

**DEPARTMENT OF ENERGY
FY 1999 CONGRESSIONAL BUDGET REQUEST
OFFICE OF ENERGY RESEARCH
SCIENCE**

(Tabular dollars in thousands, Narrative in whole dollars)

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 leading to new and improved energy technologies and to understanding and mitigating the environmental impacts of energy technologies. 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 GOALS of the BES program are:

1. To maintain U.S. world leadership in those 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;
2. To foster and support the discovery, dissemination, and integration of the results of fundamental, innovative research in these areas;
3. To provide world-class scientific user facilities for the Nation; and
4. To act as a steward of human resources, essential scientific disciplines, institutions, and premier scientific user facilities.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

The OBJECTIVES related to these goals are:

1. 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.
2. 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 fusion energy sources by using established management practices to link BES staff and BES-supported principal investigators with their counterparts in the energy technology offices and in industry. Such practices include, for example, cofunding and collocating basic research programs supported by BES with applied research programs supported by the technology offices at the DOE laboratories and the initiation in FY 1999 of the Partnerships for Academic-Industrial Research (PAIR) Program, which will link basic researchers in academia with those in industry.
3. Plan, construct, and operate premier national scientific user facilities 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 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.
4. Establish and maintain stable, essential research communities, institutions, and scientific user facilities. -- Steward important research communities and institutions 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.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

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 [Goal 1], (2) relevance to the comprehensive energy mission of the agency [Goal 2]; and (3) stewardship of research performers, essential scientific disciplines, institutions, and scientific user facilities [Goals 3 and 4]. Combining and sustaining these tenets are the management challenge of BES. The fourth area to be evaluated, 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. These include, for example, peer review of research programs and customer surveys of the scientific user facilities. However, literally dozens of other activities and indicators can be envisioned for inclusion in the matrix. An important management challenge is choosing a few significant items to target for special attention. Different activities and indicators may be targeted in successive years. In this way, a balanced system of performance measurement will evolve. For the next few years, BES will select a few activities each year that address different aspects of performance measurement and that, taken together with ongoing activities, will strengthen performance measurement.

During FY 1997, BES began two activities designed to strengthen and formalize performance measurement in the future. These were (1) codification of the peer review process for research at the DOE laboratories using a process analogous to that described in 10 CFR 605 for the university grant program and (2) development of a major new survey tool for the scientific user facilities in collaboration with the facility directors and the facility user coordinators. In addition, BES conducted a number of other activities related to performance and to the management of basic research programs including (3) initiation of a Basic Energy Sciences Advisory Committee (BESAC) review of the BES synchrotron radiation light sources; (4) initiation of a BESAC assessment of neutron science following the events at the High Flux Beam Reactor at Brookhaven National Laboratory; (5) project management reviews of two ongoing construction projects - the joint ER/Defense Programs enhancement of the Los Alamos Neutron Science Center short pulse spallation source and the Conceptual Design Report of the

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

Spallation Neutron Source; (6) sponsorship of a number of workshops to assess the frontiers of research in areas of interest to BES; (7) development of new ways to increase the number of Small Business Innovation Research (SBIR) topics promoted by BES; (8) initiation of a pilot study to assess the culture that promotes excellence in basic research at the DOE laboratories; (9) continuation of a grant to assess the impacts on industry of basic research; and (10) publication of several overview brochures aimed at general audiences providing historical retrospectives, program highlights, and descriptions of the impacts of basic research on U.S. industry.

During FY 1998, BES will (1) institute the formalized peer review process for activities at the DOE laboratories using the process developed in FY 1997, (2) establish baselines for all performance indicators for each scientific user facility using the survey tool established in FY 1997, and (3) begin peer review of the operating scientific user facilities. In addition, in order to formalize other processes for implementation in FY 1999, BES will in FY 1998 (4) determine a set of performance indicators that will be collected annually from investigators in the grant program and the DOE laboratory system; and (5) review the implementation of the criteria of the merit review system.

In FY 1999, BES will initiate construction of the Spallation Neutron Source, which will be a world-class facility used to provide beams of neutrons to probe and understand the physical, chemical, and biological properties of materials at an atomic level. In addition, (1) the development and upgrade of scientific user facilities 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 10CFR 605 for the extramural grant program and in a modification of 10CFR 605 for the laboratory programs and scientific user facilities; (4) new projects will be selected by peer review and merit evaluation; and (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.

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 several of the Nation's premier user facilities. Presented below are program accomplishments from FY 1997 including selected prizes, awards, and honors bestowed on BES principal investigators during that period and selected highlights from the scientific programs. 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 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, two

FY 1999 initiatives that will be funded with existing funds using the normal turnover in proposals, and a new program in carbon emissions management.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

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 1997 were Nobel Prizes. The Nobel Prize in Chemistry for 1996 was awarded to Richard E. Smalley (Rice University), Robert F. Curl (Rice University), and Sir Harold Kroto (University of Sussex) for their discovery of buckminsterfullerene, C₆₀. Richard Smalley was supported by BES for the work that led to the discovery of C₆₀, and Robert Curl has long been supported by BES for work in infrared spectroscopy. 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. These are the third and fourth Nobel Prizes awarded to BES principal investigators in the past four years.

Other selected major prizes and awards include:

From ACTA Metallurgica -- the Gold Medal

From the American Ceramic Society -- the James I. Mueller Memorial Award; the Edward Orton, Jr. Memorial Lecture; the George W. Morey Award

From the American Chemical Society -- the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry; the Award for Distinguished Service in the Advancement of Inorganic Chemistry; the Award in Analytical Chemistry; the Award in Spectrochemical Analysis; the Award in the Chemistry of Materials; the Berlinger Award; the E. V. Murphree Award in Industrial and Engineering Chemistry; the Henry Award; the James Van Lanen Award for Distinguished Service to the Biochemical Technology Division; the Ralph K. Iler Award in the Chemistry of Colloidal Materials; the Remsen Award; the Award in Chromotography; the Irving Langmuir Award in Chemical Physics

From the American Crystallographic Association -- the Bertram E. Warren Award

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

From the American Physical Society -- the Arthur L. Schawlow Prize in Laser Science; the Award for Outstanding Doctoral Thesis Research in Atomic, Molecular, or Optical Physics; the High Polymer Physics Prize; the Oliver E. Buckley Prize in Condensed Matter Physics; Nottingham Prize for Outstanding Graduate Thesis in the Surface Science; the Earl K. Plyer Prize in Molecular Spectroscopy

From the American Society for Mass Spectrometry -- the Biemann Award in Mass Spectrometry

From the American Society of Plant Physiologists -- the Charles Albert Shull Award; the Martin Gibbs Medal; the Dennis Robert Hoagland Award

From the American Vacuum Society -- the Peter Mark Award; the George T. Hanyo Award; the Medard W. Welch Award

From the American Welding Society -- the Charles H. Jennings Memorial Award

From the ASM International -- the Henry Marion Howe Medal

From the Australian Society of Electron Microscopy -- the President's Award

From the Electrochemical Society -- the Edward Goodrich Acheson Medal; the Olin Palladium Award

From the Geological Society of America -- the Arthur L. Day Medal for Outstanding Contributions to Geosciences Research; the Distinguished Service Award in Hydrogeology; the O. E. Meinzer Award for Hydrogeological Research

From the Institute of Electrical and Electronic Engineers -- the Magnetics Society Distinguished Lecturer; the Quantum Electronics Award

From the Institute of Materials -- the Elegant Work Prize

From the Inter-American Photochemical Society -- the Award in Photochemistry

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

From the International Union of Pure and Applied Chemistry -- the Rossini Lectureship Award

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

From the International Union of Pure and Applied Physics -- the Magnetism Award

From the Materials Research Society -- the von Hippel Award

From the Mineralogical Society of America -- the Mineralogical Society of America Award; the Harley Award

From the Minerals, Metals, and Materials Society (TMS) -- the Educator Award; the Leadership Award; the Structural Materials Distinguished Materials Scientist/Engineer Award; the Robert Lansing Hardy Award

From the North American Catalysis Society -- the Paul H. Emmett Award

From the Optical Society of America -- the Adolph Lomb Medal

From the Royal Society of Chemistry -- the Centenary Lectureship; the Structural Chemistry Award

From the Society of Analytical Chemistry -- the Robert Boyle Award

From the Society of Electroanalytical Chemistry -- the Charles N. Reilley Award

From the Society of Polymer Science (Japan) -- the Distinguished Service in Advancement of Polymer Science Award

Finally, two principal investigators received the President's National Medal of Science; two received the E. O. Lawrence Award; ten were inducted into the National Academy of Sciences; and five were inducted into the National Academy of Engineering.

Selected FY 1997 Scientific Highlights/Accomplishments

- 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 cycle of all biological organisms involves the central molecule, ATP. The energy captured from photosynthesis or released from respiration is converted into ATP where it 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. The enzyme responsible for the synthesis is ATP synthase. Dr. Boyer's work examined

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

the detailed chemical reactions involved in this synthesis and the roles specific parts of the ATP synthase molecule played in the overall synthesis. Dr. Boyer's work on the synthesis of ATP was supported in part by the Division of Energy Biosciences of the Office of Basic Energy Sciences and its predecessor organizations from 1963 until 1993 under a project entitled "Energy Capture and Use in Plants and Bacteria" to the University of California at Los Angeles.

- The Advanced Photon Source (APS) Completes Its First Year of Operation. As the floor of the APS became crowded with experimental hutches, new results emerged that took advantage of the very high brightness of this new light source and that could not have been done elsewhere. While much of the work at the APS and the other BES synchrotron radiation light sources has been and will continue to be in the area of materials sciences and condensed matter physics, many studies are also being done in the areas of biological, plant, environmental, and geosciences. For example,
 - A new structural determination and biochemical analysis of the human fragile histidine triad (FHIT) protein has been performed. The FHIT protein derives from a fragile site on human chromosome 3 that is commonly disrupted in association with cancers. The understanding of this tumor suppressor protein will focus on a diverse human HIT family member in search of their in vivo function throughout biology.
 - The first experiments were conducted with a newly constructed beamline for geosciences/soil/environmental research. Molecular-scale observations (made possible by the high brightness of the APS) enable new understanding of local structural and chemical changes that govern the mechanisms of mineral-fluid interactions. For example, the molecular form or speciation of environmental contaminants, such as chromium, arsenic, lead, uranium or plutonium, determines their toxicity and bioavailability.
 - Over 90% of the world's plants, including essentially all crops, make use of symbiotic associations with fungi. X-ray imaging studies performed on these systems using an x-ray microprobe have provided detailed information on the elemental distribution in plant roots and associated fungi. These images, with unprecedented spatial resolution, will be a key to understanding the symbiosis between the plant roots and fungi.
- New Sensor Provides Instant Litmus Test for Pathogens. A new class of colorimetric sensor materials has been invented that makes it possible to instantaneously and inexpensively detect a wide range of biological toxins and common disease-causing organisms. Building on earlier discoveries, researchers have developed a thin film consisting of receptor molecules attached to a film of linked diacetylene molecules. The film transmits blue light. The surface receptor molecules are designed to very selectively bind specific pathogens causing the film molecules to reorganize and the film to turn red. Pathogens thus far detected with good sensitivity include

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

an influenza virus, cholera toxin, botulism toxin, and the toxin produced by the bacteria responsible for 200 deaths per year in the US alone, as noted by the recent contamination of fruit drinks and fast food hamburgers. Existing tests for all of these pathogens require at least a 24 hour culture. After further development, the sensors can be placed on plastic, paper, or glass and incorporated into inexpensive packaging and portable detection devices.

