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 continuously 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;
- Foster and support the discovery, dissemination, and integration of the results of fundamental, innovative research in these areas;
- Provide world-class scientific user facilities for the Nation; 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 scientific and engineering knowledge in areas important to the BES mission, i.e., in materials sciences, chemical sciences, geosciences, plant and microbial biosciences, and engineering sciences.
- *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.
- *Plan, construct, and operate premier national scientific user facilities* — for materials research and related disciplines to serve researchers at universities, national laboratories, and industrial laboratories, 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. In addition, to 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.

- *Establish and maintain stable, essential research communities, institutions, and scientific user facilities.* — Steward important research communities and institutions in order to respond quickly and appropriately to mission need and scientific opportunity. For example, BES serves as the Nation's primary or sole supporter of such important subdisciplines as heavy element chemistry, natural and artificial solar energy conversion, catalysis, organometallic chemistry, combustion related science, separations science, neutron science, radiation chemistry, and radiation effects in materials.

Performance Measures

BES is prototypical of a large, diverse, and robust basic research program that exists within a mission agency. BES measures performance in four areas that together characterize this special role. The first three areas relate to the fundamental tenets or principles of BES, which correspond directly to the goals described above. These tenets are: (1) excellence in basic research; (2) relevance to the comprehensive energy mission of the agency; and (3) stewardship of research performers, essential scientific disciplines, institutions, and scientific user facilities. Combining and sustaining these tenets are the management challenge of BES. The fourth area that BES measures performance in, therefore, is program management.

Activities in these four areas are measured in a number of ways, which separate naturally into four categories: (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 in order to better quantify performance. 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, 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, now is completed annually by all BES facilities. An integral part of the survey tool is an assessment of user satisfaction. The tool has generated considerable interest outside of BES and has been distributed to other organizations and non-BES facilities at their request. Third, BES began formal peer reviews of its major scientific user facilities. These reviews, the first of which was documented in the 1997 Basic Energy Sciences Advisory Committee (BESAC) report on synchrotron radiation light sources ("Synchrotron Radiation Sources and Science" chaired by Professor Robert Birgeneau, MIT), assess in the aggregate, the scientific output and, to the extent possible, the outcomes of facilities. The High-Flux Isotope Reactor at Oak Ridge National Laboratory was reviewed in this manner in FY 1998. The four electron beam microcharacterization centers will be reviewed in FY 1999.

In FY 2000, (1) the development and upgrade of scientific user facilities, including the construction of the Spallation Neutron Source, will be kept on schedule and within cost, not to exceed 110 percent of estimates; (2) the operating time lost at scientific user facilities due to unscheduled downtime will be less than 10 percent of the total scheduled possible operating time, on average; (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; (5) work performed by investigators in universities and DOE laboratories will continue to be recognized as outstanding through the receipt of major prizes and awards; (6) continue Partnerships for Academic-Industrial Research where peer reviewed grants are awarded to university researchers for fundamental, high-risk work jointly defined by the academic and industrial research partners; and (7) continue fabrication of instrumentation for the short-pulse spallation source on the Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center.

Performance measurement helps determine the distribution of activities supported within BES and the individual projects supported within each activity. The funding level for each activity is derived by weighing a number of additional factors including mission need as defined by the BES and SC mission statements; scientific opportunity as determined, in part, by proposal pressure and by scientific workshops; connections with other BES and SC supported work; connections with needs expressed by the DOE technology offices and by energy-intensive industries; program balance; and budgetary constraints.

Prizes, Awards, and Honors

Annually, principal investigators funded by BES win dozens of major prizes and awards sponsored by professional societies and by others; in addition, many are elected to fellowship in organizations such as the National Academy of Sciences, the National Academy of Engineering, and the major scientific professional societies. Paramount among the honors in FY 1998 was the Nobel Prize in Chemistry. The Nobel Prize in Chemistry for 1997 was awarded to three biochemists, Paul D. Boyer (University of California at Los Angeles), John E. Walker (Medical Research Council Laboratory of Molecular Biology of Cambridge, England) and Jens C. Skou (Aarhus University in Denmark). Drs. Boyer and Walker were cited for their elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP). Dr. Boyer's work was supported in part by the BES Energy Biosciences subprogram and its predecessor organizations from 1963 until his retirement in 1993. This is the fourth Nobel Prize awarded to BES principal investigators in the past four years.

Other selected major prizes and awards for FY 1998 include:

From the American Ceramic Society — the Robert L. Coble Award; the Long-Term Service Award; the Sosman Memorial Lecture

From the American Chemical Society — the Analytical Chemistry Award in Electrochemistry; the Arthur C. Cope Scholar Award in Organic Chemistry; the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry; the E. V. Murphree Award in Industrial and Engineering Chemistry; the Award in Chromatography; the Irving Langmuir Award in Chemical Physics; the Award in Spectrochemical Analysis; the Arthur K. Doolittle Award for Best Paper at the Polymeric Materials Science and Engineering Division meeting

From the American Institute of Aeronautics and Astronautics — the Award for Distinguished Service

From the American Institute of Chemical Engineers — the Professional Progress Award; the Research Achievement Award; the Thomas Chilton Award; the Warren K. Lewis Award

From the American Institute of Chemists — the Chemical Pioneer Award

From the American Physical Society — the David Adler Lectureship Award in the Field of Materials Physics; the Davisson-Germer Prize in Atomic or Surface Physics; the Earle K. Plyler Prize in Molecular Spectroscopy; the Frank Isakson Prize for Optical Effects in Solids; the Joseph F. Keithley Award for Advances in Measurement Science; the Julius Edgar Lilienfield Prize; the Centenial Speaker Award

From the American Society for Mass Spectroscopy — the Biemann Medal; the Distinguished Contribution Award

From the American Society of Plant Physiologists — the Stephen Hales Prize

From the American Welding Society — the Burton Medal; the Masubuchi Award; the Warren F. Savage Memorial Award

From the Electrochemical Society — the Olin Palladium Award Lecture

From the Eli Lilly Corporation — the Eli Lilly Award

From the Federal Planning Division of the American Planning Association — the Best 1998 Area Development Plan (Spallation Neutron Source, ORNL)

From the Geological Society of America — the Day Medal

From the IBM Corporation — the Supercomputer Award

From the Institute of Electrical and Electronic Engineers — the Prize Paper Award

From the Inter-American Photochemical Society — the Inter-American Society Award

From the International Association for Structural Safety and Reliability — the IASSAR Research Award

From the International Electron Paramagnetic Resonance/Electron Spin Resonance Society (IES) — the Silver Metal for Chemistry

From the International Organization on Multiphase Flow — the Multiphase Flow International Prize

From the International Society of Electrochemistry — the Prix Jacques Tacussel Award

From the Japan Society for the Promotion of Science — the International Prize for Biology

From the Japan Society of Multiphase Flow — the Lifetime Achievement Award

From the Materials Research Society — the von Hippel Award; the Graduate Student Award

From the Microbeam Analysis Society — the Heinrich Award

From the Microscopy Society of America — the Outstanding Technologist Award

From the Mineralogical Society of America — the Mineralogical Society of America Award

From the North American Catalysis Society — the Robert Burwell Lectureship Award; the International Catalysis Award

From R&D Magazine — R&D 100 Awards for TRUST- Terminal Repeller Unconstrained Subenergy Tunneling; SAMMS - Self-Assembled Monolayers or Mesoporous Supports; and MICLEAN/MICARE Solvent Cleaning Systems

From the Science Museum of Virginia and the State of Virginia General Assembly — the Virginia Outstanding Scientist

From the Semiconductor Research Corporation — the Aristotle Award

From the Serbian Chemical Society — the Centenary Medal

From the Society for Technical Communication — the Technical Communcation Award

From the Society of Applied Spectroscopy, New England Section — the Lester W. Strock Award

From the Wolf Foundation — the Wolf Foundation Prize in Chemistry

From Vice President Gore — the Hammer Award

Two principal investigators received the Presidential Young Investigator Award; five were inducted into the National Academy of Sciences; one was inducted into the National Academy of Engineering. Seven principal investigators were advanced to fellowship in the American Academy of Arts and Sciences; three in the American Association for the Advancement of Science; four in the American Ceramic Society; nine in the American Physical Society; two in the American Society for Metals; and one each into the following organizations: Geological Society of America, Institute of Electrical and Electronic Engineers, the American Welding Society, National Science Foundation/Japanese Science Technology Agency, Optical Society of America, and the Royal Society of New Zealand.

Finally, principal investigators served in numerous elected offices including: President, American Chemical Society; President, International Society of Electrochemistry; President, Mineralogical Society of America; President-elect, American Ceramic Society; President-elect, American Society of Plant Physiologists; Vice President, American Physical Society; Chair, Division of Materials Physics, American Physical Society; and First Vice Chair, American Society for Testing and Materials.

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, biosciences, and engineering sciences. The program encompasses more than 2,400 researchers in 200 institutions and 17 of the Nation's premier user facilities. Presented below are program accomplishments from FY 1998. 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 often be incorporated into other scientific desciplines and into the commercial sector, and the great potential of new knowledge for future impacts in energy production and use. Following that are discussions of scientific facilities and program initiatives.

Selected FY 1998 Scientific Highlights/Accomplishments

Materials Sciences

- *Helping to Solve the Mystery of High-Temperature Superconductivity*. Understanding high-temperature superconductivity, discovered in 1987, remains *the* outstanding problem in modern condensed matter physics. Recent neutron scattering experiments suggest that the electric current in high temperature superconductors may be like “stripes” of flowing current separated by stripes where current does not flow. These stripes can be static or dynamic (like the stripes on our flags, waving in the wind). These and other experiments point to a very different electron pairing mechanism than that seen in low-temperature superconductors. Once the pairing mechanism is understood, it will be easier to find materials with higher critical superconducting temperatures and better mechanical properties.

- *Magnetic Resonance Imaging (MRI) Without Magnets.* Striking, high resolution MRI images have been obtained without the need for high field magnets or high frequency detectors normally required for MRI. The breakthrough involves MRI enhancement by noble gases magnetically polarized (100,000 fold) through laser treatment. A new ultra-low-field MRI instrument now makes it possible to obtain extremely bright MRI pictures of polarized samples in the earth’s natural magnetic field, which is thousands of times weaker than fields obtained from traditional MRI magnets (which are bulky, expensive, and often hazardous). The new instrument has been used with localized injection of polarized xenon solutions into human blood to provide the first observations of the real-time process of xenon penetrating red blood cells. (Xenon is an inert gas and an FDA-approved anaesthetic.) This combination of techniques opens the way to provide high resolution MRI images of localized areas in animal and human subjects.

- *Discovery of New Materials Using LEGO.* Of the enormous number of combinations of elements in the periodic table, only a very small fraction are used in real materials. It is quite certain that materials with optimum properties for various applications have not yet been discovered. For example, high-temperature superconductivity occurs in ceramic compounds with a most unlikely combination of elements. A new strategy using fast computers and concepts from quantum mechanics has been developed to search for "winning combinations" of atoms to produce materials with improved physical properties. This approach -- Linear Expansion in Geometric Objects (LEGO) -- recognizes that even complex crystal structures can be viewed as a collection of simple geometric objects such as dumbbells, triangles, etc. By assigning each geometric object an energy value, computers can rapidly scan hundreds of thousands of candidates looking for the lowest overall energy and, therefore, the most stable structures. LEGO has already predicted several new intermetallic compounds missed through conventional approaches.

- *Electrically Conducting Nanoscale Ropes.* Incredibly light synthetic metals with a potential electrical conductivity 50-100 times better than copper per weight are being made from carbon nanotubes doped with metals. First discovered in 1991, nanotubes are a new class of materials formed from graphite-like sheets of carbon rolled into exquisitely small cylinders. They self organize in the vapor phase during growth to form well ordered crystalline bundles of individual nanotubes. The introduction of dopant atoms, such as potassium or lithium, into the open spaces between adjacent tubes within a rope can increase electrical conductivity significantly at room temperature. Doped nanotube ropes are also attracting increased interest as constituents of novel nanoscale device structures and as replacements for pure lithium metal in Li ion batteries.

- *Molecular Bricks for Nanotechnology*. Lightweight materials are commonly composed of polymers, which are long chains of atoms. The chains are difficult to order completely, which limits their functionality and durability. Researchers have recently demonstrated new possibilities for the design of polymers using nano-objects, which can be regarded as molecular bricks. These bricks, which might have shapes as diverse as those of nature's proteins, create a toolbox for the design of lightweight materials that could self assemble into structures with surprising functionality. Using the first elements of this toolbox, a spherical nanostructure has been created that has internally continuous channels; some channels transport water and ions, while others block water but accept organic substances. These nano-sponges could trap toxic metals from water streams.

