthesize new classes of biological materials.	7,239	6,801	6,775
■ **Microbial Cell Research:** The strengths of the Energy Biosciences subprogram in microbial biochemistry and physiology will be combined with the strengths of the Biological and Environmental Research program in genomics, structural biology and computational biology in a coordinated program to establish a minimal set of genes required for bacterial growth. The Energy Biosciences subprogram will be involved in the biochemical and physiological characterization of the minimal gene set along with describing the genes (gene modules) and gene functions associated with specific physiological and biochemical processes of interest to the Department of Energy. Examples of these bioprocesses include 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 these individual gene modules and their encoded bioprocesses interact at the molecular level to permit control and stability in the entire microbial cell. Along with enabling the creation of specific microbes with specific physiological properties, this research will lead to a more complete understanding of the microbial cell, its genes, proteins and regulatory systems that define microbial life with its distinct physiological and biochemical characteristics.	0	0	2,440
■ **Climate Change Technology Initiative:** Basic research begun in FY 1999 emphasizes the biological process of photosynthesis, which is central to global carbon cycling. The focus is on studies on the mechanism of photosynthetic carbon fixation and the subsequent metabolism of the fixed carbon. Specific attention is being directed at steps in carbon fixation that regulate or limit the entire process. Another focus area of is the synthesis and biodegradation of particularly recalcitrant forms of fixed carbon. The understanding obtained from these			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
and related studies will permit the production of radical changes in photosynthetic carbon capture by manipulating both the efficacy of the photosynthetic apparatus and its function in whole plants and other photosynthetic organisms	2,435	4,873	4,873
Total, Energy Biosciences Research	29,078	29,914	32,839
SBIR/STTR Funding			
■ In FY 1999, $730,000 and $44,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	799	875
Total, Energy Biosciences	29,078	30,713	33,714

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Energy Biosciences Research	
■ Decrease in research in photosynthesis	-16
■ Decrease in research in biological synthesis	-57
■ Increase for the National Plant Genome research	+584
■ Decrease in research in metabolic interconversion	-26
■ Increase in research in microbial cells	+2,440
Total, Energy Biosciences Research	+2,925
SBIR/STTR	
■ Increase in SBIR/STTR funding because of increase in operating expenses.	+76
Total Funding Change, Energy Biosciences	+3,001

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.

Performance Measures

- Meet the cost and schedule milestones for upgrade and construction of scientific user facilities, including the construction of the Spallation Neutron Source. The cost and schedule will be kept within 10 percent of cost and schedule baselines as reflected by regular external independent reviews of project management cost and schedule.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Construction	105,400	100,000	261,900	+161,900	+161.9%
Total, Construction	105,400	100,000	261,900	+161,900	+161.9%

Detailed Program Justification

(dollars in thousands)

	FY 1999	FY 2000	FY 2001
Construction			
■ Funding for the Combustion Research Facility, Phase II was completed in FY 1999 as scheduled	4,000	0	0
■ The FY 2001 requested budget authority for the Spallation Neutron Source will provide for: detailed (Title II) design and starting fabrication of the ion source, low-energy beam transport, linac structure and magnet systems, target assemblies, experimental instruments, and global control systems; completing detailed design and starting construction of major conventional facilities; continued procurements of major			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
technical components (e.g., dipole magnets and klystrons); and continued preparation of a Safety Analysis Report for the target system and a Safety Assessment Document for the remainder of the Spallation Neutron Source facility.	101,400	100,000	261,900
Total, Construction..	105,400	100,000	261,900

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Construction	
■ The increase in funding for the Spallation Neutron Source represents the scheduled ramp up of activities.	+161,900
Total Funding Change, Construction..	+161,900

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 1999	FY 2000	FY 2001	$ Change	% Change
Advanced Light Source	31,206	31,039	35,445	+4,406	+14.2%
Advanced Photon Source	86,226	85,625	94,677	+9,052	+10.6%
National Synchrotron Light Source	32,176	32,109	36,500	+4,391	+13.7%
Stanford Synchrotron Radiation Laboratory	23,419	21,924	22,474	+550	+2.5%
High Flux Beam Reactor	22,768	19,582	17,521	-2,061	-10.5%
High Flux Isotope Reactor	30,359	34,532	34,201	-331	-1.0%
Radiochemical Engineering Development Center	7,027	6,985	7,145	+160	+2.3%
Intense Pulsed Neutron Source	12,102	11,699	13,642	+1,943	+16.6%
Manuel Lujan, Jr. Neutron Scattering Center	7,397	7,371	9,978	+2,607	+35.4%
Spallation Neutron Source	28,600	17,900	19,100	+1,200	+6.7%
Combustion Research Facility	5,024	5,003	5,831	+828	+16.6%
Partial Offset to Science General Reduction Applied to BES	1,521	0	0	0	-
Total, Major User Facilities	287,825	273,769	296,514	+22,745	+8.3%