- Joint Program Results in a New "Smart" Window. Windows with reduced transmission have been shown to be energy savers by reflecting some of the heat from solar radiation. However, such windows have fixed transmission that also reduces visible light. On a cloudy day a building or home equipped with such windows may not have adequate natural lighting. Research jointly supported by BES and the Department's Energy Efficiency program has led to the initial development of a self-powered "smart" window that can control its own transparency. Integration of two technologies, electrochromic windows and dye-sensitized solar cells, yields a smart window that darkens, reversibly, when exposed to sunlight.
- Powder Process Produces Cheaper Stronger Permanent Magnets. A collaborative team from two laboratories is a recipient of a prestigious R&D 100 Award for the processing of nanocrystalline composite powder for high-strength, permanent magnets. The permanent magnet industry is a very large global industry worth 3.2 billion dollars in 1995 and is predicted to reach 10 billion dollars by 2010. The high magnetic strength of the prize-winning neodymium-iron-boron 'super magnets' results from matching the crystallite size formed on cooling the alloy from the melt to the size of the magnetic domains. The previously used rapid cooling process that creates the fine-grained polycrystalline material is too expensive for many commercial magnet applications. It was discovered that adding titanium and carbon to the molten alloy allows a spray atomization process to create appropriately sized particles that can be consolidated into magnetic compacts.
- Fast-Transport Predicted in Subsurface Fluids. Underground flow properties of fluids containing two or more components (oil(s)/water) are a major issue for environmental remediation. New experimental work documents how upward and downward flow of different fluids can be driven by differences in their density and their tendency to diffuse. Such transport occurs much more rapidly than has been predicted by earlier models. This new research developed innovative experimental methods to test the earlier predictions, and successfully measured and modeled the effects of multiphase flow in simple porous materials. This work is a significant step towards developing improved models to make better predictions for complex and highly variable natural subsurface environments.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

- Breakthrough in Processing of Aerogel Films. A breakthrough in the processing of ceramic aerogel films won a prestigious award of the American Chemical Society and was cited as an important discovery by the Wall Street Journal. This breakthrough overcame the sixty year barrier to the large scale commercial utilization of these films. Aerogel films have a foam-like structure, exceptional lightness and transparency, and are ideal insulating materials for double-paned windows and other uses. When freshly formed from a liquid, the film can be easily torn until it has been hardened. Older processes required a toxic liquid and high pressure and temperature to dry the films. Employing a new understanding of film drying and chemical treatment of the surfaces of the pores in the film, a non-toxic, low-pressure and temperature process was developed to keep the film flexible and resilient as it formed.
- Silicon in Biology. Silicon is an element that is a principal component of glass, computer chips, coatings and numerous consumer products. There are only a few biological systems that metabolize this element. Silicon is metabolized by some simple animals, by algae to make the equivalent of glass houses, and by some higher plants (the rough feel of corn leaves comes from chards of silicates in the leaves). Recently a gene was identified that encodes a protein that is involved in binding and transporting silicon into a cell. This discovery will extend our understanding of how silicon is taken up and processed by biological systems which may lead to applications such as the mining of silicon from seawater and the manufacture of silicon-containing products.
- Cool Sounds. Air conditioning from your favorite music? Not quite yet. However, sound, or acoustic energy, has now been used to make refrigerating and heating units. These devices, called thermoacoustic refrigerators, or thermoacoustic engines when operated in a heating mode, have no moving parts and use sound waves in air or helium to transfer heat. Operation of these devices has been based upon a standing acoustic wave in a closed system, limiting their usage. Now, a radically new concept has been devised in which the air or helium would flow slowly through the device during operation. This concept would allow for heating and cooling of buildings and for other industrial air conditioning applications with an economic advantage over current technology through the elimination of the bulky heat exchangers on building roofs. First results from a test system operating as a refrigerator using helium or air have confirmed the concept. Further developments of this concept are under way.
- New Graphite Nanofibers Store Hydrogen. A new nano-phase graphitic material capable of absorbing three grams of hydrogen for each gram of carbon has been discovered by researchers studying catalyst deactivation. The origins of this material are found in studies of metal particle fracturing that occurs during Fischer-Tropsch catalysis. The graphitic microstructure of the fibers is such as to allow hydrogen to fit within the interplanar space between aligned graphitic planes. The development of synthetic routes to these new nanomaterials have been awarded a patent. Although it is not yet understood how these nanofibers absorb such a large volume of hydrogen (about 32 liters of hydrogen per gram at ambient conditions), the discovery is potentially very significant to hydrogen storage technology and perhaps also to storage of other small gases.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

- Slick and Sticky. Pencil-shaped organic molecules called "rod-coils," designed and synthesized to have half of the molecule rigid and the other half flexible, were discovered to exhibit unusual and important clustering mechanisms on several size scales. Aggregates of these molecules self-assemble into mushroom-shaped clusters with the rigid ends forming the stems and the flexible coils forming the caps. At the next level of organization, the mushroom clusters pack side by side into layered sheets to form, ultimately, a thick film. Because the building-block molecules are all oriented in the same direction, the film's properties mirror those of the individual molecules, resulting in a film whose bottom surface is sticky and top surface is slippery. Such a film has many potential applications, for example as an anti-ice coating on an airplane wing or an anti-blood-clot lining for artificial blood vessels. This new molecular organizational technique is being explored to make films with other properties by replacing the slippery and sticky groups capping the rodcoils with compounds that perform other functions, such as conducting electricity or changing their size in response to an electrical pulse.
- Controlling Natural Energy Resources through Plant Genetic Engineering. Cellulose is the most prevalent biological compound on earth. It is the principal component of all plants, wood, paper and cotton. When considered globally, cellulose constitutes an enormous supply of chemical energy, all of it renewable. Recently, several plants have been manipulated to make significantly less cellulose. This modification is important because it may now permit identification of the factors that control the synthesis and deposition of cellulose and related compounds. This development may permit the genetic engineering of plants to produce either more cellulose, or plants that produce larger amounts of other chemicals such as liquid fuels and plastics.
- New Process Forms Diamond-Like Boron Nitride Films. A process to grow diamond-like boron nitride films, the second hardest material known, has been discovered based on a new understanding of how hard nitride films are formed. Like diamond, films of boron nitride can be grown from hot gases and plasmas without the use of high pressures. However, it was recently discovered that irradiation of boron nitride films with low-energy ion beams will produce films of boron nitride that contain the hard, diamond-like form rather than the soft graphite-like form. This new process to form ultra-hard boron nitride films could revolutionize the tool industry, because, unlike diamond, boron nitride does not react with iron or steel; therefore, boron nitride is an ideal material for cutting tools.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

- "Green" Separation Process for Hanford Wastes. The radioactive components in the Hanford waste tanks comprise a mere 1/100th of a percent of the millions of gallons of contaminated waste in storage. Thus, highly selective removal of the radioactive components could significantly reduce the volume of waste which will require very costly processing and long-term storage. Fundamental studies of technetium extraction in the 1980s, followed by more recent investigations of the structural and thermodynamic aspects of the extraction of alkali metal salts with crown ethers has led to a new technetium extraction process. The crown ether binds sodium ions already present in the waste, and then extracts technetium as much as four orders of magnitude better than others ions in the waste, such as nitrate, which are present at much higher concentrations. The crown ether complex is readily decomposed by contact with water to release the extracted technetium thereby affording a convenient, safe, and economical stripping method. The crown ether is then recycled thus minimizing secondary waste production.
- New Metallocene Catalysts Lead to Commercial Applications. The new family of metallocene polymerization catalysts, in which polymerization occurs principally at a single type of metal center with a well-defined coordination environment, are a substantial advance over the prior heterogeneous polymerization catalysts. Recent advances on two fronts -- strained early transition metals and non-coordinating counterions -- have resulted in new commercial applications by Dow Chemical and by Exxon Chemical. The remarkable stereospecificity features of these new catalysts have not only led to a variety of new, advanced polymer products over a wide range of densities, but they also provide the ability to "turn a microscope on" the underlying molecular mechanisms, thus leading to continually improved catalysts and products. The new polymers produced from these catalysts are found in wide-ranging applications from food wrapping to the plastic front end front bumper combinations on automobiles. The impact of these new products can be imagined from the Dow Insite process which produces plastics with a market of about \$2,000,000,000 per year at Dow's Texas plant.
- A Microscopic Understanding of Materials Joining Enables the Intelligent Processing of Materials. Welding is a critical fabrication technology used extensively in a wide variety of industries such as energy, automotive, construction, aerospace, shipbuilding, and electronics. Weld failures are among the most common reason for unscheduled outages in power plants with the cost of replacement power often exceeding \$1,000,000 per day. Recent advances in materials joining science have improved our understanding of the welding process and welded materials. With the help of massively parallel computers, complex physical models that link both macro- and microscopic scale phenomena during the melting and solidification of a weld have been developed. Using such models it is now possible to visualize directly the solidified weld microstructure for a given set of processing conditions. The resulting knowledge has been transferred to industry thereby allowing the intelligent processing of defect-free, structurally sound and reliable welds.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

- Magnetic Refrigeration to Eliminate Harmful Freon. Conventional air conditioning of domestic and commercial buildings, and cooling in food processing and other industrial plants requires enormous quantities of electricity and uses huge amounts of environmentally harmful chlorofluorocarbons (CFCs). Magnetic refrigeration uses the magneto-caloric effect, the ability of a magnetic material to raise its temperature upon application of a magnetic field and to lower it upon removal of that field. For many years the alloys showing this effect operated only at impractically low temperatures. New understanding of thermal and magnetic behavior uncovered a gadolinium-silicon-germanium alloy that cools efficiently near room temperature. Refrigerator devices based on magneto-caloric material could cut energy costs and eliminate ozone-depleting CFCs.
- Bioproduction of Natural Gas. The few microorganisms that possess the ability to produce methane (natural gas) have been studied for a number of years in the hope of using these organisms to produce a renewable energy source. Last year the genome of a methane-producing bacterium was sequenced which showed the uniqueness of these organisms. It is now thought that these bacteria are among the first life forms ever developed on earth. Recently, procedures have been developed which will permit the genes of methane-producing bacteria to be manipulated. This development will allow scientists to determine the nature and properties of these organisms and their unusual metabolism.
- Materials Failure in a Radiation Environment. The safe storage of nuclear materials and radioactive wastes is a major challenge for the post cold-war generation. The long term effects of radiation on the physical integrity of these materials and their containers is still poorly understood. Recent work using simultaneous electron microscopy and ion irradiation experiments shows that the impact of just a single high energy ion on the surface of a material has a much greater effect than previously realized and disrupts tens of thousands of atoms near the surface of the material. The impact causes local melting, displacement of many atoms beneath the surface, and the formation of surface craters and holes. This work should lead to a correct understanding of how materials are damaged by radiation and will help explain and predict the behavior of materials used for waste storage and other applications.

Scientific Facilities Utilization

The BES program request includes \$317,012,000 to maintain support of the scientific user facilities. This funding includes increases for the synchrotron radiation light sources and for the neutron scattering facilities to adjust for increased cost-of-living expenses. In addition, in accord with the highest recommendations of the Basic Energy Sciences Advisory Committee Panel on Synchrotron Radiation Sources and Science (the Birgeneau Panel), additional funds are provided to the National Synchrotron Light Source for increased support for users and to the light source community for instrumentation and beamline construction at the light sources; the latter funds will be allocated via peer review. Research and development on the Spallation Neutron Source (SNS) is also increased and included in facility operations. Prior to

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

FY 1999, SNS research and development was funded in Materials Sciences Research. Finally, increased research activities are planned for the Combustion Research Facility, which will complete construction of Phase II in FY 1999. These increases were made possible because, in FY 1999, all funds associated with the SNS were added as an increment above the base program. Research communities that have benefitted 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 description of funding for specific facilities are given in the subprogram narratives and in the section entitled "Major User Facilities."

Spallation Neutron Source (SNS) Project

FY 1999 funding of \$157,000,000 is requested for the Spallation Neutron Source (SNS) Project to begin Title I design activities, initiate subcontracts and long-lead procurements, and continue critical research and development work necessary to reduce technical and schedule risks. 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 MW spallation source that could be upgraded to significantly higher powers in the future. 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 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 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) and the European Spallation Source project to allow joint research and development. Furthermore, a Working Group on Neutron Sources has been

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

established under the Megascience Forum of the Organization for Economic Cooperation and Development. A Steering Committee has been formed, consisting of distinguished members of the neutron science community, to provide input on instrumentation and on user needs. Finally, key management positions have been filled and the development of the project Cost Schedule Control System is proceeding as planned. Additional information on the SNS project is provided in the SNS construction project data sheet, project number 99-E-334.