- *What Makes Stainless Steel Stainless?* Corrosion damage is estimated to cost the U.S. 4.2 percent of the Gross National Product each year. Metals can be used in industrial and technological applications only when appropriately protected. In the case of stainless steel and many other metals, protection is provided by a thin oxide film that prevents further corrosion. However, the structure of these oxide films has remained a mystery despite decades of study. Recent research using surface-sensitive synchrotron x-ray diffraction with a combination of electrochemical experiments has now unambiguously determined that the oxide film on pure iron has a very fine-grained, nanocrystalline structure. Results for iron-chromium alloys (e.g., stainless steel) have shown that the oxide films are also nanocrystalline. This overturns the long accepted belief that stainless steel is corrosion resistant because its oxide film is non-crystalline. These surprising results provide a more realistic basis for understanding corrosion resistance and for the development of better corrosion protection coatings.

- *Do Cracks "Melt" Their Way through Solids?* Predicting and explaining why, how, and when solids fracture is a significant scientific challenge. The driving force for fracture is intensification of the local stress at a crack tip, yet the mechanism by which local strain is dissipated during crack propagation is not well understood. Can strain energy be dissipated via “local melting” around the crack tip? Recent computer simulations of crack formation predict this intriguing possibility. Simulations indicated that the melting in front of a crack tip can lead to catastrophic fracture. Using high-voltage electron microscopy, observations of moving crack tips in an intermetallic compound confirmed the prediction of the computer simulations and showed the development of melted and rapidly re-solidified regions adjacent to the crack tip. This new picture of fracture as a stress-induced melting process may lead to new approaches to stress-corrosion cracking in the automotive, aerospace, power generation, and ship building industries.

- *Smart Filters.* New materials with tailored pore sizes and pore chemistry can selectively remove deadly heavy metals -- such as mercury, lead, and silver -- from water. Researchers discovered that precise control over the amount of water in the pores of porous silica enabled the insertion of useful organic molecules on the walls of the pores. Using this knowledge, monolayers of organic sulfur compounds were bound to the internal surfaces of porous silica to prepare selective filter materials. The high surface area of the porous silica (a few grams have as much surface area as a football field) coupled with the bonding characteristics of the organic compounds results in high filtering capacity and high selectivity for specific contaminants. In addition, pore openings in the silica are designed to be too small for microbes to enter and digest the contaminants, later causing human illness from, for example, mercury contamination. The filter materials can purify highly contaminated water in a single treatment to a level that exceeds drinking water standards. The filters can also be recovered and reused after removing the contaminants.

- *A Line in the Sand.* Granular materials like gravel, salt, or dry chemicals are ubiquitous in our daily lives and central to many industrial processes, yet controlling their motion is both surprisingly difficult and not well understood. For example, granular material subjected to a driving force remains at rest until a minimum "critical force" is applied; then it moves in uncontrollable events like avalanches. Inefficiency in handling granular materials may result in the loss of up to 40 percent of the design capacity of industrial plants. In its retrospective of the last 50 years, *Physics Today* highlighted the emerging science of granular materials as a notable event of the last decade. Scientists have recently developed a theoretical approach to describe the motion of granular materials in a vibrating environment. This theory correctly describes the unexpected formation of stripe, square, and hexagon patterns on the surface of vibrated granular media and the formation of localized excitations called "oscillons." The theory also predicted how to control aspects of granular motion -- a prediction that was confirmed by experiment. The new theory brings the description and control of granular motion to a higher level of understanding and shows promise of substantial advances in basic granular science, which can lead to industrial applications that exploit the controlled motion of granular materials.

- *Vortex Matter -- A New Understanding of Magnetism in Superconductors*. Magnetic fields in superconductors are carried by "vortices." Each vortex consists of a tube of magnetic field surrounded by a circulating flow of electrons that move without resistance. It is this free flow of electrons that gives superconducting materials their special property. Recently, it has been shown that the system of magnetic vortices can take many forms analogous to the solid, liquid, and gaseous forms of ordinary matter. The analogy between the behavior of vortices and ordinary matter is so strong that a new term has entered the scientific vocabulary -- vortex matter. Vortex matter melts from a crystalline to a liquid state in much the same way that ice melts to water. The properties of vortex matter can be controlled over a wide range. For example, the density of vortices can be varied by a factor of 10,000 simply by changing the applied magnetic field. This remarkable control enables the study of many types of phenomena in vortex matter whose analogies in ordinary matter are difficult or impossible to observe. Thus, the identification and characterization of the melting transition in vortex matter has significant implications for phase transitions in ordinary matter, for understanding the electromagnetic properties of superconductors, and for developing applications of superconductivity.

Chemical Sciences

- *Landmark Experiment Challenges Combustion Models.* Combustion is perhaps the oldest technology in human experience, yet its complexity limits predictions of combustion processes in devices ranging from simple laboratory burners to automobile engines. The challenge is characterizing the influence of chemistry and fluid dynamics on one another. A simple experiment recently has demonstrated a major error in current models for combustion processes. The experiment allows the interaction of chemistry and turbulence to be examined in quantitative detail for the first time. A planar flame sheet is deformed by a puff of air generated by a small loudspeaker. Spectroscopic techniques are used to determine the concentrations of reaction intermediates as the flame sheet deforms. Comparisons of these experiments with computational simulations showed that the widely accepted chemical reaction mechanism for simple methane combustion is in error, thus, requiring a fundamental change in our models for combustion.

- *Fishing for Radioactive Actinides with Molecular Hooks.* The selection, separation, and removal of radioactive actinide ions from complex aqueous waste stream mixtures remain vexing technical issues. The development of new, improved separation approaches will result in significant cost savings for nuclear waste treatments as well as improve environmental safety and materials safeguard security. A new family of chelate agents or "chemical fish hooks" suitable for the reversible "catch and release" of trivalent actinide ions in highly acidic solutions has been designed, prepared, and characterized. The latest chelate derivatives show separation characteristics that are especially suited to practical, batch type waste treatments.

- *First Isolation of a Catalytic Oxidation Intermediate*. Despite worldwide efforts over the last 15 years on catalytic olefin oxidation, little progress has been made in extrapolating from ethylene (the smallest olefin) to larger olefins such as propylene. The key question -- the molecular mechanism of ethylene epoxidation (which gives us anti-freeze and polyester fibers) -- remains unresolved. Now, a combined experimental and theoretical tour de force has yielded the first definitive isolation and spectroscopic characterization of a stable intermediate in the catalytic process -- an oxametallacycle. Calculations were employed to determine the structure for the oxametallacycle on silver and to predict the infrared spectrum and molecular motions for that structure. Conclusive identification was provided by the excellent agreement between the predicted infrared spectrum and the experimental electron energy loss spectrum.

- *Liquid Crystalline Organic Semiconductors Discovered.* Liquid crystals change their optical properties as they transition between distinctive geometric states. Digital watch displays, for example, cycle between transparent and opaque forms. They, like other technologically important liquid crystals, are electrically insulating. Semiconducting crystals could have much broader application than insulating crystals, but large single crystals of these materials are difficult and expensive to produce. In a recent breakthrough, a family of liquid crystalline derivatives of perylene diimide was discovered that has semiconductor properties. The films of one compound self organize from a red, polycrystalline phase with randomly oriented crystallites into a black phase with highly ordered ribbon-like structure. The fluorescence intensity increases seven-fold during the transformation. This spontaneous change in photophysical properties makes this class of organic liquid crystals look very promising for future photoconversion applications.

- *Diode Lasers Detect Radiotoxic Isotopes.* Solid-state diode lasers, similar to those used in compact disc players, have been used in a new approach to detect the toxic radioisotope strontium-90, which received attention because of high levels found in milk after atomic weapons tests and the Chernobyl reactor accident. Diode lasers excite and efficiently ionize the strontium atoms; the resulting ions are detected using a mass spectrometer. The high efficiency allows the detection of less than one femtogram (femto = 10^{-15}, e.g., a single postage stamp compared to the area of Texas) of strontium 90. Furthermore, it is possible to selectively ionize the strontium 90 even in the presence of large excesses of the stable, naturally-occurring isotopes of strontium. Measurements can be performed in a few minutes as compared to the several weeks required previously for conventional radiochemical decay counting methods. Thus, this new approach should significantly improve the capabilities for near real-time monitoring of environmental restoration activities, nuclear weapons tests, reactor accidents, and the processing of nuclear fuels.

- *Photochemical Studies on the Light-Activated Drug Hypericin.* The popular herbal remedy St. John's wort contains the compound hypericin which, upon exposure to light, is toxic to tumors and HIV, the human AIDS virus. Now, the fundamental photochemistry of hypericin has been elucidated. A novel laser spectroscopic technique, fluorescence upconversion, was used to show definitively that the primary photochemical process is excited-state intramolecular proton or hydrogen transfer. Any incomplete proton or hydrogen atom transfers would acidfy the aqueous solution immediately surrounding hypericin, which may be of importance in its toxicity to viruses. The study is yet another example of the role that the physical sciences play in providing fundamental information relevant to a wide variety of subject areas.

Engineering and Geosciences

- *Remote Sensing of Fractures and Prediction of Failure in Rocks.* Long before catastrophic fracturing and failure of a material, sound waves transmitted through the material show a dramatic frequency shift. This shift has been documented before in fractured materials, but the observation of the shift *before* the formation of a continuous crack is a new discovery. Monitoring for the frequency shift can therefore be used to provide a warning of failure. The sound shifts to a lower frequency because the high-frequency sound (with shorter wavelengths) is preferentially absorbed or scattered. Because the frequency shift occurs prior to creation of a single fracture, there should be a network of oriented, disconnected features appearing prior to a crack that absorb or scatter the high-frequency sound in the same way as do observable cracks. Connected cracks in rocks provide pathways for water, oil, or pollutant flow. The growth of cracks can improve fluid flow or cause failure of well-bores, reservoirs, and tunnels or engineered structures; therefore, it is very important to understand how and when cracks form.

Energy Biosciences

- *The 1997 Nobel Prize in Chemistry.* Dr. Paul D. Boyer shared in the 1997 Nobel Prize in Chemistry for "elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP)." The energy captured from photosynthesis or released from respiration is converted into ATP, which is used for maintenance of cells, synthesis of cellular components, and other energy-requiring processes such as movement. ATP is frequently referred to as the "energy currency" of the cell. Dr. Boyer's work at the University of California at Los Angeles was supported in part by the Division of Energy Biosciences and its predecessor organizations from 1963 until 1993 under a project entitled "Energy Capture and Use in Plants and Bacteria."

- *Building Doors into Cells.* Before any molecule can enter a cell, it must first pass through the cell membrane—the thin, fat-containing film that covers all cells. The passage of most molecules through biological membranes is controlled by pores, defined openings made with specific proteins. The composition and structure of pore proteins can now be altered through genetic engineering. Changes in the size of the pore, the selectivity of the pore for letting different molecules pass through, and the pore's ability to open and close are three properties currently being studied by bioengineering new pore proteins. Successful attempts to engineer modified pore opening and closing properties have provided insight on how these processes can occur mechanistically as well as for developing new biotechnological applications. Among the potential products of this research are chemical triggers or molecular switches that can be used to create new sensors to detect harmful chemicals or viruses. Other potential applications are the development of small light switches and new drug delivery systems.

Scientific Facilities Utilization

The BES program request includes $311,035,000 to maintain support of the scientific user facilities. Within this overall level of support is a partial cost-of-living increase for facility operations and an increase in funding for the High-Flux Isotope Reactor at Oak Ridge National to continue activities related to the replacement of the beryllium reflector and associated beamline upgrades. The reduction in support for the scientific user facilities from that of FY 1999 is primarily a result of the decrease in R&D for the Spallation Neutron Source. Support for facility operations is maintained at as high a level as possible consistent with budgetary constraints. Research communities that have benefited from the BES supported Scientific Facilities Initiative 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 and related research in broad areas of the physical, chemical, materials, biological, and medical sciences. The SNS will be the world’s most powerful accelerator-based, pulsed neutron source producing 6-10 times more neutrons than any other such source. It 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.

The SNS will consist of a linear accelerator (linac)-ring system that will deliver short pulses of protons to a mercury target where neutrons will be produced by a nuclear reaction process called spallation. The high-energy neutrons so produced will be moderated (i.e., slowed down) to reduce their energies. The “moderated” neutron beams will then be used for neutron scattering experiments. Specially designed scientific instruments will use these pulsed neutron beams for a wide variety of investigations on all types of materials.

As the needs of our high-technology society have changed, so has the way we do R&D on new materials to meet these needs. It has become increasingly important to develop new materials that perform under severe conditions and yet are stronger, lighter, and cheaper. 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 applications. Neutron scattering will play a role in all forms of materials understanding 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 neutron science for fundamental discoveries and technological development is now universally acknowledged. The scientific justification and need for a new pulsed 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 MW spallation source that could be upgraded to significantly higher powers in the future.

The conceptual design of the SNS -- which was an interlaboratory effort involving Lawrence Berkeley National Laboratory in the ion source, Los Alamos National Laboratory in the linear accelerator, Brookhaven National Laboratory in the accumulator ring, and Argonne National Laboratory in targets and moderators -- was completed in June of 1997. The design conforms to the recommendations of the Russell Panel Report. The power will be in the 1 megawatt range or about six times that of the highest currently available worldwide, and the design will allow for significantly higher powers at a later stage. The design will further include moderators for neutrons with appropriate spectral and temporal characteristics in the epithermal, thermal, and cold energy ranges. There will be the potential for at least three target areas and for 30 to 40 instruments.