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Facilities Operations			
■ Advanced Light Source at Lawrence Berkeley National Laboratory.	31,206	31,039	35,445
■ Advanced Photon Source at Argonne National Laboratory.	86,226	85,625	94,677
■ National Synchrotron Light Source at Brookhaven National Laboratory.	32,176	32,109	36,500
■ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center	23,419	21,924	22,474
■ High Flux Beam Reactor at Brookhaven National Laboratory. The reactor has been in standby mode since December 21, 1996, awaiting a decision by the Secretary of Energy on its future. On November 16, 1999, Secretary Richardson announced the permanent closure of the reactor. The funding requested in FY 2001 represents that required to continue the transition project that will complete the shut down and provide for appropriate disposition of the scientific instruments and ancillary equipment. Surveillance will continue until the reactor is fully decommissioned and decontaminated	22,768	19,582	17,521
■ High Flux Isotope Reactor at Oak Ridge National Laboratory.	30,359	34,532	34,201
■ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory.	7,027	6,985	7,145
■ Intense Pulsed Neutron Source at Argonne National Laboratory.	12,102	11,699	13,642
■ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	7,397	7,371	9,978
■ Spallation Neutron Source at Oak Ridge National Laboratory	28,600	17,900	19,100
■ Combustion Research Facility at Sandia National Laboratories/California.	5,024	5,003	5,831
■ Partial Offset to Science General Reduction Applied to BES.	1,521	0	0
Total, Major User Facilities	287,825	273,769	296,514

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
General Plant Projects	11,194	10,500	10,625	+125	+1.2%
Accelerator Improvement Projects	8,927	8,918	13,195	+4,277	+48.0%
Capital Equipment	56,236	51,517	71,146	+19,629	+38.1%
Total, Capital Operating Expenses	76,357	70,935	94,966	+24,031	+33.9%

Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 1999	FY 2000	FY 2001	Unapprop-riated Balances
99-E-334 Spallation Neutron Source, ORNL	1,220,000	0	101,400	100,000	261,900	756,700
96-E-300 Combustion Research Facility, Phase II, SNL	26,800	22,800	4,000	0	0	0
Total, Construction		22,800	105,400	100,000	261,900	756,700

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

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp- riations	FY 1999	FY 2000	FY 2001 Request	Accept- ance Date
Short Pulse Spallation Upgrade at LANSCE – LANL	20,500	4,500	4,500	3,500	4,500	FY 2002
HB-2 Beam Tube Extension at HFIR - ORNL	5,550	0	2,800	1,600	1,150	FY 2001
SPEAR3 Upgrade	29,000[a]	0	0	0	8,000	FY 2003
ALS Beamline	6,000	0	1,500	750	1,800	FY 2003
Total, Major Items of Equipment		4,500	8,800	5,850	15,450	

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

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

(Changes from FY 2000 Congressional Budget Request are denoted with a vertical line in the left margin.)

The Total Estimated Cost and Total Project Cost have been increased and the construction schedule has been extended as a result of project restructuring during FY 1999 and the FY 2000 appropriation that was $96,100,000 less than the FY 2000 request.

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 (*Current Estimate*)	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,220,000	1,440,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Construction			
1999	101,400	101,400	37,140
2000	100,000	100,000	133,960
2001	261,900	261,900	249,900
2002	290,200	290,200	289,100
2003	222,400	222,400	224,400
2004	131,400	131,400	142,800
2005	81,600	81,600	91,600
2006	31,100	31,100	51,100

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 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 the features that make materials of technological significance for 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 has been designed to operate at an average power on target of about at least 1 megawatt (MW); the current design will produce an approximately 2 MW machine.. At this power level, the SNS will be the most powerful spallation source in the world--more than ten times that of ISIS at the Rutherford Laboratory in the United Kingdom. Furthermore, SNS will be positioned to take advantage of new technologies 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 spin 1/2, 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 1 giga electron volt (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 accelerator; accumulator ring; target station with moderators; beam transport systems; and experimental facilities capable of supporting up to 18 neutron scattering beam lines for research instruments) and attendant conventional facilities. Also included on the site will be facilities to support the needs of operations staff, technical support staff, users and capabilities for remote servicing of activated components. An initial suite of approximately 10 neutron scattering instruments is included in the TEC.