Neutron Science Activities

Facility Enhancements

BES will continue to support the ongoing enhancements of existing reactor and spallation neutron sources and will proceed with the construction of the Spallation Neutron Source (SNS). (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 state-of-the-art, short-pulse spallation source facility for neutron scattering, radiography, and science-based stockpile stewardship. (2) The beryllium reflector at the High Flux Isotope Reactor at Oak Ridge National Laboratory is scheduled to be changed in FY 1999. This is a scheduled maintenance operation, that addresses the normal lifetime limitations of the beryllium reflector. The reflector will exceed its projected operating life in November 1999. At the time of the beryllium reflector replacement, certain improvements will be made to the beam tubes and monochromators. These improvements will significantly increase the thermal neutron flux to the instruments. This work was initiated in FY 1998 and will be completed in FY 2000.

FY 1999 Initiatives

- **The Partnerships for Academic-Industrial Research (PAIR) Program will be initiated at a funding level of \$1,500,000.** This program is designed to encourage and facilitate research partnerships between academic researchers, their students, and industrial researchers. Funding for the PAIR program will be derived from normal turnover of university and DOE laboratory programs. The BES program, through support of basic research that is collocated with applied research at the DOE laboratories, has had considerable opportunity to observe that both basic and applied researchers contribute to problem definition, discovery, and understanding and that the transition from discovery to development and deployment is not a linear process. The PAIR program seeks to encourage similar interactions between basic and applied researchers in academia and industry. The PAIR program will be initiated in FY 1999 as an experiment to strengthen the linkages between academic and industrial researchers during a time when industry is restructuring its own research programs to address focused corporate needs.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

Additionally, the PAIR program is intended to encourage universities to consider novel research activities and to encourage faculty participation in nontraditional partnerships, which may have been discouraged in the past. The PAIR program encompasses the entire range of research supported by the BES program. Grants will be awarded on the basis of competitive peer review to university researchers for support of 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 time in the industrial setting.

- **A program in Complex and Collective Phenomena will be initiated at a funding level of \$3,000,000.** 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 will support 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. Funding for the initiative will be derived from normal turnover of university and DOE laboratory programs. Awards will be 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. Specific examples of work that might be funded under this initiative are given in the sections describing the BES subprograms.

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 stoichiometry; 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. As examples, high-temperature superconductors are complex compounds of four or more elements that are not stoichiometric with respect to oxygen; the glassy metal state, which has many desirable properties, has no long range order or symmetry; and many interesting and useful properties exist in atomic and molecular arrangements that have only one or two dimensions, such as is found in thin films, membranes, and quantum dots. These classes of materials, which will dominate the next generation of energy technologies, pose new challenges and opportunities because of their complexity.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

- *Functional synthesis.* Although chemists routinely synthesize molecules to desired elemental composition and structure, 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.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

Climate Change Technology Initiative

Overview

The FY 1999 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 Energy Research 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 (US/GCRP) 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 US/GCRP activities. Although the two programs, CCTI and US/GCRP, are synergistic, they are different. US/GCRP 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 science that will enable mitigation of climate change while maintaining a robust National economy.

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 Energy Research 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. Energy Research 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 Energy Research, through activities in both the Basic Energy Sciences (BES) program and the Biological and Environmental Research (BER) program, supports research that underpins both efforts.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

A research program in carbon management would include:

- (1) science for efficient technologies,**
- (2) fundamental science underpinning advances in all low/no carbon energy sources, and**
- (3) sequestration science.**

Energy Research has long-standing programs in fundamental research that already impact the three categories. Additional resources of \$16,000,000 in the BES program, provided specifically for carbon management science in the Climate Change Technology Initiative, will be a natural extension of the complementary, ongoing work in several programs in Energy Research, 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 Energy Research programs and that promise maximum impact in the area of carbon management.

Immediate Impacts of Expanded Effort in Climate Change Technology

Additional Energy Research effort will not only address an immediate societal problem, but it 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. Cross-cutting programs in nano- and meso-phase materials involve research at the forefront of materials science, chemistry, engineering, surface science, and semiconductor physics.

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

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) 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 ER 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, ER 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 ER 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. ER also has a leadership role within the USGCRP on consequence evaluation of increased greenhouse gases in global climate change, including integrated

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

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 ER 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 methane production or consumption, and will thus underpin the related activities to be undertaken by both Energy Research and the National Science Foundation LexEN (Life in Extreme Environments) program.

BES Activities

Climate Change Technology Initiative FY 1999 Budget Request

B/A
(\$000)

Materials Sciences	\$ 3,500
Chemical Sciences	4,500
Engineering and Geosciences	3,000
Energy Biosciences	<u>5,000</u>
Total	\$16,000

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 will be 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 will focus 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 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

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

molecular specific separation from complex mixtures. In the Engineering and Geosciences subprogram, research will emphasize those areas of geophysics and geomechanics that will impact carbon dioxide sequestration in subsurface geologic formations. The 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, (2) understanding multiphase fluid flow within the aquifers, and (3) understanding the geochemical reactivity within the reservoirs/aquifers. Finally, in the Energy Biosciences subprogram, research will emphasize the biological process of photosynthesis, which is central to global carbon cycling.

Included among this work, which is interdisciplinary in its nature, will be research activities for new and improved catalysts for more efficient production of fuels and chemicals and for the conversion of biomass to fuels; lower cost and more efficient photovoltaic devices to convert sunlight to electricity; higher capacity batteries to store electrical energy more effectively; fuel cells to use alternative fuels; lightweight materials to improve mileage in automobiles; high-temperature materials to increase energy efficiency in energy production and manufacturing processes; biological production of fuels to recycle carbon and reduce the use of fossil fuels; and more efficient electric generation, transmission, and use through the use of superconductors and improved magnets. Specific areas of research are described in greater detail in the narratives for the individual subprograms. The new BES research program will be closely related to DOE's technology programs and will provide the knowledge base for the development of advanced technologies to reduce CO₂ emissions. When combined with the complimentary activities within 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 \$47,905,000 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

PROGRAM MISSION - BASIC ENERGY SCIENCES - (Cont'd)

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 partners with all appropriate DOE technology offices to make the results of the BES research widely known and used. Furthermore, BES research programs are influenced by the needs of the technology offices. As a result, there have been 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 Energy Research (ER) -- 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 preliminary identification of research needs and gaps. Similar to the early photovoltaic energy systems coordination activities, it is envisioned that joint-sponsored workshops with invited specific experts will then be held to further define priority research opportunities for both offices.

Funding of Contractor Security Clearances

In FY 1999, the Department will divide the responsibility for obtaining and maintaining security clearances. The Office of Security Affairs, which has been responsible for funding all Federal and contractor employee clearances, will pay only for clearances of Federal employees, both at headquarters and the field. Program organizations will be responsible for contractor clearances, using program funds. This change in policy will enable 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 Energy Research is budgeting \$346,000 for estimated contractor clearances in FY 1999 within this decision unit.

BASIC ENERGY SCIENCES
PROGRAM FUNDING PROFILE
(Dollars in thousands)

	FY 1997 Current <u>Appropriation</u>	FY 1998 Original <u>Appropriation</u>	FY 1998 Adjustments	FY 1998 Current <u>Appropriation</u>	FY 1999 Budget <u>Request</u>
<u>Research</u>					
Materials Sciences.....	#####	\$391,595	-\$549 a/	\$391,046	\$417,216
Chemical Sciences.....	194,537	200,933	-280 a/	200,653	209,582
Engineering and Geosciences.....	40,933	41,251	-57 a/	41,194	44,413
Energy Biosciences.....	27,283	27,461	-39 a/	27,422	32,489
Subtotal, Research.....	631,221	661,240	-925 a/	660,315	703,700
Construction.....	11,500	7,000	0	7,000	132,400
Subtotal, Basic Energy Sciences.....	642,721	668,240	-925 a/	667,315	836,100
Adjustment.....	-9,731 b/	-4,780 c/	0	-4,780 c/	0
Adjustment.....	0	-925 a/	925 a/	0	0
Total, Basic Energy Sciences.....	##### d/	<u>\$662,535</u>	<u>\$0</u>	<u>\$662,535</u>	<u>\$836,100</u>

a/ Share of Science general reduction for contractor training.

b/ Share of Energy Supply, Research and Development general reduction for use of prior year balances assigned (\$9,404,000), and FY 1997 emergency flood supplemental rescission (\$327,000). The total general reduction at the appropriation level.

c/ Share of Science general reduction for use of prior year balances assigned to this program. The total general reduction at the appropriation level.

d/ Excludes \$13,916,000 which has been transferred to the SBIR program and \$833,000 which has been transferred to the STTR program.

Public Law Authorizations:

Public Law 95-91, DOE Organization Act

BASIC ENERGY SCIENCES
(Dollars in thousands)

PROGRAM FUNDING BY SITE

<u>Field Offices/Sites</u>	<u>FY 1997 Current Appropriation</u>	<u>FY 1998 Original Appropriation</u>	<u>FY 1998 Adjustments</u>	<u>FY 1998 Current Appropriations</u>	<u>FY 1999 Budget Request</u>
Albuquerque Operations Office					
Los Alamos National Laboratory	\$20,654	\$23,482	\$0	\$23,482	\$24,489
National Renewable Energy Laboratory	4,160	4,440	0	4,440	4,402
Sandia National Laboratories	30,168	28,419	0	28,419	25,378
Chicago Operations Office					
Ames Laboratory	17,498	17,996	0	17,996	16,609
Argonne National Laboratory	137,340	139,239	0	139,239	145,387
Brookhaven National Laboratory	81,843	75,023	0	75,023	77,311
Idaho Operations Office					
Idaho National Environmental Engineering	3,217	3,708	0	3,708	3,752
Oakland Operations Office					
Lawrence Berkeley National Laboratory	62,470	60,732	0	60,732	61,081
Lawrence Livermore National Laboratory	6,570	5,601	0	5,601	5,602
Stanford Linear Accelerator Center	20,562	21,279	0	21,279	21,853
Oak Ridge Operations Office					
Oak Ridge Institute for Science and Educati	1,504	999	0	999	724
Oak Ridge National Laboratory	89,481	109,431	0	109,431	244,295

<u>Field Offices/Sites</u>	<u>FY 1997 Current Appropriation</u>	<u>FY 1998 Original Appropriation</u>	<u>FY 1998 Adjustments</u>	<u>FY 1998 Current Appropriations</u>	<u>FY 1999 Budget Request</u>
Richland Operations Office					
Pacific Northwest National Laboratory	12,640	12,718	0	12,718	12,708
All Other Sites a/	154,614	165,173	-925 b/	164,248	192,509
Subtotal	<u>642,721</u> c/	<u>668,240</u>	<u>-925</u> b/	<u>667,315</u>	<u>836,100</u>
Adjustment	-9,731 d/	-4,780 e/	0	-4,780 e/	0
Adjustment	<u>0</u>	<u>-925</u> b/	<u>925</u> b/	<u>0</u>	<u>0</u>
TOTAL	\$632,990	\$662,535	\$0	\$662,535	\$836,100

a/ Funding provided to universities, industry, other Federal agencies and other miscellaneous contractors.

b/ Share of Science general reduction for contractor training.

c/ Excludes \$13,916,000 which was transferred to the SBIR program and \$833,000 which was transferred to the STTR program.

d/ Share of Energy Supply Research and Development general reduction for use of prior year balances assigned to this program (\$9,404,000) and FY 1997 emergency flood supplemental rescission (\$327,000). The total general reduction is applied at the appropriation level.

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

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**
(Tabular dollars in thousands, narrative in whole dollars)

I. 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, 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 solar energy conversion, transportation, electric power production, and petroleum refining.

Climate Change Technology Initiative. Research routes to improved carbon management in support of the Climate Change Technology Initiative include: reducing fuel consumption (and consequently emissions) via higher temperature operation through the use of improved heat and corrosion resistant alloys; reducing energy losses in motors via improved magnetic materials; and displacing fossil fuels with higher-efficiency photovoltaic cells.

Research in Complex and Collective Phenomena. It is now apparent that materials with increased complexity in their composition, atomic structure, and arrangements have created opportunities for the development of new materials with much improved properties and behavior. Research under this initiative will focus on new classes of magnetic materials and their behavior in thin films and layered arrangements; new classes of alloys; and an increased understanding of mechanical behavior between the atomic scale and the macroscopic continuum model.