Agreements are in place with Rutherford Appleton Laboratory (England), the European Spallation Source project, and the Japanese Atomic Energy Research Institute to allow joint research and development. Furthermore, a Working Group on Neutron Sources has been established under the Megascience Forum of the Organization for Economic Cooperation and Development. A User Committee has been formed, consisting of distinguished members of the neutron science community, to provide input on instrumentation and on user needs.

FY 1999 funding provided for the start of Title I design activities, initiation of subcontracts and long-lead procurements, and continued critical research and development work necessary to reduce technical and schedule risks. FY 2000 funding of $214,000,000 is requested for the SNS

Project for detailed design (Title II) for the ion source, low-energy beam transport, LINAC structure and magnet systems, target assemblies, experimental instruments, and global control systems. Detailed design will be completed for several conventional facilities in preparation for the installation of major equipment in the following fiscal year; design will be completed 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 start for some conventional facilities including roads into the site, site preparation/grading, waste systems, and retention basins. Procurement for several significant equipment items such as dipole magnets, material for the target transport systems, and klystrons will begin. Project Management and Project Integration activities, which are exceptionally important during this phase of the project, will also be conducted. The Preliminary Safety Analysis Report (PSAR) will be completed during the fiscal year and work will begin on the final report. Additional information on the SNS project is provided in the SNS construction project data sheet, project number 99-E-334.

Facility Enhancements

BES will continue to support ongoing enhancements and maintenance activities of existing reactor and spallation neutron 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) The beryllium reflector at the High Flux Isotope Reactor at Oak Ridge National Laboratory is being changed. This is a scheduled maintenance operation that addresses the normal lifetime limitations of the beryllium reflector. Work was initiated in FY 1998 and will be completed in FY 2000. At the same time that the beryllium reflector, beam tubes and shutters, and monochrometer shields are replaced, several improvements will be made to instrumentation, beam tubes, and monochrometers. The improvements will provide increases in flux to the sample by factors of 2 to 3 times that of the Institute Laue Langevin, the world's best reactor neutron source. These improvements to HFIR were recommended by BESAC.

Partnerships for Academic-Industrial Research (PAIR) Program

The Partnerships for Academic-Industrial Research (PAIR) Program. Pending the results of an evaluation of ongoing awards, an additional $1,500,000 may be allocated to the PAIR program for a total budget of $3,000,000. This program is designed to encourage and facilitate research partnerships between academic researchers, their students, and industrial researchers. The PAIR program encompasses the entire range of research supported by the BES program. Grants are awarded on the basis of competitive peer review to university researchers for support of fundamental, long-term, high-risk work that is jointly defined by the academic and industrial research partners and that supports a student or postdoctoral fellow from the university, who will spend at least four weeks per year in the industrial setting.

Complex and Collective Phenomena Program

The program in Complex and Collective Phenomena. In FY 2000, an additional $4,500,000 will be allocated to the program in Complex and Collective Phenomena for a total budget of $7,500,000. Much of the research supported by the BES program and its predecessor organizations during the past 50 years has been devoted to solving very difficult problems in idealized, simple systems. The challenge now is to use that knowledge to understand complex systems. This initiative supports work at the frontiers of basic research. Work is intended to be revolutionary rather than evolutionary, and it is expected that it may involve multidisciplinary and/or interdisciplinary efforts. Further it is expected to bridge the gap between an atomic level understanding (reductionist view) and a continuum mechanics understanding (classical view) of complex and collective phenomena. Awards are made on the basis of competitive peer review to university and DOE laboratory researchers. The initiative is open to the entire range of disciplines supported by the BES program. Some important categories of studies that might be included within the initiative in Complex and Collective Phenomena are:

Materials that are beyond binary; that lack stochiometry; that are far from equilibrium; that have little or no symmetry or low dimensionality. Often properties and behaviors that we desire exist only in "non ideal compounds," i.e., those that are made from more than a few elements, made in non stoichiometric combinations, made far from equilibrium; or made in one or two dimensions. These classes of materials, which will dominate the next generation of energy technologies, pose new challenges and opportunities because of their complexity.

Functional synthesis. The ability to *predict* structure/function relationships remains elusive. Because function can be exquisitely sensitive to even minor changes in both composition and structure and because the number of combinations is virtually boundless, we are unable to predict what combinations of elements and arrangements of atoms give rise to desired properties such as superconductivity, magnetism, ductility, toughness, strength, resistance, catalytic function, or enzymatic function.

The control of entropy. To a scientist, entropy has a precise mathematical definition; however, to a nonscientist, entropy can be viewed as synonymous with disorder. A standard maxim in physics is that "the entropy of the universe tends to increase," i.e., things become increasingly disordered with time. Interestingly, most of our energy now comes from fossil fuels that were derived from photosynthesis — the ability of plants to reduce entropy locally by absorbing sunlight and converting carbon dioxide to lower-entropy hydrocarbons, polysaccharides, and other compounds. However, even though photosynthesis has been studied for decades, we still do not completely understand it nor have we been able to duplicate or improve on it. This one example of the control of entropy — the ability to mimic the functions of plants — remains one of the outstanding challenges in the natural sciences.

Phenomena beyond the independent particle approximation. Phenomena beyond the independent particle model — that by their nature are collective — challenge our understanding of the natural world and require major advances in theory, modeling, computing, and experiment. Collective phenomena include widely diverse phenomena in the gas and condensed phases, including Bose-Einstein condensation, high-temperature superconductivity, and electron correlation.

Scaling in space and time. Research in chemistry, materials, geosciences, and biosciences covers lengths from the atomic scale to the cellular scale to the meter scale and times from femtoseconds to millennia. We understand single atoms, molecules, and pure crystals fairly well; but, when we go beyond these simple systems to larger more complex systems, our understanding is limited. Understanding phenomena over wide time scales is also important — from femtoseconds in spectroscopy to decades in the regulatory system of plants to thousands of years in radioactive waste disposal.

Climate Change Technology Initiative

Overview

The FY 2000 budget contains two carbon related programs, each of which cut across several agencies. The first is the Climate Change Technology Initiative (CCTI). That part of the CCTI that is within the Office of Science is a joint activity between the Biological and Environmental Research (BER) and Basic Energy Sciences (BES) programs. The second program is the U.S. Global Change Research Program (USGCRP) that spans eleven agencies and is coordinated through the National Science and Technology Council's Committee on Environment and Natural Resources. Within DOE, the BER program plays the lead role in USGCRP activities. Although the two programs, CCTI and USGCRP, are synergistic, they are different. USGCRP research focuses on developing the fundamental understanding of the comprehensive climate system and the global and regional adaptations to it. The CCTI focuses on the underpinning fundamental science that will enable mitigation of climate change while maintaining a robust National economy. All research in the CCTI will be peer-reviewed fundamental scientific research; no funds will be devoted to policy studies.

Eighty-five percent of our Nation's energy results from the burning of fossil fuels, a process that adds carbon to the atmosphere — principally in the form of carbon dioxide — from the sequestered fossil reservoir. Because of the potential environmental impacts of increases in atmospheric carbon dioxide, carbon management has become an international concern and has become a focus of the Climate Change Technology Initiative. A comprehensive research and development program that meets the needs of the Climate Change Technology Initiative addresses the diverse aspects of this problem. The Office of Science is well positioned to make significant contributions to the many solutions needed for this problem, as it is set to build on the fundamental discoveries of its core programs and extend them to the new discoveries needed to make carbon management practical and efficient. Science core programs include research on both carbon and non-carbon energy sources and on both carbon sequestration and carbon recycling. These core activities can now be exploited in the generation of the carbon management science that will underpin the technologies of the future. The theme of efficiency in energy production and use must span the entire range of research activities. Research on carbon energy sources, and their impacts, is a focal point of interagency activity through the U.S. Global Change Research Program (USGCRP). Research on non-carbon energy sources is also a focal point of intra-agency activities and is led by the DOE Office of Energy Efficiency and Renewable Energy. The DOE Office of Science, through activities in both the Basic Energy Sciences (BES) program and the Biological and Environmental Research (BER) program, supports research that underpins both efforts.

A research program in carbon management would include:

- science for efficient technologies,
- fundamental science underpinning advances in all low/no carbon energy sources, and
- sequestration science.

Science has long-standing programs in fundamental research that already impact the three categories. In the BES program, funds in the amount of $19,504,000, are provided specifically for carbon management science in the Climate Change Technology Initiative. This work will be a natural extension of the complementary, ongoing work in several programs in Science, and it will build on the foundation of excellent and relevant research already underway. Focus areas will be those that build on strengths of the current Science programs and that promise maximum impact in the area of carbon management.

Immediate Impacts of Expanded Effort in Climate Change Technology

Additional science efforts will not only address an immediate societal problem, but they will also have a major effect on many scientific disciplines by advancing the state of knowledge and by training students in areas of research that are important to carbon management. For example, biochemistry, molecular and cellular biology, structural biology, and genome science will be impacted, because the production of fuels and chemicals by plants and microorganisms and the interconversion of greenhouse gases requires a better understanding of metabolism, of the structure and function of sub-cellular components, and of enzymes. Similarly, the state-of-the-art in biochemistry, molecular biology, and ecology will be impacted. All of these biological processes are important in understanding the role of marine microorganisms in sequestering carbon. Improvements in combustion to reduce carbon emissions require a fundamental understanding in chemical dynamics and theoretical chemistry and physics. Conversion of sunlight to energy requires an understanding in many areas of science, including photochemistry, photosynthesis, metabolism, and solid state physics. The search for increased efficiency in energy production and use requires fundamental knowledge in ceramics, metals, polymers, solid state chemistry, and condensed matter physics for materials that can withstand higher temperatures, have lower coefficients of friction, and are stronger and lighter. Enhanced recovery of fuel resources and of disposal of carbon dioxide requires a fundamental understanding of geometric, structural, and hydrologic properties of reservoirs and of multiphase, nonlinear transport of fluids in porous and fractured structures. Crosscutting programs in nano- and meso-phase materials involve research at the forefront of materials science, chemistry, engineering, surface science, and semiconductor physics.

The new research efforts supporting advances in low/no carbon energy technologies, as well as existing activities, will be closely coordinated with DOE's technology programs and will provide the knowledge base for the development of advanced technologies to reduce carbon dioxide emissions. Many of the activities will impact the Office of Energy Efficiency and Renewable Energy (EE) and the energy and transportation industry by providing options for increasing efficiency in automobiles by reducing weight; for increasing efficiency in the use of electricity by increasing the efficiency of electric motors and generators with better magnets; for increasing efficiency in the transmission of electricity by using superconductors; and for reducing energy consumption in manufacturing with improved sensors, controls, and processes. Much of this research program will provide the knowledge base needed to increase the use of renewable resources with research aimed at understanding the metabolism of carbon dioxide and the metabolic pathways to the production of methane and other biofuels. Other aspects of the research program impact the Office of Fossil Energy (FE) by providing a foundation for effective and safe underground sequestration, new materials, a better understanding of combustion, and improved catalysts.

Funding will be provided for areas of research in carbon cycle management including appropriate areas that will be jointly identified and implemented by the Biological and Environmental Research and Basic Energy Sciences programs. Solicitations will be used for individual research projects. Additionally, proposal notifications may be developed jointly with the DOE energy technology programs with the intention of establishing multi-disciplinary centers at universities and national laboratories that will use the full capabilities of the institutions for a research program in carbon cycle management encompassing, for example, topics in the following areas: integration and assessment; separations; efficiency; clean fuels; bioenergy; storage and conversion; enhanced natural terrestrial cycles; and enhanced use of major scientific user facilities to support carbon management research.

Interagency Environment

The Office of Science program in fundamental science supporting energy technologies will be closely coordinated with, and synergistic to, the activities in its sister agencies (e.g., NASA, NSF, NOAA, USDA, DOI, and EPA) within the USGCRP. Through its leadership role in decade to century climate prediction, the Office of Science has developed the research capability for comprehensive and large scale modeling of carbon dioxide impacts on climate, on ecology, and on ocean sciences, and this expertise is augmented by complementary activities in the other agencies. Similarly, the network of carbon flux measurements and ecological experiments that the Office of Science has developed serve as a backdrop to those of many other agencies, and the state-of-the-art can thus be pushed ahead more rapidly by capitalizing on the more rapidly growing base of knowledge. The Office of Science also has a leadership role within the USGCRP on consequence evaluation of increased greenhouse gases in global climate change, including integrated assessments that address both scientific and societal (including economic) impacts of carbon management. Finally, through its pre-eminent role in the Human Genome Program and its development of the complementary Microbial Genome Program, the Office of Science program is ideally placed to support research that will focus on the application of genetic information of microorganisms to increase metabolic efficiency related to both carbon dioxide and conversion to fuels through photosynthesis.