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 funding of $281,000,000 (includes other project costs) is requested for the SNS Project for conducting detailed (Title II) design and starting fabrication of the ion source, low-energy beam transport, linac structure and magnet systems, target assemblies, experimental instruments, and global control systems. Construction will begin on several conventional facilities such as the front end building, linac tunnel, ring-service building, and the klystron hall. Construction will be completed on roads into the site and site preparation. Production will continue on several significant equipment items such as magnets, target systems, and klystrons.

Project management and integration activities, which are exceptionally important during this phase of the project, will also be conducted. Work will continue on the Safety Assessment Document for all the facility except for the target system, for which a Safety Analysis Report will be prepared.

4. Details of Cost Estimate

(dollars in thousands)

	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 10% of construction costs	127,100	166,900
Construction management at approximately 1% of construction costs	15,400	26,300
Project management at approximately 11% of construction costs	135,200	102,900
Land and land rights	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	27,100	28,600
Buildings	151,800	176,700
Other structures	600	600
Utilities (electrical, water, steam, and sewer lines)	25,800	30,500
Technical Components	433,200	417,900
Standard Equipment	2,700	1,100
Major computer items	7,600	12,000
Removal cost less salvage	0	0
Design and project liaison, testing, checkout and acceptance	5,200	9,700
Subtotal	931,700	973,200
Contingencies at approximately 31 percent of above costs	288,300	186,300
Total Line Item Cost	1,220,000	1,159,500
Less: Non-Agency Contribution	0	0
Total, Line Item Costs (TEC)	1,220,000	1,159,500

5. Method of Performance

The SNS project is being carried out by a partnership of five DOE national laboratories, led by ORNL, as the prime contractor to DOE. The other four laboratories are Argonne, Brookhaven, Lawrence Berkeley, and Los Alamos National Laboratories. 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 - Linac; Oak Ridge - Target. Project execution is the responsibility of the SNS Project Director with the support of a central SNS Project Office at ORNL, which provides overall project management, systems integration, ES&H, quality assurance, and pre-commissioning support. The SNS Project Director has prime authority for directing the efforts at all five partner laboratories and exercises ultimate financial control over all project activities. The ORNL Management and Operating Contractor has subcontracted to an Industry Team for design and construction management services. The Industry Team consists of an Architect-Engineer for the conventional facilities design and a Construction Manager for construction installation, equipment procurement, testing and pre-operational support. Procurements by all five 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 1999	FY 2000	FY 2001	Outyears	Total
Project Cost						
Facility Cost [a]						
Line Item TEC	0	37,140	133,960	249,900	799,000	1,220,000
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	0	37,140	133,960	249,900	799,000	1,220,000
Other project costs						
R&D necessary to complete project [b]	21,600	26,837	16,820	16,000	14,097	95,354
Conceptual design cost [c]	15,303	0	0	0	0	15,303
Decontamination & Decommissioning (D&D)	0	0	0	0	0	0
NEPA Documentation costs [d]	1,500	400	0	0	0	1,900
Other project-related costs [e]	0	800	900	3,000	101,700	106,400
Capital equipment not related construction [f]	100	563	180	100	100	1,043
Total, Other project costs	38,503	28,600	17,900	19,100	115,897	220,000
Total project cost (TPC)	38,503	65,740	151,860	269,000	914,897	1,440,000

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 $1,220,000,000.

b A research and development program at an estimated cost of $95,354,000 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 $15,303,000 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 Estimated costs of $1,900,000 are included to complete the Environmental Impact Statement.

e Estimated costs of $106,400,000 are included to cover pre-operations costs.

f Estimated costs of $1,043,000 to provide test facilities and other capital equipment to support the R&D program.

7. Related Annual Funding Requirements

	(FY 2000 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	106,700	N/A