II. Funding Schedule:

<u>Program Activity</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
Materials Sciences Research	\$169,212	\$195,860	\$189,066	\$- 6,794	- 3.5%
Facilities Operations	191,950	185,915	218,246	+32,331	+17.4%
SBIR/STTR	0	9,271	9,904	+ 633	+ 6.8%
Congressional Direction	<u>7,306</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>-----</u>
Total, Materials Sciences	<u>\$368,468</u>	<u>\$391,046</u>	<u>\$417,216</u>	<u>\$+26,170</u>	<u>\$+ 6.7%</u>

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Materials Sciences Research</u>			
<p>-Basic research is conducted on synthesis and processing; theory and modeling; atomic scale structural characterization; and mechanical and physical behavior. The purpose of this research is to understand the relationship among the synthesis, processing, microscopic structure and the mechanical and physical behavior of materials. This research includes topics in lattice defects; diffusion and transport; phase transformations; magnetic, superconducting, semiconducting and alloy ordering behaviors; radiation damage; corrosion; deformation and fracture; and microstructural and microchemical characterizations by means of electron beams, neutron beams, and x-rays. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$650,000. Capital equipment is required for items such as high-temperature components for electron microscopes, atomic probes, crystals, x-ray detectors, spectrometers, tomographic instruments, and computer controls. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.</p>		\$68,168	\$72,264\$75,390
<p>-Basic research on the physical properties of materials, largely in the area of condensed matter physics, is conducted to determine the positions and movements of atoms in solids and liquids and the effects of these on the electronic states. This activity encompasses experiments in neutron and x-ray scattering; experiments to determine transport properties of solids, such as electrical and thermal conductivity, superconductivity, magnetism, and</p>	64,682	65,260	68,430

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
experiments on the effects of light and other radiation on materials. There are also theoretical investigations and computer simulations to gain understanding of the experiments and to model the behavior of materials. Within this category of research, new work in a complex and collective phenomena is expected to be funded at approximately \$650,000. Capital equipment is required for items such as high field magnets, neutron and x-ray beam lines and instrumentation, detectors, energy filters, and magneto-optical instrumentation. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.			
-Research on the chemical properties of materials is conducted to understand the effects of chemical reactivity on the behavior of materials and to synthesize new chemical compounds and structures from which better materials can be made. This activity includes research in solid state chemistry, surface chemistry, polymer chemistry, crystallography, synthetic chemistry, and colloid chemistry. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$200,000. Capital equipment is required for items such as spectrometers, reflectometers, computer workstations for simulations and modeling, and instrumentation to study surfaces at the atomic scale. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.	21,616	24,021	25,131

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:

FY 1997

FY 1998

FY 1999

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

EPSCoR DISTRIBUTION OF FUNDS BY STATE

(Dollars in thousands)

	FY 1997 <u>Actual</u>	FY 1998 <u>Estimate</u>	FY 1999 <u>Estimate</u>
Alabama	\$ 750	\$ 725	\$ 725
Kentucky	750	725	725
Louisiana	659	725	**
Maine	600	725	**
Montana	750	725	**
Nevada	750	725	725
Puerto Rico	750	725	725
South Carolina	550	725	725
Wyoming	730	725	725
Other*	<u>514</u>	<u>290</u>	<u>2,465</u>
Totals	\$6,803	\$6,815	\$6,815

* Includes technical support of Experimental Program to Stimulate Competitive Research (EPSCoR).

** The funding commitments for awards to Louisiana, Maine, and Montana expire in FY 1998. The uncommitted funds in FY 1999 will be competed among all EPSCoR states that do not have an active award to begin new "initiation" awards. (Eligible states are Arkansas, Idaho, Kansas, Louisiana, Maine, Mississippi, Montana, Nebraska, North Dakota, Oklahoma, South Dakota, Vermont, and West Virginia.) In addition to the normal initiation awards, which support cluster activities statewide, some funds may be used to support individual grants to scientists from EPSCOR states.

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>-The Experimental Program to Stimulate Competitive Research (EPSCoR) provides financial assistance to states that historically have received relatively less Federal research funding. The EPSCoR program was included in the BES program at the direction of Congress in FY 1996.</p>	6,803	6,815	6,815
<p>-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.</p>	0	4,500	4,500
<p>-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.</p>	0	0	3,500
<p>-Replacement of High Flux Isotope Reactor Monochromator Drums.</p>	0	0	1,800
<p>-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. In FY 1999, SNS research funding in support of construction is reflected in the facility operations section of this budget.</p>	7,943	23,000	0

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>-Basic research in carbon management for the Climate Change Technology Initiative will focus on three areas: high temperature materials, magnetic materials, and semiconductor materials. (1) 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 surface physics and chemistry of oxide layers, which is expected to produce alloys and coatings that have improved corrosion resistance at high temperatures. (2) 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. (3) 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 focus would be to improve 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</p>	0	0	3,500

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
sunlight, which, when coupled to electron transport structures, would provide new ways to convert sunlight to electricity.			
Subtotal Materials Sciences Research	169,212	195,860	189,066
<u>Facilities Operations</u>			
-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 described 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. 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	191,950	185,915	218,246

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
provided below. Additional funds for facility operations for some of these facilities are included in the Chemical Sciences subprogram of this budget.			
Subtotal Facilities Operations	191,950	185,915	218,246
<u>Facilities</u>			
National Synchrotron Light Source	\$ 19,990	\$ 23,047	\$ 24,422
High Flux Beam Reactor	34,450	22,900	22,900
Intense Pulsed Neutron Source	10,692	11,230	11,920
Stanford Synchrotron Radiation Laboratory	3,650	4,002	4,002
Manuel Lujan, Jr. Neutron Scattering Center	7,343	6,588	7,502
Advanced Light Source	32,877	30,708	31,600
Advanced Photon Source	81,441	82,368	87,300
Spallation Neutron Source	0	0	28,600
High Flux Isotope Reactor	0	3,972	0
Partial Offset to ESRD General			
Reduction Applied to BES	1,507	1,100	0
Total	<u>\$191,950</u>	<u>\$185,915</u>	<u>\$218,246</u>
<u>SBIR/STTR Funding</u>	0	9,271	9,904
In FY 1997 \$7,956,000 and \$475,000 were transferred to the SBIR and STTR programs, respectively. The FY 1998 and FY 1999 amounts are the estimated requirement for the continuation of these programs.			
Subtotal SBIR/STTR Funding	0	9,271	9,904

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Congressional Direction</u>	7,306	0	0
<p>Funds Rose Hulman Institute of Technology; Alabama Mineral Research Center, Tuscaloosa; and University of Alabama, Birmingham in FY 1997 (per Congressional direction). No additional funds were provided for these projects by the Congress in FY 1997.</p>			
Total Materials Sciences	<u>\$368,468</u>	<u>\$391,046</u>	<u>\$417,216</u>

EXPLANATION OF FUNDING CHANGES FROM FY 1998 TO FY 1999:

Increase research and development funds and provide capital equipment for the SNS in support of the FY 1999 construction start.	\$+ 5,600,000
Initiate a program of fundamental research in carbon emissions management for the Climate Change Technology Initiative.	+ 3,500,000
Initiate a program of fundamental research in complex and collective phenomena.	+ 1,500,000
Initiate the Partnerships for Academic Industrial Research (PAIR) program.	+ 750,000
Provide increased support for the major scientific user facilities.	+ 7,703,000
Provide AIP funds for extension of HB-2 beam tube at HFIR for thermal neutron scattering.	+ 3,500,000
Reduce AIP funds following completion of beam tube upgrades at HFIR.	- 3,972,000

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

Provide capital equipment funds for new monochromator drums at HFIR for thermal neutron scattering.	+ 1,800,000
Increase in research for characterization of materials.	+ 1,956,000
Increase SBIR/STTR funding due to increase in operating expenses.	+ 633,000
Increase for peer reviewed research at the synchrotron radiation light sources.	+ 3,000,000
Beginning in FY 1999, this program will budget \$200,000 for the estimated costs of obtaining and maintaining security clearances for contractor employees under the Chicago Operations Office and the Oak Ridge National Laboratory.	+ 200,000
Total Funding Change, Materials Sciences	<u>\$+26,170,000</u>

MAJOR ISSUES:

- Neutron science is a critical tool in materials sciences and related disciplines that are crucial to the U.S. knowledge base for advanced technologies, particularly those related to energy technologies. The U.S. currently lags far behind both Europe and Japan in neutron science. Planned new neutron sources in Europe and Japan could increase their lead even further in materials science and related research using neutrons. To maintain a strong U.S. position in the field of neutron science, funds to begin construction of the SNS are required in FY 1999. In addition, funds to continue neutron source enhancements such as the Los Alamos Neutron Science Center (LANSCE) instrumentation enhancement and enhanced thermal neutron flux capacity at the High Flux Isotope Reactor are included in this request.
- 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

**BASIC ENERGY SCIENCES
MATERIALS SCIENCES**

reactor and associated equipment in safe operating condition. The HFBR will continue to be maintained in this state while the Department evaluates options for its future. The Basic Energy Sciences Advisory Committee has recommended that the HFBR be restarted. This recommendation, along with input from the new contractor at Brookhaven National Laboratory, input from the local community on Long Island, and the Environmental Impact Statement will be used by the Secretary of Energy in determining the future of the HFBR.

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

(Tabular dollars in thousand, narrative in whole dollars)

I. 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 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 C₆₀ (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 disciplinary areas address fundamental interactions of atoms, molecules and ions with photons and electrons that define the underlying chemical science needed to address carbon management. These areas enable more efficient combustion and new understanding of the photochemical conversion of CO₂ and the direct conversion of solar radiation to electricity. The other major component of the research program is comprised of inorganic chemistry, physical chemistry, organic chemistry, analytical chemistry, separations science, heavy element chemistry and aspects of chemical engineering sciences. The separations science, physical chemistry and inorganic chemistry disciplinary areas provide a better molecular level understanding of homogeneous and heterogeneous reactions occurring at surfaces, interfaces and in bulk media. These disciplinary areas provide 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.

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

Research on Complex and Collective Phenomena. Chemical Sciences research under complex and collective phenomena would fall in the areas of AMO physics with a focus on phenomena beyond the independent particle approximation; improved predictive capability in catalysis; combustion models; and separations systems and processes through advances in understanding scaling in space and time as well as functional synthesis; and improved photochemical processes for solar energy conversion and "green synthesis" through the control of entropy and functional synthesis. The greatest potential technological impact would be in energy efficiency and renewable energy, but impacts would also be realized in environmental management and fossil energy.

II. Funding Schedule:

<u>Program Activity</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
Chemical Sciences Research	\$124,908	\$128,852	\$137,515	\$+8,663	+6.7%
Facilities Operations	64,221	67,335	67,319	- 16	----
SBIR/STTR	0	4,466	4,748	+ 282	+6.3%
Congressional Direction	<u>5,408</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>----</u>
Total, Chemical Sciences	<u>\$194,537</u>	<u>\$200,653</u>	<u>\$209,582</u>	<u>\$+8,929</u>	<u>+4.4%</u>

III. Performance Summary- Accomplishments:

Chemical Sciences Research

-The program supports experimental and theoretical research devoted to study of atoms, molecules, ions and light and their interactions- areas that may have broad fundamental impact on much of chemistry. Molecular processes related to combustion of fossil fuels and catalysis as well as the conversion of solar energy to other useful energy forms are also studied. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$475,000. Capital equipment is required for such items as mass spectrometers, electronic waveform digitizers, oscilloscopes, detection equipment, optical spectrometers, and vacuum equipment. AIP

	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
	\$67,171	\$68,797	\$70,610

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

III. Performance Summary

FY 1997

FY 1998

FY 1999

funding is also required for additions and modifications to accelerator and reactor facilities supported by the Chemical Sciences subprogram. The total estimated cost of each AIP project will not exceed \$5,000,000. The Chemical Sciences subprogram also provides General Purpose Equipment (GPE) and General Plant Projects (GPP) funds, for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems at the Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of Basic Energy Sciences landlord responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed \$5,000,000. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.

-The program supports a broad, well-integrated continuum of effort that uses atomic and molecular level information to understand homogeneous and heterogeneous catalysis as well as separations and analysis methodologies including studies of the actinide elements. Certain engineering areas are also supported such as turbulence related to combustion and thermodynamics. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$425,000. Capital equipment is required for such items as high resolution area detectors, catalytic reactors, analytical instrumentation, lasers, and optical spectrometers. The Chemical Sciences subprogram also

57,737

60,055

62,405

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

III. Performance Summary

FY 1997

FY 1998

FY 1999

provides General Purpose Equipment (GPE) and General Plant Projects (GPP) funds, for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems at the Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of Basic Energy Sciences landlord responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed \$5,000,000. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.