BES Activities

Climate Change Technology Initiative

	(dollars in thousands)	
	FY 1999	FY 2000
Materials Sciences	1,708	3,415
Chemical Sciences	2,197	4,394
Engineering and Geosciences	1,464	6,822
Energy Biosciences	2,436	4,873
Total	7,805	19,504

As noted above, an inclusive climate change technology research and development program must address diverse aspects of the problem including: (1) carbon recycling; (2) improved efficiency in the use of fossil carbon energy sources; (3) new and improved non-carbon energy sources; and (4) carbon dioxide sequestration. The BES program has long supported fundamental research that impacts these categories and has particularly strong programs related to the first three. A comprehensive program in issues relating specifically to carbon management, therefore, finds a natural home with the scientific communities supported by BES.

Focus areas 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, research emphasizes atomic and molecular level understanding of chemical processes to enable predictive capability. A major component of the research will aim 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 will include research to: (1) understand the mechanical stability of porous and fractured reservoirs/aquifers; (2) understand multiphase fluid flow within the aquifers; and (3) understand the 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.

All of the BES activities in CCTI are closely related to DOE's technology programs and will provide the knowledge base for the development of advanced technologies to reduce CO_2 emissions. When combined with the complimentary activities within the Biological and Environmental Research program, this initiative will lead to the comprehensive carbon management research program described above.

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 support 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 totalling $6,300,000 in this category also addresses the 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, photoassisted 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.

BES engages in appropriate partnerships to make the results of the BES research widely known and used. Examples include partnerships with the DOE technology offices and with other federal agencies. As a result, BES engages in many joint activities. For example, in photovoltaics, the Office of Energy Efficiency and Renewable Energy (EE) and BES together sponsored a workshop in 1993. Based on this workshop, a jointly funded project was started at NREL that resulted in record-breaking photovoltaic efficiencies. In general, research activities in biomass, wind energy, photovoltaics, hydrogen, and solar photoconversion are coordinated with EE through Coordinating Committees in the Department, through ad hoc meetings, through workshops, and through joint funding at universities and at the Department's laboratories.

In November, 1997, more than 30 program staff from the Office of Science (SC) — primarily from BES — and from EE Offices of Utility Technologies and Transportation Technologies met to discuss programs in the areas noted above. The EE programs involved include those of photovoltaic energy systems, solar thermal, hydrogen technologies, wind technologies, biomass power, and biofuels (transportation). Follow on one-on-one meetings between program managers of both offices are now being held for identification of research needs, gaps and areas of opportunity of possible joint program development. For example, in May 1998, BES program staff participated in a Workshop on Biohydrogen Production sponsored by EE's Hydrogen program and by the Engineering Directorate at NSF; BES staff further provided reviews of EE projects in the area of biological hydrogen production and recommendations for the overall direction of that program. Another outcome of the November 1997 meeting has been the re-establishment of a Department-wide technical committee in the area of bioenergy which includes program representatives from BES and EE and also from the Office of Environmental Management (EM) and the Office of Fossil Energy (FE). The purposes of the revitalized DOE Bio-Energy Coordinating Committee (BECC) are to: (a) achieve effective coordination of all DOE bio-energy research and development; (b) assure optimum use of DOE’s existing expertise in the field of bio-energy research and development; and (c) achieve the most rapid communication among DOE program representatives of new developments, opportunities, and issues in the areas of bio-energy research, development, demonstration and commercialization. In a related effort, BES and EE’s Office of Fuels Development are drafting a joint research topic on biofuels for the FY1999 SBIR Program Solicitation.

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 budgeting $346,000 and $313,000 for estimated contractor clearances in FY 1999 and FY 2000, respectively, within this decision unit.

Scientific Simulation Initiative

This budget also includes the BES program’s contribution to DOE’s Scientific Simulation Initiative (SSI), an integrated effort bringing together computational and communication resources, focused research in scientific disciplines, and research in computer science and other enabling technologies to solve the complex problems that characterize DOE’s scientific research needs. The SSI couples research in advanced scientific applications in the programs of the Office of Science (SC) with research in computer science and enabling technologies and advanced computing and communications facilities. It is a joint program between the Computational and Technology Research (CTR) program and the other programs in SC. The overview of the integrated program is given in the overview of the CTR budget; however, the specific contributions of the BES program are described below.

BES, through its Chemical Sciences subprogram manages the SSI Combustion Systems integrated applications effort. BES's participation in the SSI also represents an important contribution to the broader Presidential initiative in information technology. The Chemical Sciences subprogram has been involved in combustion research for over two decades. The goal of this research effort is to develop, through simulation and modeling, a sufficiently deep and detailed understanding of combustion processes to accelerate the development, characterization, and validation of design tools for advanced combustion devices. Eighty-five percent of current U.S. energy use is derived from the combustion of fossil fuels. This dependence on fossil fuels is not likely to change in the coming decades. For transportation technologies alone, preliminary calculations suggest that improvement in direct-injection diesel thermal efficiency of 35% is possible, which could result in energy savings of 3.7 quads or $26 billion and reductions of carbon dioxide ($CO_{2)}$ emissions of 250 million tons per year. Combustion has been and remains one of the primary causes of lowered air quality in urban environments. Providing the knowledge that can lead to improved efficiency of the fossil fuel combustion process while reducing unwanted emissions remains one of among the highest priorities in the Nation's research portfolio. High fidelity combustion simulation and modeling may well be the path to significant breakthroughs in the ability of engineers to characterize, and therefore optimize and control, all aspects of combustion devices.

At present, engineers have neither sufficient knowledge nor the computational tools to understand and predict the chemical outcome of combustion processes. The design of combustion devices remains an Edisonian process dependent on intuition, experience, and time consuming trial and error. Computational models to guide the design process currently are of limited use because of the extraordinary complexity of the combustion process. This complexity derives from:

- the hundreds of chemical reactions that comprise combustion chemistry;
- fluid dynamics with turbulence scales covering 6 orders of magnitude; and
- interactions between chemistry and fluid dynamics involving time and spatial scales that cover 12 orders of magnitude.

The anticipated accomplishments of this research effort will allow the complete characterization of the chemistry and fluid dynamics of combustion processes and systems. The computational tools developed under this program, along with the new level of understanding of complex combustion phenomena, will allow engineers to design a new generation of combustion devices optimized for energy efficiency and pollution reduction.

The combustion modeling and simulation component of the SSI will be managed in a manner consistent with the way BES manages other projects and facilities. A program manager in the Office of Basic Energy Sciences will be appointed to be responsible for the effort. This manager will be assisted by a technical management and coordination office located at one of the DOE laboratories whose role is to ensure that the subelements remain tightly integrated. Research teams at laboratories and universities, as well as the technical management and coordination office, will be competitively selected in response to a published announcement and following peer review.

Funding Profile

(dollars in thousands)

	FY 1998 Current Appropriation	FY 1999 Original Appropriation	FY 1999 Adjustments	FY 1999 Current Appropriation	FY 2000 Request
Basic Energy Sciences					
Research					
Materials Sciences	381,828	417,216	-2,530	414,686	407,636
Chemical Sciences	196,127	209,582	-2,745	206,837	215,577
Engineering and Geosciences	40,151	44,413	-1,674	42,739	37,545
Energy Biosciences	26,710	32,489	-2,627	29,862	31,226
Subtotal, Research	644,816	703,700	-9,576	694,124	691,984
Construction	7,000	105,400	0	105,400	196,100
Subtotal, Basic Energy Sciences	651,816	809,100	-9,576	799,524	888,084
Use of Prior Year Balances	-4,852 [a]	-4,002[a]	0	-4,002[a]	0
General Reduction for Policy Papers for CCTI		-8,000	8,000	0	0
General Reduction		-1,576	1,576	0	0
Total, Basic Energy Sciences	646,964 [b]	795,522	0	795,522	888,084

Public Law Authorization:

Public Law 95-91, “Department of Energy Organization Act”

[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 $14,622,000 which has been transferred to the SBIR program and $877,000 which has been transferred to the STTR program.

Funding by Site

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory	23,613	24,673	25,906	+1,233	+5.0%
National Renewable Energy Laboratory . . .	4,515	4,193	3,744	-449	-10.7%
Sandia National Laboratories	28,764	26,600	22,008	-4,592	-17.3%
Total, Albuquerque Operations Office	56,892	55,466	51,658	-3,808	-6.9%
Chicago Operations Office					
Ames Laboratory	18,659	17,114	16,967	-147	-0.8%
Argonne National Laboratory, East	139,894	143,436	145,096	+1,660	+1.2%
Brookhaven National Laboratory	76,722	77,586	77,331	-255	-0.3%
Princeton Plasma Physics Laboratory	700	675	0	-675	-100.0%
Total, Chicago Operations Office	235,975	238,811	239,394	+583	+0.2%
Idaho Operations Office					
Idaho National Environmental and Engineering Laboratory	3,478	3,609	3,020	-589	-16.3%
Oakland Operations Office					
Lawrence Berkeley National Laboratory . . .	62,160	62,553	62,095	-458	-0.7%
Lawrence Livermore National Laboratory . .	5,933	6,044	5,236	-808	-13.4%
Stanford Linear Accelerator Facility (SSRL)	21,684	22,686	21,968	-718	-3.2%
Total, Oakland Operations Office	89,777	91,283	89,299	-1,984	-2.2%
Oak Ridge Operations Office					
Oak Ridge Inst. For Science & Education . .	2,003	1,258	1,541	+283	+22.5%
Oak Ridge National Laboratory	110,219	217,848	302,898	+85,050	+39.0%
Thomas Jefferson National Accelerator Facility	200	0	0	0	0.0%
Total, Oak Ridge Operations Office	112,422	219,106	304,439	+85,333	+38.9%
Richland Operations Office					
Pacific Northwest National Laboratory	12,868	12,788	12,947	+159	+1.2%
All Other Sites [a]	140,404	178,461	187,327	+8,866	+5.0%
Subtotal, Basic Energy Sciences	651,816	799,524	888,084	+88,560	+11.1%
Use of Prior Year Balances	-4,852 [b]	-4,002 [b]	0	+4,002	+100.0%
Total, Basic Energy Sciences	646,964 [c]	795,522	888,084	+92,562	+11.6%

[a] Funding provided to laboratories, universities, industry, other Federal agencies and other miscellaneous contractors.

[b] 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.

[c] Excludes $14,622,000, which has been transferred to the SBIR program and $877,000, which has been transferred to the STTR 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 leading experts on magnets, superconductors, and quasicrystals that incorporate rare earth elements. Recent innovations include the use of a rare earth alloy and the magnetocaloric effect to achieve efficient refrigeration without gases that are harmful to the atmosphere. The BES Chemical Sciences subprogram supports studies of heterogeneous electron transfer in self-assembled monolayers, 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 continues to provide leadership in analytical chemistry with strength in organometallic based catalysis and heavy metal extraction chemistry important to high level wastes.

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 in broad areas of materials, chemical, and geosciences, and it is 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 batteries and coal chemistry; 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 centers 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 by the Secretary of Energy, 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. 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 **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 in 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 two BES supported user facilities -- the National Synchrotron Light Source (NSLS) and the High Flux Beam Reactor (HFBR).

The Materials Sciences subprogram emphasizes experiments that make use of the NSLS and the HFBR. 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 centers for pulsed radiolysis research at BNL. With the recent completion of a new innovative short-pulse radiation chemistry facility, BNL is well poised to contribute significantly to radiation sciences research for the next decade. There is also a forefront research project 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 and lipid metabolism 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 1998, over 600 students who earned doctorate degrees used the NSLS in their thesis research.

The **High Flux Beam Reactor**, commissioned in 1965, is a heavy-water cooled and moderated reactor designed to produce neutrons for scattering. In contrast to most reactors, which are designed to minimize the escape of neutrons from the core, the HFBR was expressly designed to maximize the number of neutrons available in external beams. The HFBR supports a range of neutron-based research in solid-state and nuclear physics, chemistry, and structural biology. The reactor's 9 beam tubes deliver neutrons to 15 experimental facilities. Before the HFBR was put in standby mode in December, 1996, about 250 researchers conducted experiments at the facility annually. The HFBR will continue to be maintained in this standby mode while the Department evaluates options for its future.

Idaho National Environmental and Engineering Laboratory

Idaho National Engineering and Environmental 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, 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; and the structures of magnetic, optical, and electrical thin films and coatings. In the Center for Advanced Materials, research is conducted in the processing, mechanical fatigue, and high-temperature corrosion of structure ceramics and ceramic coatings; the synthesis, structure and properties of advanced semiconductor and semiconductor-metal systems; polymers; surface science and catalysis; and structure, development and magnetic properties of high performance metals and alloys. The Chemical Sciences subprogram has long excelled in 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 excellence 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 a new concept in catalysis, that of 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 an 800 MeV proton linac that is the basis for 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. 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 comprises a high-power 800-million-electron-volt 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 30 Tesla magnet is being developed for use with neutron scattering.

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 this 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 synthesis related to catalysis and to advanced battery research addressing high-efficiency, thin-film cathodes based on doped vanadium and manganese oxides. The BES Energy Biosciences subprogram funds programs to examine the mechanisms of photosynthetic oxygen evolution.

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 writing of annual BES subprogram summary books, the administration of topical scientific workshops, and provides support for other activities such as for the review of the Spallation Neutron Source Conceptual Design Report.

ORISE manages the **Shared Research Equipment Program** (SHaRE) at ORNL. The SHaRE Program has made 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 and Engineering Development Center (REDC). ORNL also leads the five-laboratory collaboration that will design and construct 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 programs such as the energy efficiency program in superconductivity. Research is supported 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 Facility.

The Chemical Sciences subprogram supports research in analytical chemistry, particularly in the area of mass spectrometry, separations 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 crustal rocks. Engineering research supports the Center for Engineering Systems Advanced Research with emphasis in 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.

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 experiment 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 are high-resolution laser spectroscopy for analysis of trace metals on ultra small samples, understanding 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 funds 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 focussed 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/A), with sites in Livermore, California (SNL/L), 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/A are relevant to the overall mission of the laboratory. Included among these are projects on the processing and properties sol-gel chemistry of ceramic coatings; 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/L.

The BES geophysics research effort at SNL/A 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/L 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 25 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 world leaders in photoemission studies of high-temperature superconductors and in x-ray scattering.

Thomas Jefferson National Accelerator Facility

Thomas Jefferson National Accelerator Facility (TJNAF) is a program-dedicated laboratory (Nuclear Physics) located on 273 acres in Newport News, Virginia. The Basic Energy Sciences program funds a research project at TJNAF related to fourth generation light sources based on linac-driven free electron lasers.

All Other Sites

The BES program funds research at 135 colleges/universities located in 43 states. This line also includes funding of 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, metals and ceramics 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.

Climate Change Technology Initiative. Research routes to improved carbon management in support of the Climate Change Technology Initiative include improved heat and corrosion resistant alloys to increase the efficiency of power generation, reducing energy losses in motors via improved magnetic materials, and displacing fossil fuels with higher-efficiency photovoltaic cells.

Performance Measures

- Continue Partnerships for Academic-Industrial Research where peer reviewed grants are awarded to university researchers for fundamental, high-risk work jointly defined by the academic and industrial research partners.
- Continue fabrication of instrumentation for the short-pulse spallation source at the Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center.

Funding Schedule

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
Materials Sciences Research	195,752	187,793	188,342	+549	+0.3%
Facilities Operations	186,076	217,104	209,599	-7,505	-3.5%
SBIR/STTR	0	9,789	9,695	-94	-1.0%
Total, Materials Sciences	381,828	414,686	407,636	-7,050	-1.7%

Detailed Program Justification

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
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 dimensionally restricted forms (films, dots) of materials. This activity provides world-class scientific user facilities to the Nation through the operation of four complementary and network interfaced electron beam microcharacterization user centers. These centers contain a variety of highly specialized instruments that complement each other in terms of their ability to characterize localized atomic positions and configurations, chemical gradients, interatomic bonding forces, etc. Major activities in FY 2000 will be responsive to the increasing demand for advanced facilities and models with capabilities to characterize and interpret the atomic structure, composition, bonding, and physical properties of materials with improved resolution and accuracy. Capital equipment needs for FY 2000 are expected to relate to facility refurbishment and upgrade.	24,455	25,655	25,390
■ **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			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
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 2000 will include continued development of experimental techniques and methods for the characterization of properties, the advancement of models and theories for interpretation, and the design and investigation of new materials and material structures. Capital equipment is needed for mechanical testing machines, especially with high-temperature capabilities, furnaces, and characterization equipment.	15,223	15,965	15,800
■ **Physical Behavior:** These activities support 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 2000 will continue fundamental studies of the mechanisms governing material response to aqueous, galvanic, and high-temperature gaseous corrosion; the processing and investigation of semiconductor materials and structures leading to enhanced solar energy conversion efficiencies; crystal defects, grain boundaries and interfaces for high-temperature superconductors; mechanisms controlling material response to hostile environments; and the structure and behavior of ceramic electrolytes for advanced fuel cells. Capital equipment is needed for corrosion studies and for electronic and spectroscopy instruments for the characterization of electronic, optoelectronic properties, and electrical properties of semiconductors, superconductors, and fuel cell electrolytes.	13,562	14,225	14,078

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ **Engineering Behavior:** These activities support basic research in the engineering behavior of materials. The research includes the synthesis and processing of materials with new or improved behavior, for minimization of waste, and with hard and wear resistant surfaces to reduce friction and wear; 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; 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 that makes available small quantities of specialized research quality materials for research purposes that are not commercially or otherwise available. Major activities for FY 2000 will include continued work on design of new material compositions and structures, synthesis and processing new and enhanced materials, and characterization and interpretation of material behavior. Capital equipment includes furnaces, lasers, processing equipment, plasma and ion sources, and deposition equipment.	20,211	21,205	20,985
■ **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 2000, measurements			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
of particular interest will include neutron and x-ray scattering from materials which exhibit complex phenomena resulting from 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 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 such items as detectors, monochromators, mirrors, and beamline instrumentation.	18,739	19,700	19,495
■ **Experimental Condensed Matter Physics:** This activity supports fundamental experimental research in condensed matter physics. This 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 instruments including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy are major			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
components 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. The major efforts in FY 2000 will include continued support for investigations of materials with increasingly complex behavior, composition and structures with strongly competing interactions among the electronic charge and spin, and the crystalline lattice. A major new activity will be the synthesis and fabrication of unusual materials systems with pulsed laser ablation epitaxy, self-organized structures, and engineered materials and structures to provide insight into unusual behavior. Capital equipment is provided for items such as lasers, scanning tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets and computers.	26,147	27,450	27,165
■ **Condensed Matter Theory, Particle-Solid Interactions, and Engineering Physics:** This activity supports basic research in theory and simulations, the use of ion beams to modify the properties of materials, and engineering applications. The theory activity complements much of the experimental work by guiding and stimulating experiments. The centers are group thrust areas in which individual scientists from widely different backgrounds work together to work on common research areas or making use of a common research facility. Included among these are the Center for X-ray Optics and the Center for Advanced Materials at LBNL and the Surface Modification and Characterization Facility at ORNL. Additionally, the design and construction of new, unique research instruments, such as the 100 Tesla Pulsed Field Magnet and the actinide photoelectron spectrometer at LANL, are supported in this activity. The emphasis in engineering physics is on the use of fundamental science to advance technology. Engineering physics includes activities			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
such as the application of sound waves for refrigeration; the fabrication of small, machined structures using x-rays; and the development of new, electron microscopy techniques such as the Z-contrast electron microscope at ORNL. This activity is science driven. Capital equipment is provided for items such as computer work stations, sample chambers, and high resolution electron microscopes. BES will provide opportunities for college faculty and students to spend time at DOE laboratories, to participate in world-class research projects. Faculty/Student Science Teams will visit our labs during the academic/summer semesters, be involved in conducting research, writing proposals, utilizing technology and pursuing techncial or scientific careers. Primary goals of the Science Teams are to build long-term partnerships among DOE laboratories and provide faculty/students with a deeper understanding of DOE science associated needs for research and development. Funds will be provided to pay for faculty/student stipends, travel, housing, and subsidize laboratory scientists' time for this activity ($1,947,000).	19,553	20,555	22,341
■ **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 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			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
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, electrode-electrolyte interfaces, catalysis, surface science and synchrotron x-ray micro-characterization have stimulated increased emphasis for these areas. 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.	23,547	24,715	24,458
■ **Experimental Program to Stimulate Competitive Research:** This activity supports basic research spanning the entire range of research supported by the Department in states that have historically received relatively less Federal research funding. The EPSCoR program supports research cluster activities at nine EPSCoR states through block grants and to individual investigator projects in all EPSCoR states and Puerto Rico. The EPSCoR states include Alabama, 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. 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 2000, this program will include new work that will make use of the DOE National Laboratories and the world-class facilities at these labs. This program will be science-driven and will support the most meritorious proposals based on peer review. Workshops and discussions have been held with representative scientists from EPSCoR states to acquaint them with the facilities and personnel at the DOE Laboratories.	6,815	6,815	6,815

EPSCoR Distribution of Funds by State

(dollars in thousands)

	FY 1998 Actual	FY 1999 Estimate	FY 2000 Estimate
Alabama	800	825 [a]	75
Arkansas	50	100	100
Idaho	50	100	100
Kansas	50	91	95
Kentucky	800	650 [a]	200
Louisiana	814 [a]	152	146
Maine	150	750 [a]	0
Mississippi	0	50	50
Montana	800 [a]	75	75
Nevada	850	855 [a]	96
North Dakota	0	47	46
Oklahoma	0	100	100
Puerto Rico	800	800 [a]	50
South Carolina	250	800	800
South Dakota	50	50	50
Vermont	25	25	25
West Virginia	100	100	100
Wyoming	800	800	800
Other	426 [b]	445 [b]	3,907 [b]
Totals	6,815	6,815	6,815

[a] In FY 1998 the funding commitments for awards to the States of Louisiana and Montana expire. In FY 1999, the funding commitments to the States of Alabama, Kentucky, Maine, Nevada, and Puerto Rico will expire.

[b] Includes technical support for the Experimental Program to Stimulate Competitive Research (EPSCoR). Uncommitted funds in FY 2000 will be competed among all EPSCoR states that do not have active Research Implementation Awards to begin new Research Implementation Awards.

	(dollars in thousands) FY 1998	FY 1999	FY 2000
■ **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	4,500	6,000
■ **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 $5,900,000 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.	0	3,500	2,400
■ **Replacement of High Flux Isotope Reactor Monochrometer Drums.**	0	1,800	0
■ **Spallation Neutron Source (SNS):** Conceptual design of the Spallation Neutron Source (SNS) was completed in FY 1997. FY 1998 funding will support continued Pre-Title I research and development on the SNS. Beginning in FY 1999, SNS research funding in support of construction is reflected in the facility operations section of this budget.	23,000	0	0

■ **Climate Change Technology Initiative:** Basic research in carbon management for the Climate Change Technology Initiative will focus on three areas: high temperature materials, magnetic materials, and semiconductor materials. A major goal in a carbon management program is the derivation of materials that can withstand higher temperatures for more efficient combustion and for improved properties in applications. Research will focus on attaining an atomic-level understanding and a predictive capability for bulk metallic glasses, which have the potential to make significant contributions in corrosion and wear resistance in fossil fueled power plants, and on structural ceramics, which will be used in high temperature applications such as engine components. Additional work will focus on a fundamental understanding of the

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
surface physics and chemistry of oxide layers, which is expected to produce alloys and coatings that have improved corrosion resistance at high temperatures. A second goal is the derivation of magnetic materials to reduce energy loss during use. Research on the microstructure of permanent magnetic materials to understand the optimum grain structure is expected to result in stronger magnets, and research in the processing of magnetic materials is expected to optimize magnetic properties. Taken together, research in magnetic materials is critical to energy efficiency, since electric motors consume about two-thirds of U.S. electric power. A final goal in the areas of materials sciences is 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. The research will focus on improving the efficiency of the conversion of light to electricity. For example, research in the physics of quantum confinement might lead to new nanoscale structures that can be tuned to absorb the full spectrum of sunlight, which, when coupled to electron transport structures, would provide new ways to convert sunlight to electricity.	0	1,708	3,415
Total, Materials Sciences Research	195,752	187,793	188,342

Facilities Operations

- **Operation of National User Facilities:** The facilities included in Materials Sciences are: National Synchrotron Light Source, High Flux Beam Reactor (currently not operating), 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 construction of the Spallation Neutron Source is also included. The facility operations budget request, which includes operating funds, capital equipment, and Accelerator and Reactor Improvements (AIP) funding under $5,000,000, is

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
provided in a consolidated manner later in this budget. AIP funding will support additions and modifications to accelerator and reactor facilities which are supported in the Materials Sciences subprogram. Included in the AIP funding are funds for the HFIR upgrade. Capital equipment is needed at the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front end components, monochromators, and power supplies. A summary of the funding for the facilities included in the Materials Sciences subprogram is provided below. Additional funds for facility operations for some of these facilities are included in the Chemical Sciences subprogram of this budget.	186,076	217,104	209,599

	(dollars in thousands)		
Facilities	FY 1998	FY 1999	FY 2000
National Synchrotron Light Source	23,047	24,094	24,523
High Flux Beam Reactor	22,986	22,568	22,580
Intense Pulsed Neutron Source	11,230	11,982	11,985
Stanford Synchrotron Radiation Laboratory	4,077	3,946	4,029
Manuel Lujan, Jr. Neutron Scattering Center	6,588	7,397	7,547
Advanced Light Source	30,708	31,166	31,732
Advanced Photon Source	82,368	86,226	87,703
Spallation Neutron Source	0	28,600	17,900
High Flux Isotope Reactor	3,972	0	1,600
Partial Offset to Science General Reduction Applied to BES	1,100	1,125	0
Total, Facilities	186,076	217,104	209,599

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
SBIR/STTR Funding			
■ In FY 1998 $8,696,000 and $522,000 were transferred to the SBIR and STTR programs, respectively. The FY 1999 and FY 2000 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	9,789	9,695
Total, Materials Sciences	381,828	414,686	407,636