Basic research in carbon management for the Climate Change Technology Initiative 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 CO₂ from complex mixtures or new concepts for economical oxygen

0

0

4,500

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

III. Performance Summary

FY 1997 FY 1998 FY 1999

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 the catalytic process to enable new catalysts for carbon dioxide insertion into chemicals; understanding the complex relationship between chemical reaction dynamics and turbulence that are critical to improving the efficiency of fossil fuel combustion processes.

Subtotal Chemical Sciences Research

124,908 128,852 137,515

Facilities Operations

-Operation of national user facilities. 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. 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,

64,221 67,335 67,319

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

III. Performance Summary

FY 1997

FY 1998

FY 1999

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.

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. Included in FY 1999 is the second major increment to the HFIR operating budget of \$2,360,000. This increment is 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 will begin in FY 1998 and will be completed in FY 2000, is a recurring activity that must be performed every 10-12 years. The present reflector will reach its end of life in November 1999.

Subtotal Facilities Operations

64,221

67,335

67,319

**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

III. Performance Summary	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Facilities</u>			
National Synchrotron Light Source	\$ 7,429	\$ 7,949	\$ 8,190
High Flux Isotope Reactor	27,383	29,798	29,061
Radiochemical Engineering Development Center	6,705	6,705	7,127
Stanford Synchrotron Radiation Laboratory .	16,912	17,277	17,851
Combustion Research Facility	5,256	5,161	5,090
Partial Offset to ESRD General Reduction Applied to BES	<u>536</u>	<u>445</u>	<u>0</u>
Total	<u>\$64,221</u>	<u>\$67,335</u>	<u>\$67,319</u>
 <u>SBIR/STTR Funding</u>	 0	 4,466	 4,748
 In FY 1997 \$4,248,000 and \$255,000 were transferred to the SBIR and STTR programs, respectively. The FY 1998 and FY 1999 amounts are the estimated requirement for the continuation of these programs.			
Subtotal SBIR/STTR Funding	<u>0</u>	<u>4,466</u>	<u>4,748</u>
 <u>Congressional Direction</u>	 5,408	 0	 0
 Funds Rose-Hulman Institute of Technology; Alabama Mineral Research Center, Tuscaloosa; and University of Alabama, Birmingham in FY 1997 (per Congressional direction). No additional funds were provided for these projects by the Congress in FY 1997.			
Subtotal Congressional Direction	<u>5,408</u>	<u>0</u>	<u>0</u>

Total Chemical Sciences	<u>\$194,537</u>	<u>\$200,653</u>	<u>\$209,582</u>
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**BASIC ENERGY SCIENCES
CHEMICAL SCIENCES**

EXPLANATION OF FUNDING CHANGES FROM FY 1998 to FY 1999:

Initiate a program of fundamental research in carbon emissions management for the Climate Change Technology Initiative. \$+4,500,000			
Initiate a program of fundamental research in complex and collective phenomena.		+ 900,000	
Initiate the Partnerships for Academic Industrial Research (PAIR) program.		+ 450,000	
Provide increased support for the major scientific user facilities.		+ 1,223,000	
Reduce operating funds to support the beryllium replacement at HFIR.		- 1,239,000	
Provide funds for increased research at the CRF.		+ 1,000,000	
Increase in research for atomic level understanding of catalysis and chemical processes.		+1,687,000	
Increase SBIR/STTR funding due to increase in operating expenses.		+ 282,000	
Beginning in FY 1999, this program will budget \$126,000 for the estimated costs of obtaining and maintaining security clearances for contractor employees under the Chicago Operations Office and the Oak Ridge National Laboratory.		+126,000	
 Total Funding Change, Chemical Sciences			<hr/> \$+8,929,000

**BASIC ENERGY SCIENCES
ENGINEERING AND GEOSCIENCES**
(Tabular dollars in thousands, narrative in whole dollars)

I. 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 carbon dioxide injection technologies, reservoir storage capacities, and long-term storage stability. Research concerning the physics of multiphase flow in fractured rock systems will provide the basis not only for advancing the predictability of terrestrial carbon dioxide sequestration, but also for providing the basis for improved efficiency of fossil energy and geothermal energy production.

Research on Complex and Collective Phenomena. This research will address: (1) the coupling between geochemical, hydrodynamic, mechanical, and thermal processes in shallow crustal conditions, (2) the effects of heterogeneity and scale on geological structures, transport processes, and properties, and (3) non-linear controls in processing.

II. Funding Schedule

<u>Program Activity</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
Engineering Research	\$16,691	\$16,853	\$17,754	\$+ 901	+5.3%
Geosciences Research	21,510	23,301	25,534	+2,233	+9.6%
SBIR/STTR	0	1,040	1,125	+ 85	+8.2%
Congressional Direction	<u>2,732</u>	<u>0</u>	<u>0</u>	<u>0</u>	<u>----</u>
Total, Engineering and Geosciences	<u>\$40,933</u>	<u>\$41,194</u>	<u>\$44,413</u>	<u>\$+3,219</u>	<u>+7.8%</u>

**BASIC ENERGY SCIENCES
ENGINEERING AND GEOSCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Engineering Research</u>			
<p>-The Engineering Research program supports basic research in selected areas to provide the fundamental scientific base necessary for current engineering practice and to broaden the technical and conceptual base for solving future engineering problems in the energy technologies. Research efforts include single and multiphase flow in reservoirs and pipes, progress in understanding how fracture and fatigue arise in stressed energy structures for early detection and prevention of structure failure, chemical process control to improve production efficiency, instrumentation for environmental sensors, improved understanding of chaotic systems bearing on industrial scale mixing methods, principles underlying environmentally benign manufacturing methods, and continuing support for graduate training fellowships in environmentally sustainable manufacturing. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$125,000. Capital equipment is required for items such as instrumentation and diagnostics for experiments on the control of plasma processing of materials and fracture and fatigue in stressed structures. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.</p>	\$16,691	\$16,853	\$17,754
Subtotal Engineering Research	<u>16,691</u>	<u>16,853</u>	<u>17,754</u>

BASIC ENERGY SCIENCES

ENGINEERING AND GEOSCIENCES

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Geosciences Research</u>			
<p>The Geosciences Research program supports basic research to improve the level of understanding necessary for advances in, and choices among, current and emerging energy and environmental technologies. 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; advances in geophysical imaging and interpretation to provide new windows on subsurface structure and properties in the context of energy and environmental technologies; 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. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$175,000. Capital equipment is required for laboratory and in-situ studies of geologic systems, including facilities for microanalysis (e.g., synchrotron based methods) and facilities for characterizing the thermo-mechanical and transport behavior of rocks. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.</p>	21,510	23,301	22,534
<p>Basic research in carbon management for the Climate Change Technology Initiative will emphasize those areas of geophysics and geomechanics that will impact carbon dioxide sequestration in subsurface geologic</p>	0	0	3,000

**BASIC ENERGY SCIENCES
ENGINEERING AND GEOSCIENCES**

III. Performance Summary- Accomplishments:

FY 1997

FY 1998

FY 1999

formations. A basic 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, (2) understanding multiphase fluid flow within the aquifers, and (3) understanding the geochemical reactivity 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, and fluid-fluid transport at ambient and injection conditions, fluid-fluid-mineral interactions including wetting behavior, and surface tension effects. Better understanding of the geochemical reactivity of reservoirs/aquifers under conditions of flowing and stagnant CO₂ rich multiphase fluids and in the presence of multi-component mineral systems will be needed to fully evaluate the reservoirs and adequately model these systems for sequestration potential and safety. Specifically, research will address: (1) geometric, structural, and hydrological reservoir descriptions including rock properties, fluid content, and fluid distribution, (2) changes in reservoir characteristics with drilling and reservoir production including fluid injection, and (3) the physics of multiphase flow in fractured rock systems.

Subtotal Geosciences Research

21,510

23,301

25,534

**BASIC ENERGY SCIENCES
ENGINEERING AND GEOSCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>SBIR/STTR Funding</u>	0	1,040	1,125
<p>In FY 1997 \$1,017,000 and \$61,000 were transferred to the SBIR and STTR programs, respectively. The FY 1998 and FY 1999 amounts are the estimated requirement for the continuation of these programs.</p>			
Subtotal SBIR/STTR Funding	<u>0</u>	<u>1,040</u>	<u>1,125</u>
<u>Congressional Direction</u>			
Funds Rose-Hulman Institute of Technology; Alabama Mineral Research Center, Tuscaloosa; and University of Alabama, Birmingham in FY 1997 (per Congressional direction). No additional funds were provided for these projects by the Congress in FY 1997.	2,732	0	0
Subtotal Congressional Direction	<u>2,732</u>	<u>0</u>	<u>0</u>
Total Engineering and Geosciences	<u><u>\$40,933</u></u>	<u><u>\$41,194</u></u>	<u><u>\$44,413</u></u>

**BASIC ENERGY SCIENCES
ENGINEERING AND GEOSCIENCES**

EXPLANATION OF FUNDING CHANGES FROM FY 1998 to FY 1999:

Initiate a program of fundamental research in carbon emissions management for the Climate Change Technology Initiative. \$+3,000,000

Initiate a program of fundamental research in complex and collective phenomena.
+ 300,000

Initiate the Partnerships for Academic Industrial Research (PAIR) program. + 150,000

Redirection of base program research funds to support initiatives.
- 336,000

Increase SBIR/STTR funding due to increase in operating expenses. + 85,000

Beginning in FY 1999, this program will budget \$20,000 for the estimated costs of obtaining and maintaining security clearances for contractor employees under the Chicago Operations Office and the Oak Ridge National Laboratory. + 20,000

Total Funding Change, Engineering and Geosciences \$ +3,219,000

**BASIC ENERGY SCIENCES
ENERGY BIOSCIENCES**

(Tabular dollars in thousands, narrative in whole dollars)

I. Mission Supporting Goals and Objectives: The Energy Biosciences subprogram supports research to provide a basic understanding of the biological phenomena associated with the capture, transformation, storage and utilization of energy. The research on plants and non-medical microorganisms focuses on a range of biological processes including photosynthesis, bioenergetics, primary and secondary metabolism, the synthesis and degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of growth and development, thermophily, e.g., bacterial growth under high temperature, and other phenomena with the potential to impact biological energy production and conversion. The research supported is fundamental and is selected to broadly support Department of Energy's goals and objectives in energy production, environmental management, and energy conservation.

Climate Change Technology Initiative. The scientific disciplines actively involved in this research are plant science and fermentative microbiology. 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 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 recycling the carbon or providing fixed carbon for longer term sequestration.

Research in Complex and Collective Phenomena. The interactions between biological macromolecules is responsible for self-assembly and other properties both structural and functional. Studies will be supported to examine both the fundamental nature of these interactions and the resulting effects of the intercommunication.