Explanation of Funding Changes From FY 1999 to FY 2000

	FY 2000 vs. FY 1999 ($000)
Materials Sciences Research	
■ Decrease in research for structure of materials.	-265
■ Decrease in research for mechanical behavior and radiation effects.	-165
■ Decrease in research for physical behavior.	-147
■ Decrease in research for engineering behavior	-220
■ Decrease in research for neutron and x-ray scattering.	-205
■ Decrease in research for experimental condensed matter physics.	-285
■ Decrease in materials research for condensed matter theory, particle-solid interactions, and engineering physics.	-161
■ Increase in funding will provide opportunities for college faculty and students to spend time at DOE laboratories to participate in world class research projects.	+1,947
■ Decrease in research for materials chemistry.	-257
■ Increase in capital equipment for LANSCE instruments	+1,500
■ Decrease in capital equipment funds for extension of HB-2 beam tube at HFIR for thermal neutron scattering because of completion of scheduled activities	-1,100
■ Decrease in capital equipment funds for monochromator drums on HB-1 and HB-3 because of completion of scheduled activities	-1,800
■ Increase support for Climate Change Technology Initiative.	+1,707
Total, Materials Sciences Research	+549

	FY 2000 vs. FY 1999 ($000)
Facilities Operations	
■ Decrease in SNS research and development funds because scheduled activities supporting construction are nearing completion	-10,700
■ Slight increase in support for the operation of major scientific user facilities.	+1,595
■ Increase in AIP funds for HB-4 beamline enclosure at HFIR.	+ 1,600
Total, Facilities Operations	-7,505
SBIR/STTR	
■ Decrease SBIR/STTR funding due to decrease in operating expenses.	-94
Total Funding Change, Materials Sciences	-7,050

Chemical Sciences

Mission Supporting Goals and Objectives

The Chemical Sciences subprogram has two major components. The disciplinary areas within each component are connected to and address needs of the principal DOE and BES mission goals and objectives. One major component is comprised of atomic, molecular and optical (AMO) physics; chemical physics; photochemistry; and radiation chemistry. 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. Completely unanticipated benefits from this research often result. For example, research supported by the Chemical Sciences subprogram on small atomic clusters led to the discovery of the new forms of carbon named the fullerenes, typified by C_{60} (buckminsterfullerene). The 1996 Nobel Prize in chemistry was awarded to the scientists who made this discovery. The other major component of the research program is comprised of inorganic chemistry, organic chemistry, analytical chemistry, separations 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 and to new catalysts for the production of fuels and chemicals, better analytical methods in a wide variety of applications in energy processes and environmental sciences, 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.

Climate Change Technology Initiative. The chemical physics and photochemistry components of the research program provide the underlying chemical science needed to address carbon management. These areas enable more efficient combustion and new understanding of the photochemical conversion of CO_2 and the direct conversion of solar radiation to electricity. The component of the research program, comprised of separations science, physical chemistry and inorganic chemistry, provides the basis for new and improved catalysts for conversion of fuels to carbon dioxide and hydrogen, potentially for carbon dioxide conversion to chemicals, separation of the conversion components, and new electrochemical energy production and storage systems.

Scientific Simulation Initiative. This subprogram includes the Combustion Systems Integrated Applications component of DOE’s Scientific Simulation Initiative (SSI), an integrated effort bringing together computational and communication resources, focused research in scientific disciplines, and research in computer science and other enabling technologies to solve the complex problems that characterize DOE’s scientific research needs.

Funding Schedule

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
Chemical Sciences Research	128,452	132,750	139,230	+6,480	+4.9%
Facilities Operations	67,675	68,928	71,430	+2,502	+3.6%
SBIR/STTR	0	4,672	4,917	+245	+5.2%
Congressional Direction	0	487	0	-487	-100.0%
Total, Chemical Sciences	196,127	206,837	215,577	+8,740	+4.2%

Detailed Program Justification

(dollars in thousands)

FY 1998	FY 1999	FY 2000

Chemical Sciences Research

- **Photochemistry and Radiation Research:**
  - The photochemistry research program investigates, at the molecular level, fundamental processes that capture and convert solar energy. Fundamental concepts of light-induced charge separation at the molecular level are developed for application to photodriven endothermic reactions for the conversion of light energy to chemical energy. In addition, photochemistry presents opportunities for altering chemical reaction pathways so that high volume industrial intermediates and specialty chemicals can be produced by less polluting processes. The program encompasses organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry. Naturally occurring photosynthetic reaction centers and antenna systems are studied as models of biomimetic/ photocatalytic assemblies that can carry out efficient photoinduced charge separation.

	FY 1998	FY 1999	FY 2000
	(dollars in thousands)		

- Related to the photochemistry program but using different techniques is the radiation chemistry research program. This program supports research on the chemical effects produced by the absorption of energy from ionizing radiation. A major goal is to obtain molecular level information on chemical reactivity in solution, reactive transient intermediates, the kinetics and mechanisms of chemical reactions and processes at the solid/liquid interface. Frequently the studies are on systems that are not amenable to investigation by other techniques. Results from this research provide information on transients in solution and intermediates at liquid/solid interfaces for resolving important issues in solar photochemical energy conversion, environmental waste management and remediation; and intermediates relevant to nuclear energy production.

- Recent workshops entitled "Research Opportunities in Photochemical Sciences" and "Research Needs and Opportunities in Radiation Chemistry" have helped identify issues for FY 2000 emphasis. These include: the fundamental mechanisms of inorganic and organic semiconductor electrode corrosion and passivation; improved theoretical models of heterogeneous electron and hole transfer across semiconductor interfaces; studies of the photophysics and chemistry of molecular excited states; control of the energetics of water splitting redox chemistry; and better understanding of the fundamental principles of photoinduced energy and charge transfer in natural and artificial photosystems as functions of structure, energetics, and medium.

	FY 1998	FY 1999	FY 2000
▸ Capital equipment is provided for such items as lasers, microscope scanners, liquid chromatographs, and temperature controllers.	24,907	23,927	22,982

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ **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.	26,713	27,836	27,401

■ **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. 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.

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
Furthermore, work in AMO science has produced measurement techniques and instrumentation that is widely used by other scientific disciplines and by industry and medical sciences.			
▸ A recent workshop entitled "Atomic, Molecular, and Optical Physics Workshop" has helped define areas of priority for BES for FY 2000 and beyond. That workshop was the first in a series of annual workshops that will link the BES-supported AMO science community with other scientific and technical communities. Program priorities include a detailed understanding of the interactions of photons, electrons, ions, and heavy particles with matter including a fundamental understanding of the interaction of optical electromagnetic fields with matter in the high field regime; novel states of matter induced by such interactions; and the control of matter by these light fields. Priority research also incudes studies of novel materials such as nanostructured materials, quantum dots, and artificial atoms; and heavy-ion and highly-charged ion collisions.			
▸ Capital equipment is provided for such items as pulse processing electronics, laser upgrades, position sensitive and solid state (SiLi) detectors.	9,926	10,200	10,213
■ **Catalysis and Chemical Transformations:**			
▸ This activity supports basic research related to chemical transformations and conversions that are fundamental to new or existing concepts of energy production and storage. The emphasis is on understanding the fundamental chemical principles underlying the 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; the conversion of biomass and related cellulosic wastes; and the			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
chemistry of precursors to advanced materials. The disciplines of organic, organometallic, inorganic, physical, and thermochemistry are central to these programs.			
▸ 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 that they replace or which function as energy-saving media themselves. These activities are linked with other catalyst related activities in BES in the materials chemistry and chemical physics programs; to other activities in the Department (Office of Heavy Vehicle Technology and the Office of Industrial Technology within EE, the Office of Fossil Energy, and the Office of International Development), and to programs at NSF.			
▸ For FY 2000, new opportunities identified through workshops and changing directions within this field of science are in aqueous catalytic chemistry, understanding the interface between water and catalytic oxides, and in catalytic activation and conversion of chlorofluorocarbons. Another area associated with the Climate Change Technology Initiative is the development of catalysts and catalytic processes for the transformation of carbon dioxide, i.e., the development of chemistry for new or improved CO_2 sequestration concepts.			
▸ Capital equipment is provided for such items as ultrahigh vacuum equipment, Fourier-transform infrared instrumentation, and high-field, solid-state NMR spectrometers.	21,883	23,401	22,854

	(dollars in thousands)	
FY 1998	FY 1999	FY 2000

- **Separations and Analysis:**
  - The separations science activity supports basic research to improve our understanding of methods for separating mixtures of gases, liquids, solids, and their component molecules, cations, and anions. The program covers a broad spectrum of separations concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. The research addresses the fundamental molecular level questions underlying the single most energy consuming of all industrial processes -- separations. The science has wide applicability and the potential for significant savings. There are strong links between this effort and the separations and analysis efforts in the Environmental Management Science Program.
  - The analysis activity supports research on phenomena basic to analytical methods with the goal of improving the sensitivity, reliability, and/or productivity of analytical determinations. Chemical and physical principles that can lead to entirely new methods of analysis are investigated; however, this program does not support instrument development. Rather, the program is aimed at obtaining a thorough understanding of the basic chemistry of analytical techniques so that their utility can be realized.
  - Several opportunities have been identified for FY 2000 that would provide the foundations needed to advance new technologies. These include advances in ceramic membranes, improved understanding of supercritical fluids for separations, applications of combinatorial chemistry to ligand design, reliable calibration methods for laser ablation sources, and improved understanding of surface-enhanced Raman spectroscopy.
  - Capital equipment is provided for such items as computational workstations and inductively-coupled plasma atomic emission spectrometers. . . . .

	FY 1998	FY 1999	FY 2000
Separations and Analysis	14,248	13,528	13,406

	FY 1998	FY 1999	FY 2000
(dollars in thousands)			

- **Heavy Element Chemistry:**

  - This program focuses on the chemical and certain physical properties of the actinide elements, principally the transuranium elements. A variety of investigations are pursued, including organometallic chemistry, chemistry of excited spectroscopic states, thermochemistry of actinide elements and compounds, chemistry of actinides in near-neutral aqueous solutions, the reactions of aqueous actinide ions with various complexing agents, development of preparative methods for actinide metals, and compounds and characterization of actinides in the solid state under pressure. This research is performed principally at the national laboratories because of the special facilities required for handling radioactivity.

  - This program is the principal source of support in fundamental chemistry of the actinide elements for the Nation. The Department has assumed 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.

  - For FY 2000, new opportunities have been identified in the emerging areas of aqueous coordination chemistry, solid-state speciation and reactivity, and advanced theoretical methods for the prediction of electronic and molecular structure and reactivity.

	FY 1998	FY 1999	FY 2000
▸ Capital equipment is provided for such items as an x-ray diffractometer and equipment for a synchrotron light source end station.	6,239	6,862	6,774

(dollars in thousands)

FY 1998	FY 1999	FY 2000

- **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. Areas of research include anode, cathode, and electrolyte systems and their interactions with emphasis on improvements in battery size, weight, life, and recharge cycles. The 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.

  - This activity provides support for those fundamental chemical engineering sciences that underpin nearly all energy intensive industrial chemical processes; particular emphasis is placed on electrochemical storage and turbulence both in combustion and in fluid flow where significant energy savings are possible. There are strong links with the combustion efforts in chemical physics and with other combustion efforts within the Department coordinated through the Combustion Coordinating Committee. The battery research efforts are coordinated with those in the Office of Transportation Technologies and the federal interagency battery consortium.

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
‣ For FY 2000 a new opportunity has been identified associated with the need to couple the current emphasis of the program in molecular simulations with molecular level theory.	8,044	8,869	8,448
■ **Climate Change Technology Initiative:** Basic research in carbon management will emphasize atomic and molecular level understanding of chemical processes to enable predictive capability. A major component of the research will aim 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 particular, multidisciplinary efforts are required that focus on improved understanding of new and existing chemical and physical separation processes, transport mechanisms, and membrane systems with selective chemical functionality; this work will address issues that are critical to clean and efficient fuels in a reduced green-house-gas economy, such as separation of CO_2 from complex mixtures or new concepts for economical oxygen separation from air for partial oxidation schemes. In addition, work will be initiated using supercritical carbon dioxide as a reagent for the catalytic and photochemical reduction of carbon dioxide to specialty chemicals or hydrocarbons, thus preventing their release into the atmosphere. 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.	0	2,197	4,394

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ **Scientific Simulation Initiative, Combustion Simulation and Modeling:** This research effort, part of the overall DOE Scientific Simulation Initiative, will develop, through simulation and modeling, a deep and detailed understanding of combustion processes to accelerate the development, characterization, and validation of design tools for advanced combustion devices. Combustion processes are extraordinarily complex, consisting of hundreds of chemical reactions that comprise combustion chemistry, fluid dynamics with turbulence scales covering 6 orders of magnitude, and interactions between chemistry and fluid dynamics involving time and spatial scales that cover 12 orders of magnitude. To address this complexity, the problem will be broken into computational regimes: device scale, subgrid, and chemistry models. The chemistry models, using modern quantum mechanical computational methods, will calculate the rates of component, combustion reactions that cannot be measured. The subgrid models incorporate the detailed interaction of chemistry with fluid dynamics at a scale that is independent of the combustion device and provide data on material and energy balance required by the device scale models. The device scale model completes the simulation, incorporating the results and parameters supplied by the other two regimes into a description of the overall device performance. Models for each of the three regimes can and will be developed concurrently and interactively. The fundamental physical laws that govern combustion behavior are known. Computational codes that can take advantage of parallel computer architectures are already under development for each of the three regimes. Provision of sufficient fidelity in the prediction of combustion device performance, particularly the emission characteristics of combustion devices, will require computational resources of the scale being planned for the overall Scientific Simulation Initiative. The knowledge gained will be used by the combustion engineering community to develop design and optimization codes for new combustion devices.	0	0	6,828

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ **General Plant Project (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 GPP funding is included in the Facilities Operations justification. The total estimated cost of each GPP project will not exceed $5,000,000.	9,992	10,275	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.	6,500	5,655	5,655
Subtotal, Chemical Sciences Research	128,452	132,750	139,230

Facilities Operations

- **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.

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
Included in FY 2000 is the third and final major increment to the HFIR operating budget of $5,979,000 for the replacement of the beryllium reflector. The reflector replacement includes fabrication of the new reflector, disassembly and reassembly of the reactor and beam room, and associated safety and engineering activities. Reflector replacement, which began in FY 1998 and will be completed in FY 2000, is a recurring activity that must be performed every 10-12 years. 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.	67,675	68,928	71,430

	(dollars in thousands)		
Facilities	FY 1998	FY 1999	FY 2000
National Synchrotron Light Source	7,949	8,082	8,233
High Flux Isotope Reactor	29,798	29,659	32,974
Radiochemical Engineering Development Center	6,705	7,027	7,168
Stanford Synchrotron Radiation Laboratory	17,607	18,740	17,939
Combustion Research Facility	5,161	5,024	5,116
Partial Offset to Science General Reduction Applied to BES	455	396	0
Total, Facilities	67,675	68,928	71,430

	FY 1998	FY 1999	FY 2000
SBIR/STTR Funding			
■ In FY 1998 $4,270,000 and $256,000 were transferred to the SBIR and STTR programs, respectively. In FY 1999 and FY 2000 the amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	4,672	4,917
Congressional Direction			
■ Funds research related to identification of trace element isotopes in environmental samples at the University of Nevada - Las Vegas (per Congressional Direction).	0	487	0
Total, Chemical Sciences	196,127	206,837	215,577

(dollars in thousands)

Explanation of Funding Changes From FY 1999 to FY 2000

	FY 2000 vs. FY 1999 ($000)
Chemical Sciences Research	
■ Decrease in research for photochemistry and radiation research.	-945
■ Decrease in research for chemical physics.	-435
■ No change in atomic, molecular and optical sciences research	+13
■ Decrease in research for catalysis and chemical transformations	-547
■ Decrease in research for separations and analysis	-122
■ Decrease in research for heavy element chemistry	-88
■ Decrease in research for chemical energy and chemical engineering	-421

	FY 2000 vs. FY 1999 ($000)
■ Increase support for the Climate Change Technology Initiative.	+2,197
■ Initiate the Combustion Simulation and Modeling Research effort as part of the overall DOE Scientific Simulation Initiative.	+6,828
Total, Chemical Sciences Research	+6,480
Facilities Operations	
■ Provide increase for scientific facilities, except for the beamline at SSRL that was completed in FY 1999. Also includes support of the beryllium reflector replacement at HFIR	+2,502
SBIR/STTR	
■ Increase SBIR/STTR funding due to increase in operating expenses	+245
Congressional Direction	
■ Funding completed on Congressionally directed project..	-487
Total Funding Change, Chemical Sciences	+8,740

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 environmental remediation of polluted sites.

Climate Change Technology Initiative. The Geosciences Research Program will enhance the scientific underpinning necessary for improving the characterization of subsurface formations and their host potential for carbon dioxide sequestration. Geomechanical studies and research on rock-fluid interactions will support evaluations of carbon dioxide injection technologies, reservoir storage capacities, and long-term storage stability. Research concerning the physics of flow for multiple reactive fluid phases in fractured rock systems will provide the basis for predicting the viability of terrestrial carbon dioxide sequestration and for improved efficiency of fossil energy and geothermal energy production. Additional research in geochemistry will complement the research activities in geophysics with investigations to enhance understanding of the geochemical reactivity within the reservoirs/aquifers under static and dynamic flow conditions for fluids enriched in constituents important for CO_2 sequestration.

Funding Schedule

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
Engineering Research	17,296	17,471	14,500	-2,971	-17.0%
Geosciences Research	22,855	24,189	22,097	-2,092	-8.6%
SBIR/STTR	0	1,079	948	-131	-12.1%
Total, Engineering and Geosciences	40,151	42,739	37,545	-5,194	-12.2%

Detailed Program Justification

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
Engineering Research			
■ **Engineering Research:** The Engineering Research activity supports work in three technical areas: (1) mechanical systems including fluid mechanics, heat transfer, and solid mechanics; (2) systems sciences including process control, instrumentation, and intelligent machines and systems; and (3) 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 2000, funding will be terminated for research in turbulence, control systems, integrated manufacturing, and combustion. Research will be decreased in fluid dynamics and flow through porous research in bodies.	17,296	17,471	14,500
Geosciences Research			
■ **Geosciences Research:** The Geosciences Research activity supports basic research in geophysics and geochemistry to improve the level of understanding necessary for advances in and choices among current and emerging energy and environmental technologies. Geochemical research focuses on fundamental understanding of mineral-fluid interactions to provide a better foundation for oil, gas, and geothermal resource recovery and control of contaminants in groundwater flow; new fundamental thermodynamic and physical property information on rocks, minerals, and geologic fluids for resource recovery and contaminant assessment and monitoring; and extending the applicability of isotopic tracer methods for evaluation of natural and human-perturbed processes in the geologic environment. This information, in concert with other geosciences research, is providing the basis for efforts leading to quantitative predictive capabilities for processes that take place in the			

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
Earth's crust. In FY 2000, funding will be terminated on mechanical stability of porous reservoirs and multi-phase flow through porous bodies. Funding will be reduced in geochemistry and geophysics.	22,855	22,725	15,275
■ **Climate Change Technology Initiative:** Basic research in carbon management for the Climate Change Technology Initiative will emphasize those aspects of geosciences and engineering that will provide the understanding needed for sequestration of carbon dioxide in subsurface reservoirs. The research program will focus on three areas where improved understanding is needed to evaluate the potential for deep underground sequestration: (1) understanding the mechanical stability of porous and fractured reservoirs/aquifers during injection and over the long times required for sequestration; (2) understanding flow of fluids with multiple phases within the aquifers; and (3) understanding the geochemical reactivity within and among fluids, and between fluids and rock material within the reservoirs/aquifers. In order to understand the mechanical stability of formations, a better understanding of the stress-strain-poroelasticity- viscoelasticity-thermoelasticity constitutive relationships are necessary, as are fracture mechanics models, improved seismic models, and inversion codes to track mechanical stability of rocks at reservoir depths and scales. Fluid flow studies are need to understand mixing, fingering and phase retardation, fluid-fluid transport at ambient and injection conditions, fluid-fluid-mineral interactions including wetting behavior, and surface tension effects. In order to understand the mechanical stability of potential storage formations, a better understanding of the geochemical reactivity of reservoirs/aquifers -- under conditions involving fluids rich in constituents important for CO_2 sequestration and in the presence of interacting mineral-fluid system -- will be needed to fully evaluate these systems in terms of sequestration potential and safety..	0	1,464	6,822
Total, Geosciences Research	22,855	24,189	22,097

	FY 1998	FY 1999	FY 2000
	(dollars in thousands)		
SBIR/STTR Funding			
■ In FY 1998 $984,000 and $59,000 were transferred to the SBIR and STTR programs, respectively. The FY 1999 and FY 2000 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.	0	1,079	948
Total, Engineering and Geosciences	40,151	42,739	37,545

Explanation of Funding Changes From FY 1999 to FY 2000

	FY 2000 vs. FY 1999 ($000)
Engineering Research	
■ Termination of engineering research on turbulence, control systems, integrated manufacturing, and combustion and decrease in research on fluid dynamics. . . .	-2,971
Geosciences Research	
■ Termination of geosciences research on mechanical stability of porous reservoirs and multi-phase flow through porous bodies and decrease in geochemistry and geophysics to provide increase in Climate Change Technology Initiative and other priority areas..	-7,450
■ Increase in Climate Change Technology Initiative.	+5,358
Total, Geosciences Research	-2,092
SBIR/STTR	
■ Decrease SBIR/STTR funding due to increase in operating expenses.	-131
Total Funding Change, Engineering and Geosciences	-5,194

Energy Biosciences

Mission Supporting Goals and Objectives

The Energy Biosciences subprogram supports mechanistic research on fundamental biological processes related to capture, transformation, storage and utilization of energy. The research focuses on plants and non-medical microorganisms to form a broad scientific foundation for support of Department of Energy's goals and objectives in energy production, environmental management, and energy conservation. Basic research on plants includes photosynthetic mechanisms and bioenergetics in algae, higher plants, and photosynthetic bacteria; control mechanisms that regulate plant growth and development; fundamental aspects of gene structure, function, and expression; plant cell wall structure, function and synthesis; and mechanisms of transport across membranes. Research supported in these areas seeks to define and understand the biological mechanisms that effectively transduce light energy into chemical energy, to identify the biochemical pathways and genetic regulatory mechanisms that can lead the efficient biosynthesis of potential fuels and petroleum-replacing compounds, and to elucidate the capacity of plants to remediate contaminated environments by transporting and detoxifying toxic substances. The research focus in the microbiological sciences includes the degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of microbial growth and development, thermophily, e.g., bacterial growth under high temperature, and other phenomena with the potential to impact biological energy production, conversion and conservation. Organisms and processes that offer unique possibilities for research at the interface of biology and the physical, earth and engineering sciences are also studied.

Climate Change Technology Initiative. Biological systems, particularly plants, algae, and microbes, play a major role in the capture and release of atmospheric carbon dioxide. Photosynthetic organisms use sunlight to convert carbon dioxide into more complex organic compounds, while many non-photosynthetic organisms use the energy in various inorganic and organic compounds to fix 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.

Funding Schedule

	(dollars in thousands)				
	FY 1998	FY 1999	FY 2000	$ Change	% Change
Energy Biosciences	26,710	29,088	30,410	+1,322	+4.5%
SBIR/STTR	0	774	816	+42	+5.4%
Total, Energy Biosciences	26,710	29,862	31,226	+1,364	+4.6%

Detailed Program Justification

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000

Energy Biosciences

- **Energy Biosciences**: This activity supports basic research in the energy-related biosciences forming the mechanistic foundation for the development of future biotechnologies related to energy. This work provides the knowledge necessary to use biological systems associated with the capture, transformation, storage and utilization of energy, and other significant missions of the Department of Energy. Those programs within the Department that are active in creating or exploiting technologies are supported through numerous interactions at both the manager and the researcher level. The Basic Energy Sciences program is scientifically heterogeneous and many efforts are made to encourage the development of truly interdisciplinary research activities. The Energy Biosciences subprogram is actively involved with other federal agencies funding basic plant and microbial research to encourage effective and efficient management of the total federal research portfolio.

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
The successes of this subprogram, along with other federal research efforts, are developing an expanding science knowledge base leading to the rapid expansion of biotechnological applications using both plants and microbes. The formation of numerous large "life science" corporations is indicative of this trend. Ongoing basic research is leading to numerous new and unexploited research opportunities, including functional plant genomics, organellar and chromosome-level bioengineering, elucidation of new biochemistries, and determiantion of cellular and morphological development. Each of these areas have the potential to be commercially applied, resulting in major economic and societal impacts ranging from the revitalization of the rural economy through dispersal of the nation's manufacturing base to the formation of a new generation of bio-based industries; in addition to having a major impact on the nation's production and use of energy expensive chemicals and fuels. Recently, private and charitable research foundations have responded to both the opportunities and impacts of fundamental research in these areas and are building large basic research institutes in St. Louis and San Diego. They have the resources to build the needed facilities, but are relying on the federal government to provide the long-term support of the research activities and to provide the required scientific personnel. Capital Equipment is provided for items used for structure determination and for special analysis of biomaterials. .	26,710	26,652	25,537

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ **Climate Change Technology Initiative:** Basic research in carbon management for the Climate Change Technology Initiative begun in FY 1999 emphasized the biological process of photosynthesis, which is central to global carbon cycling. The primary current focus of these photosynthesis activities is the biophysics and biochemistry of energy capture and structural studies on the photosynthetic apparatus. There are a number of unexplored opportunities that complement this work with studies on the mechanism of photosynthetic carbon fixation and the subsequent metabolism of the fixed carbon. An example of the research supported are studies to provide a fundamental understanding of chloroplasts, which are small membrane bound entities in the cytoplasm of plant cells where photosynthesis occurs. Chloroplasts contain DNA and are able to control their development and replication. The new research will investigate the principals underlying the biochemical and molecular genetic mechanisms of chloroplast development and reproduction along with critical interactions of chloroplasts with the cytoplasm and nucleus. The understanding obtained from these 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.	0	2,436	4,873
Total, Energy Biosciences	26,710	29,088	30,410
SBIR/STTR Funding			
■ In FY 1998 $672,000 and $40,000 were transferred to the SBIR and STTR programs, respectively. The FY 1999 and FY 2000 amounts shown are the estimated requirement for the continuation of the SBIR/STTR programs.	0	774	816
Total, Energy Biosciences	26,710	29,862	31,226

Explanation of Funding Changes from FY 1999 to FY 2000

	FY 2000 vs. FY 1999 ($000)
Energy Biosciences	
■ Decrease in support of research providing the fundamental understanding of life processes in plant and microbes.	-1,115
■ Increase in support for Climate Change Technology Initiative.	+2,437
Total, Energy Biosciences	+1,322
SBIR/STTR	
■ Increase in SBIR/STTR funding due to increase in operating expenses.	+42
Total Funding Change, Energy Biosciences	+1,364

Construction

Mission Supporting Goals and Objectives

Construction is needed to support the research in each of the subprograms in the Basic Energy Sciences program. Experiments necessary in support of basic research require that state-of-the-art facilities be built or existing facilities modified to meet unique research requirements. Reactors, radiation sources, and neutron sources are among the expensive, but necessary, facilities required. The budget for the BES program includes funding for the construction and modification of these facilities.