II. Funding Schedule:

<u>Program Activity</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
Energy Biosciences	\$26,437	\$26,711	\$31,644	\$+4,933	+18.5%
SBIR/STTR	0	711	845	+ 134	+18.8%
Congressional Direction	846	0	0	0	----
Total, Energy Biosciences	<u>\$27,283</u>	<u>\$27,422</u>	<u>\$32,489</u>	<u>\$+5,067</u>	<u>+18.5%</u>

**BASIC ENERGY SCIENCES
ENERGY BIOSCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>-The Energy Biosciences subprogram supports a broad research portfolio of molecular and mechanistic research in the microbial and plant sciences. Efforts to increase the understanding of the molecular interactions between microbial systems and geologic components critical in environmental restoration and the biological modification of inorganic materials are continuing. Research efforts to determine the mechanisms of plant tissue development are being enhanced to more fully understand the formation of the tissues involved in energy storage. A recent advance in this area was the identification of three genes that when mutated led to significant reductions in the cellulase deposited in the cell walls of the model plant, <i>Arabidopsis thaliana</i>. Research efforts on the biochemistry and physiology of microbes with the potential for energy use are continuing with special emphasis on the field of microbial physiology, a subdiscipline that is critical to scaling up and deploying new biotechnologies in an industrial setting (e.g., fermentation, pharmaceutical and chemical industries). The recent development of experimental procedures to modify the genes of methane-producing bacteria should greatly facilitate determining the biological roles of genes in these unusual organisms. Within this category of research, new work in complex and collective phenomena is expected to be funded at approximately \$300,000. Small capital equipment items are needed to maintain the basic experimental infrastructure required for the advancement of this program's objectives. Education activities for improving science education for students and faculty in America's schools, colleges and universities are also funded in this program.</p>	\$26,437	\$26,711	\$26,644

**BASIC ENERGY SCIENCES
ENERGY BIOSCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>Basic research in carbon management for the Climate Change Technology Initiative will emphasize the biological process of photosynthesis, which is central to global carbon cycling. The current primary focus of the 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. This process is tightly controlled with indications that several levels of regulation exist. Technologies recently developed in the medical community using microarrays of genes may be used to discern the genes responsible for these levels of regulation. An understanding of the complex metabolic and regulatory networks along with other molecular mechanistic studies in metabolism and molecular genetics may lead to new strategies for (1) the replacement of fossil fuels with biologically fixed carbon, including fuels and chemical feedstocks and (2) altering the steady-state levels of carbon fixed in the biosphere. Finally, the fixation mechanisms active in nonphotosynthetic organisms offer the potential to use biobased systems in the context of carbon management through an interconversion of simple carbon containing compounds.</p>	0	0	5,000
<p><u>SBIR/STTR Funding</u> In FY 1997 \$695,000 and \$42,000 were transferred to the SBIR and STTR programs, respectively. The FY 1998 and FY 1999 amounts are the estimated requirement for the continuation of these programs.</p>	0	711	845
<p style="padding-left: 40px;">Subtotal SBIR/STTR Funding</p>	0	711	845

**BASIC ENERGY SCIENCES
ENERGY BIOSCIENCES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Congressional Direction</u>	846	0	0
Funds Rose-Hulman Institute of Technology; Alabama Mineral Research Center, Tuscaloosa; and University of Alabama, Birmingham in FY 1997 (per Congressional direction). No additional funds were provided for these projects by the Congress in FY 1997.	_____	_____	_____
Subtotal Congressional Direction	846	0	0
Total Energy Biosciences	<u>\$27,283</u>	<u>\$27,422</u>	<u>\$32,489</u>

EXPLANATION OF FUNDING CHANGES FROM FY 1998 to FY 1999:

Initiate a program of fundamental research in carbon emissions management for the Climate Change Technology Initiative.	\$+5,000,000
Initiate a program of fundamental research in complex and collective phenomena.	+ 300,000
Initiate the Partnerships for Academic Industrial Research (PAIR) program.	+ 150,000
Redirection of base program research funds to support initiatives.	- 517,000
Increase SBIR/STTR funding due to increase in operating expenses.	+ 134,000
Total Funding Change, Energy Biosciences	<u>\$+5,067,000</u>

**BASIC ENERGY SCIENCES
CONSTRUCTION**

(Tabular dollars in thousands, narrative in whole dollars)

I. 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.

II. Funding Schedule:

<u>Program Activity</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
Construction	\$ 11,500	\$ 7,000	\$132,400	\$+125,400	+1,791.4%
Total, Construction	<u>\$ 11,500</u>	<u>\$ 7,000</u>	<u>\$132,400</u>	<u>\$+125,400</u>	<u>+1,791.4%</u>

III. Performance Summary- Accomplishments:

	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
-Funding for the Combustion Research Facility, Phase II is completed in FY 1999 as scheduled.	\$ 9,000	\$7,000	\$ 4,000
-Funding for Accelerator and Reactor Improvements and Modifications in excess of \$2,000,000 was provided for construction of a liquid hydrogen cold source at the High Flux Isotope Reactor.		2,500	0
-Funding to begin construction of the Spallation Neutron Source Title I design activities and long-lead procurements will begin in FY 1999.		0	128,400
Total Construction	<u>\$11,500</u>	<u>\$ 7,000</u>	<u>\$132,400</u>

**BASIC ENERGY SCIENCES
CONSTRUCTION**

EXPLANATION OF FUNDING CHANGES FROM FY 1998 to FY 1999:

The decrease in funding for the construction of the Combustion Research Facility, Phase II project is a scheduled ramp down of effort. \$- 3,000,000

The increase in funding for the Spallation Neutron Source represents the initiation of construction of this facility. +128,400,000

Total Funding Change, Construction \$+125,400,000

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**
(Tabular dollars in thousands, narrative in whole dollars)

- I. 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.

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.

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

II. Funding Schedule:

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

<u>Facilities</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$Change</u>	<u>%Change</u>
National Synchrotron Light Source	\$27,419	\$30,996	\$32,612	\$+1,616	+ 5.2%
High Flux Beam Reactor	34,450	22,900	22,900	0	----
Intense Pulsed Neutron Source	10,692	11,230	11,920	+690	+ 6.1%
High Flux Isotope Reactor	27,383	33,770	29,061	-4,709	-13.9%
Radiochemical Engineering Development Center ..	6,705	6,705	7,127	+422	+ 6.3%
Stanford Synchrotron Radiation Laboratory	20,562	21,279	21,853	+574	+ 2.7%
Manuel Lujan, Jr. Neutron Scattering Center	7,343	6,588	7,502	+914	+13.9%
Combustion Research Facility	5,256	5,161	5,090	-71	- 1.4%
Advanced Light Source	32,877	30,708	31,600	+892	+ 2.9%
Advanced Photon Source	81,441	82,368	87,300	+4,932	+ 6.0%
Spallation Neutron Source	0	0	28,600	+28,600	----
Partial Offset to ESRD General Reduction Applied to BES	<u>2,043</u>	<u>1,545</u>	<u>0</u>	<u>-1,545</u>	<u>0.0%</u>
TOTAL	<u>\$256,171</u>	<u>\$253,250</u>	<u>\$285,565</u>	<u>\$+32,315</u>	<u>+12.8%</u>

III. Performance Summary- Accomplishments:

-National Synchrotron Light Source at Brookhaven National Laboratory: This synchrotron provides 79 experimental stations for research using infrared, visible, ultraviolet, and x-ray radiation. The FY 1999 request includes an increase for support of users in accord with the recommendations presented in the Birgeneau Report.

	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
	\$27,419	\$30,996	\$32,612

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>-High Flux Beam Reactor at Brookhaven National Laboratory: This high-flux reactor operates at 30 megawatts to provide neutrons for 9 beam tubes and 16 instruments. 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 spend 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 HFBR will continue to be maintained in this state while the Department evaluates options for its future.</p> <p>The funding requested in FY 1999 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. The level of funding for both FY 1998 and FY 1999 was set by using a formal review of cost, schedule, and technical scope of the required modifications.</p>	34,450	22,900	22,900
<p>- Intense Pulsed Neutron Source at Argonne National Laboratory: This pulsed spallation neutron source operates at 6.7 kilowatts with 12 instruments.</p>	10,692	11,230	11,920
<p>-High Flux Isotope Reactor at Oak Ridge National Laboratory: The HFIR operates at 85 megawatts. A major use of the HFIR is</p>	27,383	33,770	29,061

for

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
neutron-scattering experiments in fundamental studies of materials of interest to solid-state physicists, chemists, biologists, polymer scientists, metallurgists, and colloid scientists. Another purpose of the HFIR is the production of isotopes for research, industrial, and medical applications. Beyond these contributions, the HFIR also provides for a variety of irradiation tests and experiments that benefit from the exceptionally high neutron flux available. There will be a continuation of increased operating support in FY 1999 to take advantage of the new cold source with 3 new experimental stations and to support the scheduled replacement of the beryllium reflector. Also, as noted in the Material Sciences subprogram narrative, major item of equipment funds are provided for extension of HB-2 in order to provide beam access for six thermal neutron scattering instruments.			
-Radiochemical Engineering Development Center at Oak Ridge National Laboratory: This facility is used to process the isotopes produced in the High Flux Isotope Reactor.	6,705	6,705	7,127
-Stanford Synchrotron Radiation Laboratory at Stanford University: This synchrotron provides 22 experimental stations for x-ray scattering research with an additional 4 stations under construction.	20,562	21,279	21,853

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

III. Performance Summary- Accomplishments:	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<p>-Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory: This pulsed spallation neutron source operates at 60 kilowatts with 7 instruments for neutron scattering and is part of the Los Alamos Neutron Science Center, a facility supported jointly by the Office of Basic Energy Sciences and the Office of Defense Programs. Additional neutron scattering instruments will be added to accommodate more users with new capabilities.</p>	7,343	6,588	7,502
<p>-Combustion Research Facility at Sandia National Laboratories/California: This facility provides lasers for research in chemical dynamics and spectroscopy.</p>	5,256	5,161	5,090
<p>-Advanced Light Source at Lawrence Berkeley National Laboratory: This new, third-generation synchrotron light source provides high-brilliance visible and ultra-violet light and low energy x-rays to 22 experimental stations including 4 that are under construction. Following the receipt of the BESAC Panel Report "Synchrotron Radiation Sources and Science" (the "Birgeneau Report") in November, 1997, BES adjusted the FY 1998 funding for its four synchrotron radiation light sources to address the highest priority recommendations of the Birgeneau Panel. In order to provide funding for at least part of the recommended increases at the National Synchrotron Light Source, the Stanford Synchrotron Radiation Laboratory, and the Advanced Photon Source, it was necessary to reduce FY 1998 support at the Advanced Light Source by \$2,500,000. It is important to note, however, that it is not the intention of BES to close the Advanced Light Source or to permanently reduce its operations. Indeed, the</p>	32,877	30,708	31,600

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

III. Performance Summary- Accomplishments:

FY 1997

FY 1998

FY 1999

most important recommendation of the Birgeneau Panel was that the shutdown of any one of the four BES synchrotron light sources over the next decade would do significant harm to the Nation's science research capabilities and would considerably weaken our international competitive position in this field.

Furthermore, the most important conclusion of the Birgeneau Panel was that over the past 20 years in the United States synchrotron radiation research has evolved from an esoteric endeavor practiced by a small number of scientists primarily from the fields of solid state physics and surface science to a mainstream activity that provides essential information in the materials and chemical sciences, the life sciences, molecular environmental science, the geosciences, nascent technology and defense-related work. The user community at U.S. synchrotron facilities continues to grow exponentially, having reached more than 4,000 on-site users annually in FY 1997. The Birgeneau Report noted that the research carried out at the four BES synchrotron sources is both very broad and often exceptionally deep. Therefore, a high priority of the BES program is to strengthen the scientific program at the Advanced Light Source in order that the facility may evolve into a world-class VUV/soft X-ray light source. To do so, BES is supporting an international workshop in March, 1998, at the Advanced Light Source to determine scientific directions for the facility and a roadmap for achieving the vision. Funding for the Advanced Light Source in FY 1999 represents a modest cost of living increase over the *reduced*

**BASIC ENERGY SCIENCES
MAJOR USER FACILITIES**

III. Performance Summary- Accomplishments:

FY 1998 level; however, it is anticipated that this funding could increase based on successful proposals both from the user community and from the facility itself following the workshop in March, 1998.

-Advanced Photon Source at Argonne National Laboratory:
This new, third-generation synchrotron light source provides high-energy x-rays to at least 20 experimental stations with more under construction.

-Spallation Neutron Source at Oak Ridge National Laboratory:
This next-generation neutron source will have a power in the 1 megawatt range. Continued research and development is necessary to support construction of the SNS. Prior to FY 1999, research and development activities were funded in the Materials Sciences research section of this budget.

-Partial Offset to ESRD General Reduction Applied to BES.