Funding Schedule

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
Construction	7,000	105,400	196,100	+90,700	+86.0%
Total, Construction	7,000	105,400	196,100	+90,700	+86.0%

Detailed Program Justification

(dollars in thousands)

	FY 1998	FY 1999	FY 2000
Construction			
■ Funding for the Combustion Research Facility, Phase II was completed in FY 1999 as scheduled.	7,000	4,000	0
■ The FY 2000 requested budget authority will provide for: continuation of Title I design, the start of Title II design activities, initiation of construction of conventional facilities, procurement of several significant technical components, and continued research and development activities for the Spallation Neutron Source.	0	101,400	196,100
Total, Construction	7,000	105,400	196,100

Explanation of Funding Changes From FY 1999 to FY 2000

	FY 2000 vs. FY 1999 ($000)
Construction	
■ The decrease in funding for the construction of the Combustion Research Facility, Phase II project is a result of the scheduled completion of this project .	-4,000
■ The increase in funding for the Spallation Neutron Source represents the scheduled ramp up of activities.	+94,700
Total Funding Change, Construction	+90,700

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 operation of these facilities is provided in the Materials Sciences and Chemical Sciences subprograms.

	(dollars in thousands)				
	FY 1998	FY 1999	FY 2000	$ Change	% Change
National Synchrotron Light Source	30,996	32,176	32,756	+580	+1.8%
High Flux Beam Reactor	22,986	22,568	22,580	+12	-+0.1%
Intense Pulsed Neutron Source	11,230	11,982	11,985	+3	0.0%
High Flux Isotope Reactor	33,770	29,659	34,574	+4,915	+16.6%
Radiochemical Engineering Development Center	6,705	7,027	7,168	+141	+2.0%
Stanford Synchrotron Radiation Laboratory	21,684	22,686	21,968	-718	-3.2%
Manuel Lujan, Jr. Neutron Scattering Center	6,588	7,397	7,547	+150	+2.0%
Combustion Research Facility	5,161	5,024	5,116	+92	+1.8%
Advanced Light Source	30,708	31,166	31,732	+566	+1.8%
Advanced Photon Source	82,368	86,226	87,703	+1,477	+1.7%
Spallation Neutron Source	0	28,600	17,900	-10,700	-37.4%
Partial Offset to Science General Reduction Applied to BES	1,555	1,521	0	-1,521	-100.0%
Total, Major User Facilities	253,751	286,032	281,029	-5,003	-1.7%

Detailed Program Justification

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
Facilities Operations			
■ National Synchrotron Light Source at Brookhaven National Laboratory.	30,996	32,176	32,756

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ High Flux Beam Reactor at Brookhaven National Laboratory. On December 21, 1996, the High Flux Beam Reactor (HFBR) was shut down for normal refueling. However, before the reactor was restarted, the announcement was made that a plume of tritium, believed to emanate from the reactor spent fuel pool, was contaminating the ground water south of the reactor. The reactor has remained in standby mode since that time. Because the reactor contains radioactive fluids in the primary cooling system, nearly a full staff is necessary to maintain the reactor and associated equipment in safe operating condition. The funding requested in FY 2000 represents that required to maintain the reactor and to proceed with safety modifications that are required regardless of whether the reactor is restarted or is decommissioned.	22,986	22,568	22,580
■ Intense Pulsed Neutron Source at Argonne National Laboratory.	11,230	11,982	11,985
■ High Flux Isotope Reactor at Oak Ridge National Laboratory. There will be a continuation of increased operating support in FY 2000 to take advantage of the new cold source with 3 new experimental stations and to support the scheduled replacement of the beryllium reflector. Also, includes AIP funding of $3,972,000 in FY 1998 for HB-2 tube upgrades and $1,600,000 in FY 2000 for HB-4 Beamline Enclosure.	33,770	29,659	34,574
■ Radiochemical Engineering Development Center at Oak Ridge National Laboratory.	6,705	7,027	7,168
■ Stanford Synchrotron Radiation Laboratory at Stanford University. The decrease is the result of scheduled completion of Beamline 11.	21,684	22,686	21,968
■ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.	6,588	7,397	7,547
■ Combustion Research Facility at Sandia National Laboratories/California.	5,161	5,024	5,116

	(dollars in thousands)		
	FY 1998	FY 1999	FY 2000
■ Advanced Light Source at Lawrence Berkeley National Laboratory.	30,708	31,166	31,732
■ Advanced Photon Source at Argonne National Laboratory.	82,368	86,226	87,703
■ Spallation Neuron Source.	0	28,600	17,900
■ Partial Offset to ESRD General Reduction Applied to BES.	1,555	1,521	0
Total, Major User Facilities	253,751	286,032	281,029

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 1998	FY 1999	FY 2000	$ Change	% Change
General Plant Projects	10,342	10,625	10,625	0	0.0%
Accelerator Improvement Projects . .	11,502	7,108	8,195	+1,087	+15.3%
Capital Equipment	49,809	57,114	55,178	-1,936	-3.4%
Total, Capital Operating Expenses . . .	71,653	74,847	73,998	-849	-1.1%

Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp- riations	FY 1998	FY 1999	FY 2000	Unapprop- riated Balance
99-E-334 Spallation Neutron Source, ORNL	1,159,500	0	0	101,400	196,100	862,000
96-E-300 Combustion Research Facility, Phase II, SNL	26,800	15,800	7,000	4,000	0	0
Total, Construction		15,800	7,000	105,400	196,100	862,000

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

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp- riations	FY 1998	FY 1999	FY 2000	Accept- ance Date
Short Pulse Spallation Upgrade at LANSCE - LANL	20,500	0	4,500	4,500	6,000	FY 2001
HB-2 Beam Tube Extension at HFIR - ORNL	5,900	0	0	3,500	2,400	FY 2000
Total, Major Items of Equipment . .		0	4,500	8,000	8,400	

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

(Changes from FY 1999 Congressional Budget Request are denoted with a vertical line in the left margin.)

Significant Changes

The Total Estimated Cost and Total Project Cost have been increased and the construction schedule has been extended. The schedule delay and increased costs are a result of the planned FY 1999 funding being reduced by $27,000,000 in the FY 1999 appropriation.

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 (*Current Estimate*)	1Q 1999	4Q 2003	3Q 2000	1 Q 2006	1,159,500	1,360,000

2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
Construction			
1999	101,400	101,400	53,700
2000	196,100	196,100	166,200
2001	267,900	267,900	263,800
2002	262,500	262,500	274,100
2003	193,600	193,600	207,300
2004	78,300	78,300	131,700
2005	49,200	49,200	47,200
2006	10,500	10,500	15,500

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 next century.

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.

Neutron probes 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 1996 Russell Panel Report, the SNS has been designed to operate at an average power on target of about 1 MW. At this power level, the SNS will be the most powerful spallation source in the world--six times that of ISIS at the Rutherford Appleton Laboratory in the United Kingdom. However, the SNS has been deliberately designed to allow for economical upgrading to substantially higher powers once the technology is developed to make this possible. 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 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 they have spin, neutrons have a magnetic moment and can be used to study magnetic structure and magnetic properties of materials. Because their interactions are known with great accuracy, neutron scattering is far more easily interpreted than either photon scattering or electron scattering.

However, the same properties that make neutrons an ideal probe of matter also result in their most significant disadvantage. Because neutrons interact only weakly with matter, most neutrons pass through a sample without producing a detectable interaction. Therefore, neutron scattering experiments are said to be extremely "flux limited." This situation is further exacerbated because, unlike photons and charged particles, neutrons cannot be focused. Therefore, high brilliance (i.e., highly focused) neutron beams are very difficult to make. The combination of weak interaction and inherent low brilliance has driven the quest for high-flux neutron sources. 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 next century and to address the mix of needs associated with the user community, the operations staff, security, contamination control, noise, etc.

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 1999 budget authority allowed the start of Title I design activities, initiation of subcontracts and long-lead procurements, and continuation of critical research and development work necessary to reduce technical and schedule risks in this project. Initiation of most long-lead procurements is delayed until FY 2000 due to the reduction in the FY 1999 appropriation.

FY 2000 funding of $214,000,000 is requested for the SNS Project for detailed design (Title II) for the ion source, low-energy beam transport, linac structure and magnet systems, target assemblies, experimental instruments, and global control systems. Detailed design will be completed for several conventional facilities in preparation for the installation of major equipment in the following fiscal year; design will be completed 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 start for some conventional facilities including roads into the site, site preparation/grading, waste systems, and retention basins. Procurement for several significant equipment items such as dipole magnets, material for the target transport systems, and klystrons will begin. Project Management and Project Integration activities, which are exceptionally important during this phase of the project, will also be conducted. The Preliminary Safety Analysis Report (PSAR) will be completed during the fiscal year and work will begin on the final report.

4. Details of Cost Estimate [a]

(dollars in thousands)	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 26% of construction costs	166,900	166,900
Construction management at approximately 4% of construction costs	26,300	26,300
Project management at approximately 15% of construction costs	102,900	96,800
Land and land rights	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks)	28,600	28,600
Buildings	176,700	176,700
Other structures	600	600
Utilities (electrical, water, steam, and sewer lines)	30,500	30,500
Technical Components	417,900	406,300
Standard Equipment	1,100	1,100
Major computer items	12,000	12,000
Removal cost less salvage	0	0
Design and project liason, testing, checkout and acceptance	9,700	6,700
Subtotal	973,200	952,500
Contingencies at approximately 19 percent of above costs	186,300	186,300
Total Line Item Cost	1,159,500	1,138,800
Less: Non-Agency Contribution	0	0
Total, Line Item Costs (TEC)	1,159,500	1,138,800

5. Method of Performance

The ORNL Management and Operating Contractor will provide overall project management and integration, design and ultimate procurement of the target station, beam transport, and experiment systems, and will subcontract for the services of an Industry Team for design and construction management services. The Industry Team will consist of an Architect-Engineer for the conventional facilities design and a Construction Manager for construction, installation, equipment procurement, testing and preoperational support. Other DOE laboratories will, through intra laboratory agreements, become members of the overall project's management, design and R&D team, particularly in the areas encompassed by the linac, the accumulator ring, instrumentation, and the target. Procurement and

a The cost estimate is based on a conceptual design completed in FY 1997. The DOE Headquarters Economic Escalation indices were used as appropriate over the project cycle.

construction will be accomplished, to the extent feasible, by fixed-priced subcontracts awarded to industry on the basis of competitive bidding.

6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 1998	FY 1999	FY 2000	Outyears	Total
Project Cost						
Facility Cost [a]						
Line Item TEC	0	0	53,700	166,200	939,600	1,159,500
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	0	53,700	166,200	939,600	1,159,500
Other project costs						
R&D necessary to complete project [b]	200	21,400	25,300	16,300	26,200	89,400
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]	0	1,500	400	0	0	1,900
Other project-related costs [e]	0	0	800	900	89,097	90,797
Capital equipment not related construction [f]	0	100	2,100	700	200	3,100
Total, Other project costs	15,503	23,000	28,600	17,900	115,497	200,500
Total project cost (TPC)	15,503	23,000	82,300	184,100	1,055,097	1,360,000

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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 $1,159,500,000.

b A research and development program at an estimated cost of $89,400,000 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 $90,797,000 are included to cover pre-operations costs.

f Estimated costs of $3,100,000 to provide test facilities and other capital equipment to support the R&D program.

7. Related Annual Funding Requirements [a]

	(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

[a] Expressed in FY 2006 dollars, the first full year of operation.