Total Major User Facilities

FY 1997

FY 1998

FY 1999

81,441

82,368

87,300

0

0 28,600

2,043

1,545

0

\$256,171

\$253,250

\$285,565

BASIC ENERGY SCIENCES
CAPITAL OPERATING EXPENSES AND CONSTRUCTION SUMMARY
(Dollars in thousands)

	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>	<u>\$ Change</u>	<u>% Change</u>
<u>Capital Operating Expenses</u>					
General Plant Projects (total).....	\$8,894	\$10,762	\$9,275	\$-1,487	-13.8%
AIP under \$5 million (total).....	7,602	11,109	7,110	-3,999	-36.0%
Capital Equipment (total).....	45,870	49,740	60,097	+10,357	+20.8%

Construction Project Summary (both Operating and Construction Funded)

<u>Project No.</u>	<u>Project Title</u>	<u>TEC</u>	<u>Previous Appropriated</u>	<u>FY 1997 Appropriated</u>	<u>FY 1998 Request</u>	<u>FY 1999 Request</u>	<u>Unapprop. Balance</u>
99-E-334	Spallation Neutron Source, ORNL	#####	\$0	\$0	\$0	\$128,400	#####
97-E-305	Accelerator and Reactor Improvements & Modifications, Various Locations	2,500	0	2,500	0	0	
96-E-300	Combustion Research Facility, Phase II, SNL	26,800	6,800	9,000	7,000	4,000	
Total Basic Energy Sciences		<u>XXXXXX</u>	\$6,800	\$11,500	\$7,000	\$132,400	#####

<u>Detailed Breakouts</u>	<u>Total CDR Cost</u>	<u>Previous Appropriated</u>	<u>FY 1997 Appropriated</u>	<u>FY 1998 Request</u>	<u>FY 1999 Request</u>	<u>Unapprop. Balance</u>
CDR's - Exceeding \$3 million						
1. Spallation Neutron Source - Conceptual Design	\$15,478	\$7,535	\$7,943	\$0	\$0	\$0

<u>Major Items of Equipment (CE \$2 million and above)</u>	<u>TEC</u>	<u>Previous Appropriated</u>	<u>FY 1997 Appropriated</u>	<u>FY 1998 Request</u>	<u>FY 1999 Request</u>	<u>Acceptance Date</u>
1. Short Pulse Spallation Upgrade at LANSCE - LANL	20,500	0	0	4,500	4,500	Sept-2001
2. HB-2 Beam Tube Extension at HFIR-ORNL	5,900	0	0	0	3,500	Sept-2000

DEPARTMENT OF ENERGY
 FY 1999 CONGRESSIONAL BUDGET REQUEST

SCIENCE
 (Tabular dollars in thousands. Narrative material in whole dollars.)

Basic Energy Sciences

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334	2b. Construction Funded
3a. Date A-E Work Initiated (Title I Design Start Scheduled)	Preliminary Estimate 1st Qtr. FY 1999	Title I Baseline <u>a/</u> TBD	Current Baseline Estimate TBD
3b. A-E Work (Title I & II) Duration:	60 Months	TBD	TBD
4a. Date physical Construction Starts:	3rd Qtr. FY 2000	TBD	TBD
4b. Date Construction Ends:	4th Qtr. FY 2005	TBD	TBD
5. Total Estimated Cost (TEC) --	Preliminary Estimate \$1,138,800	Title I Baseline <u>a/</u> TBD	Current Baseline Estimate TBD
6. Total Project Cost (TPC) --	\$1,332,800	TBD	TBD

a/ To be determined upon completion of Title I design.

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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7. Financial Schedule (Federal Funds):

<u>Fiscal Year</u>	<u>Appropriations</u>	<u>Adjustments</u>	<u>Obligations</u>	<u>Costs</u>
1999	\$128,400		\$128,400	\$ 52,500
2000	196,100		196,100	135,200
2001	254,900		254,900	294,000
2002	253,200		253,200	276,100
2003	184,900		184,900	207,300
2004	78,300		78,300	130,700
2005	43,000		43,000	43,000

8. 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.

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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8. Project Description, Justification, and Scope (continued)

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.

1. Title and Location of Project: Spallation Neutron Source (SNS)
Oak Ridge National Laboratory (ORNL)
Oak Ridge, Tennessee

2a. Project No.: 99-E-334
2b. Construction Funded

8. Project Description, Justification, and Scope (continued)

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

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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systems that will meet performance requirements.

8. Project Description, Justification, and Scope (continued)

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 requested budget authority will allow 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.

1. Title and Location of Project: Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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9. Details of Cost Estimate^{a/}

	<u>Item Cost</u>	<u>Total Cost</u>
a. Design and Management Costs		\$ 290,000
(1) Engineering, design, and inspection at approximately 26% of items c and f below .	\$ 166,900	
(2) Construction management at approximately 4% of items c and f below	26,300	
(3) Project management at approximately 15% of items c and f below	96,800	
b. Land and land rights		0
c. Construction costs.		642,700
(1) Improvements to land (grading, paving, landscaping, and sidewalks)	28,600	
(2) Buildings	176,700	
(3) Other structures	600	
(4) Utilities (electrical, water, steam, and sewer lines)	30,500	
(5) Technical components	406,300	
d. Standard Equipment		1,100
e. Major computer items		12,000
f. Removal cost less salvage.		0
g. Design and project liaison, testing, checkout and acceptance		<u>6,700</u>
Subtotal		\$ 952,500
h. Contingency at approximately 20% of above costs		<u>186,300</u>
Total line item cost (Section 11.a.1.(a))		\$1,138,800
i. Less: Non-Federal Contribution		<u>0</u>
Net Federal total estimated cost (TEC)		\$1,138,800

^{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.

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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10. 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 construction will be accomplished, to the extent feasible, by fixed-priced subcontracts awarded to industry on the basis of competitive bidding.

1. Title and Location of Project: Spallation Neutron Source (SNS)
 Oak Ridge National Laboratory (ORNL)
 Oak Ridge, Tennessee

2a. Project No.: 99-E-334
 2b. Construction Funded

11. Schedule of Project Funding and Other Related Funding Requirements

	FY	Previous FY	FY	FY	FY	FY	FY	FY	FY
	Years	1999	2000	2001	2002	2003	2004	2005	TOTAL
a. Total project costs									
(1) Total facility costs									
(a) Line Item (Section 9)	\$ 0	\$ 52,500	\$135,200	\$294,000	\$276,100	\$207,300	\$130,700	\$43,000	\$1,138,800
(b) Plant Engineering & Design . . .	0	0	0	0	0	0	0	0	0
(c) Expense-funded equipment . . .	0	0	0	0	0	0	0	0	0
(d) Inventories	0	0	0	0	0	0	0	0	0
Total direct cost (Federal and Non-federal)	0	52,500	135,200	294,000	276,100	207,300	130,700	43,000	1,138,800
(2) Other project costs									
(a) R&D necessary to complete project	21,600	25,700	16,297	11,700	7,800	3,700	2,600	0	89,397
(b) Conceptual design cost	15,303	0	0	0	0	0	0	0	15,303
(c) Decontamination & Decommissioning (D&D)	0	0	0	0	0	0	0	0	0
(d) NEPA Documentation costs . . .	1,500	0	0	0	0	0	0	0	1,500
(e) Other project related costs	0	800	900	1,300	1,900	6,400	16,000	57,400	84,700
(f) Capital equipment not related to construction	100	2,100	700	100	100	0	0	0	3,100
Total other project costs	38,503	28,600	17,897	13,100	9,800	10,100	18,600	57,400	194,000
Total project costs (TPC)	38,503	81,100	153,097	307,100	285,900	217,400	149,300	100,400	1,332,800
(g) Less: Non-federal contribution	0	0	0	0	0	0	0	0	0
Net Federal total project costs (TPC)	\$38,503	\$81,100	\$153,097	\$307,100	\$285,900	\$217,400	\$149,300	\$100,400	\$1,332,800

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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11. Schedule of Project Funding and Other Related Funding Requirements (Continued)

b. Related annual funding ^{a/} (estimated life of project: 40 Years)		
(1) Facility operating costs	\$21,300
(2) Facility maintenance and repair costs	25,300
(3) Programmatic operating expenses directly related to the facility	22,500
(4) Capital equipment not related to construction but related to the programmatic effort in the facility	2,100
(5) GPP or other construction related to the programmatic effort in the facility	1,000
(6) Utility costs	30,400
(7) Accelerator Improvement Modifications (AIMs)	<u>4,100</u>
Total related annual funding	\$ 106,700

^{a/} Expressed in FY 2006 dollars, the first full year of operation.

12. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total Project Cost

(1) Total facility costs

(a) Line Item (Section 9)

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 \$1,138,800,000.

(b) Plant Engineering and Design

No narrative required

12. Narrative Explanation of Total Project Funding and Other Related Funding Requirements (continued)

1. Title and Location of Project: Spallation Neutron Source (SNS)
Oak Ridge National Laboratory (ORNL)
Oak Ridge, Tennessee

2a. Project No.: 99-E-334
2b. Construction Funded

(c) Expense funded equipment

No narrative required

(d) Inventories

No narrative required

(2) Other project costs

(a) R&D necessary to complete construction

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.

(b) Conceptual design costs

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.

(c) Decontamination & Decommissioning

No narrative required

12. Narrative Explanation of Total Project Funding and Other Related Funding Requirements (Continued)

1. Title and Location of Project:	Spallation Neutron Source (SNS) Oak Ridge National Laboratory (ORNL) Oak Ridge, Tennessee	2a. Project No.: 99-E-334 2b. Construction Funded
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(d) NEPA Documentation costs

Estimated costs of \$1,500,000 are included to complete the Environmental Impact Statement.

(e) Other project related costs

Estimated costs of \$84,697,000 are included to cover pre-operations costs.

(f) Capital equipment not related to construction but related to the programmatic effort in the facility.

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

b. Related Annual Funding (estimated life of the facility: 40 years)

Costs shown are the estimated annual operating costs for the facility in FY 2006 dollars, the first full year of operation.

13. Design and Construction of Federal Facilities

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

DEPARTMENT OF ENERGY
 FY 1999 CONGRESSIONAL BUDGET REQUEST

SCIENCE
 (Tabular dollars in thousands. Narrative material in whole dollars.)

Basic Energy Sciences

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded
		Preliminary Estimate	Title I Baseline	Current Baseline Estimate
3a.	Date A-E Work Initiated (Title I Design Start Scheduled) 1998	N/A		N/A 1st Qtr. FY
3b.	A-E Work (Title I & II) Duration:	N/A	N/A	12 months
4a.	Date physical Construction Starts:	N/A	N/A	4th Qtr. FY 1998
4b.	Date Construction Ends: Qtr. FY 1999	N/A		N/A 4th
		Preliminary Estimate	Title I Baseline	Current Baseline Estimate a/
5.	Total Estimated Cost (TEC) --	N/A	N/A	\$26,800
6.	Total Project Cost (TPC) --	N/A	N/A	\$30,020

a/ Current Baseline Estimate is the latest baseline which reflects the approved changes to the Title I baseline.

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

7. Financial Schedule: (Federal Funds)

<u>Fiscal Year</u>	<u>Appropriation</u>	<u>Adjustments</u>	<u>Obligations</u>	<u>Costs</u>
Prior Years <u>a/</u>	\$ 4,800		\$ 4,800	\$ 4,205
1995	0	0	4	
1996	2,000	2,000	685	
1997	9,000	9,000	7,347	
1998	7,000	7,000	8,476	
1999	4,000	4,000	6,083	

a/ Prior year funds transferred from 87-R-405.

8. Project Description, Justification and Scope

Phase II of the Combustion Research Facility (CRF) will add approximately 32,300 gross square feet to the existing 51,100 square-foot multibuilding CRF facility (Project No. 78-13-B, TEC \$9,400,000) at Sandia National Laboratories, Livermore (SNL/L). Phase II will add 21,200 square feet to the existing 16,400 square-foot laboratory building and 11,100 square feet to the existing 25,000 square-foot office building. The project will include such site modifications and improvements as yard paving, walkways, landscaping, fencing, signage, and east entrance road relocation.

The project has been delayed due to budget constraints from FY 1989 through FY 1995. The appropriations totaling \$4,800,000 in FY 1987 and FY 1988 were used for site preparation and design and construction of the shell of the laboratory building addition. The appropriations in FY 1996-FY 1998 will complete the balance of the project.

The laboratory building addition will be an L-shaped extension to the south and east of the existing building. Construction of the addition will match the existing building in architectural style, materials, and finishes, color, and floor-to-floor heights. The laboratory building

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California		2a. Project No. 96-E-300 2b. Construction Funded
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8. Project Description, Justification and Scope (Continued)

addition will provide sixteen new laboratory spaces and two facility laser laboratories. The new facility laser rooms will be connected to serve any Lab in the facility, via the Laser Duct and Periscope System.

Once-through conditioned ventilation will be provided from existing building fans for existing and new laboratory spaces to carry off fuel gases or vapors and products of combustion, with systems included to minimize the discharge of contaminants to the atmosphere. An electronic safety monitoring and control system will provide back-up to the ventilation system.

The existing system of ducts used for diagnostic laser beam transmission from the central laser rooms will be extended to all new laboratories. Other existing building systems such as power distribution, lighting, communications, security alarms, fire and evacuation alarms, automatic fire sprinkler, and piping and plumbing will also be extended to the addition.

The office building addition will provide space for thirty-four new offices, an open office secretarial and file area, computer terminal rooms, and conference rooms. The addition will be a two-story wing added to the north of the existing office building and will match it in architectural style, materials and finishes, color, and floor-to-floor height.

Design of the existing mechanical building allowed space for the expansion of some services. Included in this project will be an additional chiller, pumps, and heat exchangers. Additional fan equipment providing recirculated conditioned air for the laboratory building and its addition will be in the loft space above the laboratory buildings. An additional electrical substation and process-cooling water system will also be provided.

Existing site utilities such as domestic and fire protection water, sanitary sewer, natural gas, site lighting, and electrical power and special systems will be modified and extended to service the additional facilities.

1. Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a. Project No. 96-E-300 2b. Construction Funded
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8. Project Description, Justification and Scope (Continued)

A key feature of the Combustion Research Facility is the availability of specially designed lasers for optical diagnostics. The Facility lasers developed in Phase I will continue to be used, and will be supplemented by two new Facility lasers: a high-power pulsed, high-repetition rate tunable ultraviolet laser (UV) and a subpicosecond laser. The laser beam directing system will be extended so that the existing and new laboratories have the capability of receiving the beam from any of the Facility lasers.

Other equipment includes a gas-chromatograph-mass spectrometer, infrared, visible, and ultraviolet spectrometers, elemental analyzers, optical signal processing equipment, and fast laser image processing devices.

Existing equipment from current facilities at SNL/L will be relocated to eleven of the new labs, although some of these experiments will be modified and some equipment will be upgraded. Two labs will be furnished with new equipment within the project TEC, and three labs will be furnished with new equipment by future users of the facilities.

This project will add vitally needed capacity and important new capabilities to the Combustion Research Facility at SNL, Livermore. The principal objective of this construction is to provide combustion research resources that can adequately deal with the critical needs of the 1990s and beyond. To accomplish this goal requires the addition of a new laboratory wing that emphasizes centralized next-generation laser diagnostic facilities and specially designed laboratories not available in CRF Phase I.

The overall scope of this project is the doubling of space available for experiments. Equipment funds are required for a new central laser system and special purpose laboratory equipment. A modest enlargement of the office building is included to house the rapidly increasing population of visiting scientists. These enhancements will consolidate the combustion-related resources at a single site readily accessible to visiting scientists.

There is a continuing need for the CRF to advance combustion-related science and technology to a higher level. The improvements included in the Phase II project will address this need. For example, special lasers and equipment will be developed to provide the ability to measure quantitatively entire two- and three-dimensional images of a system's physical and chemical properties with better resolution, and far greater

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

8. Project Description, Justification and Scope (Continued)

speed than is now possible. It is this type of advance in the science of combustion that will allow the pursuit of the increasingly more difficult and complex problems that face our country.

CRF Phase II will enable attacking many complex problems directly associated with combustion. An important example is the need for improved combustion processes that incorporate high efficiency together with minimum production of pollutants such as NO_x and air toxics. Rapid progress on these problems both in engines and in furnaces requires Phase II's next-generation diagnostic capabilities. Completion of Phase II will also enable using the tools and expertise developed in Phase I to address broader challenges facing the country. CRF basic research in laser diagnostics, for example, will underpin remote sensing applications that contribute to global-change research and to nonproliferation of weapons. Basic research in chemically reacting flows will continue to support improved U.S. competitiveness in semiconductor processing and will support the development of new industrial materials. Basic research in chemistry will address new processes, such as supercritical water oxidation, for destroying hazardous wastes with minimal environmental impact.

The implementation of Phase II will develop and make available a new class of lasers. Phase II will include a specially designed high repetition rate laser system. This laser will be optimized for laser photochemistry combustion research and for high speed planar imaging of transient combustion phenomena. A second laser system will be designed to study combustion phenomena occurring on extremely short time scales (subpicosecond time scales). The new laser systems will enable significant extension of our knowledge in a broad range of topics in fundamental combustion science.

The normal increase in both the quantity and sophistication of combustion research by Sandia staff, together with the heightened requirements of visiting scientists, have completely saturated the facilities provided under CRF Phase I. During the past ten years the number of scientists who visit the CRF long enough to participate in research has almost tripled. In fiscal year 1993 forty professional staff hosted eighty nine such visits. Many important experiments cannot be carried out in the existing facilities because of a lack of space. Access to the unique capabilities of the CRF (such as the Facility lasers and computer resources) is essential for studying trade-offs between combustion efficiency and the pollution that results from existing and alternative fuels. However, much of the combustion

1. Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a. Project No. 96-E-300 2b. Construction Funded
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research and diagnostics development

8. Project Description, Justification and Scope (Continued)

work at Sandia is currently being done in facilities that are widely scattered throughout Sandia/CA where the researchers do not have access to these unique capabilities. Additional laboratories will permit the consolidation of these experiments at the CRF, thus providing the necessary access to the unique capabilities at the Facility. It will also provide adequate space and ready access to visiting scientists.

The number of offices required to support visiting researchers and staff must also be increased as each year of operation brings a large number of requests from qualified researchers to do work here who stay longer.

This addition is crucial to continuation of the lead role the CRF now plays in developing, improving, and applying advanced research methods for combustion science. As a result of successful technology transfer from the CRF to visiting scientists, there has been a significant advance in the research methods practiced by the combustion community. Given the increasingly difficult challenges faced in the use of fuel resources, the CRF mission must continue to emphasize advancing the frontiers of combustion science.

Without Phase II the technology at the CRF will stagnate, and opportunities for important new scientific research will be missed. The major advances in lasers and computers will not be brought to bear on pressing problems, nor made available to combustion researchers and designers in this country. CRF Phase II is also crucial to the success of programs in combustion research and diagnostics development. Currently, progress is hampered by the fractionation of the research effort. A significant amount of the experimental activities are housed in other buildings without direct access to the Facility lasers and other resources. Some of the activities are in security areas where it is difficult or impossible for uncleared visiting researchers to work. Moreover, the major portion of the diagnostics research is housed in a converted warehouse. It is essential that this activity be moved to an area that provides cleaner air, better temperature control, improved safety, access to the facility lasers, and unrestricted availability to users.

Finally, without the Phase II addition to the Facility, the size of the visiting scientist (user) program will have to be curtailed, due to the saturation of laboratory and office space. As a result, the ability for the combustion community to move on to more complex, yet

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

realistically important research topics, will be constrained.

1.	Title and Location of Project: Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300 2b. Construction Funded
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9.	<u>Details of Cost Estimate</u>	<u>Unit Cost</u>	<u>Item Cost</u>	<u>Total Cost</u>
a.	Engineering, design, and inspection (ED&I)			\$4,200
	1. Engineering, design, and inspection at approximately 22 percent of construction		3,000	
	2. Construction management costs		900	
	3. Project management		300	
b.	Construction costs			13,800
	1. Improvements to land		1,000	
	Paving, walkways, landscaping, fencing, signage, road relocation parking lot rearrangement			
	2. Buildings		12,000	
	(a) Office Building (11,100 SF \$193/SF)	2,100		
	(b) Laboratory Building (21,200 SF \$432/SF)	9,200		
	(c) Mechanical Building (Existing)	700		
	3. Utilities		800	
	Water, sanitary sewer, natural gas, site lighting, electrical power, signal systems			
c.	Standard equipment			6,800
	Lasers, spectrometers, analyzers, processing equipment			
	Subtotal			24,800
d.	Contingency at approximately 8 percent of above costs			2,000
	Total line item cost			\$26,800

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

9. Details of Cost Estimate (Continued)

ED&I costs for Title I and II reflect negotiated contract fees. ED&I for Title III is based on a negotiated fee plus an allowance for an extended period of construction, and for escalation. Construction costs and equipment costs have been escalated to mid points of construction and equipment procurement and installation. Escalation rates are in agreement with the DOE Price Change Index dated August 1993 for DOE construction projects, published by the DOE Independent Cost Estimating Staff.

Contingency is judged to be adequate for the remainder of the project. Construction of the laboratory shell was completed in FY 1990. Design was completed for the balance of the construction work in FY 1989. As a result of zero appropriations in FY 1989 through FY 1995 and the consequential schedule extension, some remaining ED&I and Project Management funds will be expended on obsolete Title II design elements prior to going to bid for remaining construction.

10. Method of Performance

Engineering, design, and inspection will be performed under negotiated architect and engineer contracts. Construction, procurement of equipment, and occupancy will be accomplished by fixed price contracts awarded on the basis of competitive bidding.

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

11. Schedule of Project Funding and Other Related Funding Requirements

	Prior	<u>Years</u>	<u>FY 1995</u>	<u>FY 1996</u>	<u>FY 1997</u>	<u>FY 1998</u>	<u>FY 1999</u>
<u>Total</u>							
a. Total project funding							
1. Total facility costs							
(a) Line item	<u>\$4,205</u>	<u>\$ 4</u>	<u>\$ 685</u>	<u>\$ 7,347</u>	<u>\$ 8,476</u>	<u>\$6,083</u>	<u>\$26,800</u>
Total direct cost	4,205	4	685	7,347	8,476	6,083	26,800
2. Other project costs							
(a) Other project costs . .	220	0	0	500	750	750	2,220
(b) Capital equipment . . .	<u>0</u>	<u>0</u>	<u>0</u>	<u>500</u>	<u>250</u>	<u>250</u>	<u>1,000</u>
Total other project costs	<u>220</u>	<u>0</u>	<u>0</u>	<u>1,000</u>	<u>1,000</u>	<u>1,000</u>	<u>3,220</u>
Total project cost (TPC) .	\$4,425	\$ 4	\$ 685	\$8,347	\$ 9,476	\$7,083	\$30,020
b. Related annual costs a/ (estimated life of building: 50 years)							
1. Facility operating costs					\$ 300		
2. Programmatic operating expenses directly related the facility					2,400		
3. Capital equipment not related to construction but related to the programmatic effort in the facility					400		
4. GPP or other construction related to programmatic effort in the facility					200		
5. Other costs					<u>0</u>		
Total related annual costs					\$ 3,300	a/	

a/ Estimated costs in thousands escalated to 1999-year dollars. The related annual funding displayed is related to CRF, Phase II project only. These amounts are in addition to annual funding for the existing CRF operations.

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

12. Narrative Explanation of Total Project Funding and Other Related Funding Requirements

a. Total project costs:

1. Total facility costs

(a) Construction Line Item as described in previous items.

2. Other project costs

(a) Other project costs

\$220,000 of operating funds have been paid to architect engineering firms for preparation of conceptual designs/conceptual design reports and supplemental information for this project. \$500,000 in FY 1997, \$750,000 in FY 1998, and \$750,000 in FY 1999, are operating costs associated with the new facility.

(b) \$500,000 in FY 1997, \$250,000 in FY 1998, and \$250,000 in FY 1999 is for capital equipment associated with the new facility.

b. Related annual costs:

1. Facility operating costs

This cost represents the annual operating expenses for utilities, maintenance, and janitorial service incurred due to the increase of 32,300 gross square feet in laboratory and office space.

2. Programmatic operating expenses

Staff increase resulting from this project is estimated to be six people. Costs also include acquisition of computer resources that will serve both resident staff and visiting scientists.

3. Capital equipment not related to construction

The increase in annual capital equipment is estimated at \$400,000. This is in addition to capital equipment funds currently allocated to the CRF.

4. Maintenance, repair, GPP or other construction related to programmatic effort

The annual GPP needs for Phase II are expected to be approximately \$200,000. This is in addition to GPP funds presently allocated to the CRF.

5. Other costs - No other costs are anticipated.

1.	Title and Location of Project:	Combustion Research Facility, Phase II Sandia National Laboratories Livermore, California	2a.	Project No. 96-E-300
			2b.	Construction Funded

13. Design and Construction of Federal Facilities

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