DEPARTMENT OF ENERGY

FISCAL YEAR 1980 CONGRESSIONAL BUDGET REQUEST

ENERGY SUPPLY RESEARCH AND DEVELOPMENT

VOLUME 3

BASIC RESEARCH

TABLE OF CONTENTS

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

PROGRAM OVERVIEW

Basic Research

The Basic Research category includes four programs: (1) Basic Energy Sciences (BES); (2) Technical Assessment Projects (TAP); (3) University Research Support (URS); and (4) Technology Program and Policy Analysis. These programs are carried out under the legal requirements of P.L. 95-91, Section 209, which sets forth the duties and responsibilities of the Director, Office of Energy Research. All four of the programs are dedicated to maintaining a strong national energy program that will provide a base of pertinent knowledge which future scientists, engineers and mathematicians can apply to the development and improvement of energy alternatives to meet the Nation's ever-increasing energy needs.

The Basic Energy Sciences program strengthens the base for advances in energy production, conversion, and conservation, by improving our understanding of existing phenomena and discovering new phenomena in the physical and biological sciences, engineering and mathematics. BES supports outstanding talent at institutions carrying out technology-oriented energy research and development programs, sponsors major involvement of university scientists and their students, and interacts strongly with other Department of Energy programs in choosing research tasks and in communicating research results. BES assembles, encourages and supports a body of highly competent researchers in physics, chemistry, biology, the materials sciences, engineering, geosciences and mathematics in order to provide new ideas, instruments, materials, processes and techniques for application in the development of various energy technologies. In addition, the program will continue to support the construction and operation of pioneering and/or unique research facilities for use by scientists throughout the Nation. The program is expected to continue to expand during the next few years to ensure that a balanced research program is maintained which supports the long-term requirements of the Department of Energy technology programs in a manner consistent with the Department's long-range plans. BES program managers will continue to maintain liaison with other Department of Energy programs, other Federal agencies and with the scientific, academic and industrial research communities in order to ensure the early and optimum application of their research to the Department's programs.

The primary output of basic research is new fundamental knowledge which is expected to influence significantly the long-term energy capability of the Nation. Direct commercialization of results from basic research has occurred fairly often; however, more often the benefits accrue as the accumulated knowledge and understanding of detailed processes and properties become an integral part of the body of data on which applied technologies rest. The following are two accomplishments which are representative of the types of advances which have come out of the BES program. A new technique for preparing the high critical field superconductor (niobium-aluminum-germanium) was developed using a powder metallurgy process involving infiltration of niobium compacts with a liquid mixture of aluminum-germanium. The multifilamentary wire produced has the highest critical current yet reported and has potential use in high magnetic field applications such as magnetic fusion, magnetohydrodynamics and energy storage. In addition, a very fast, accurate, automatic analysis of oxygen in coal, heretofore lacking for coal conversion development, has been developed using charged particle activation analysis. This is an important new method of providing analytical data required by the coal industry. Other recent major accomplishments have occurred in a wide variety of areas such as catalysis; scale formation phenomena in geothermal processes; nuclear data measurements; combustion; coal conversion development; nuclear waste processing; computer software development; and metallurgy. These accomplishments are discussed in greater detail below in the narrative justification. The provision of separated isotopes to the research community, done within the Nuclear Sciences portion of the BES program, is the only direct revenue-producing activity within the program. Revenues from this activity in FY 1980 are estimated to be about $1,500,000.

The Technical Assessment Projects program provides the capability for independent and rigorous assessment of the base of research that underlies a variety of energy technologies, including a complete evaluation of the Solar Powered Satellite (SPS) concept. Such independent assessments are very important to ensure that the Department's basic research effort enhances both the short-term and long-term objectives of the applied programs. These efforts are intended to provide the Director, Office of Energy Research with the information required to fulfill his role of providing advice and recommendations to the Secretary on Department-wide research and development issues and strategy. This program, initiated late in FY 1978 with reprogrammed funds, has performed assessments of superconducting electric generation for utility applications, applications of remote instrumentation and automated systems (robotics), and future uranium resources. In FY 1979 new assessments, including identification of long-range research needs for fossil energy and examination of solar energy alternatives, have begun.

The University Research Support program provides institutional support for university-based research on long-range energy problems and aids in the preparation and training of future energy professional manpower through research participation by advanced graduate students. It includes an activity aimed at increasing the involvement of smaller, traditionally minority institutions in the National energy program. Eight research awards were made in this program in FY 1978 and a similar number is planned in FY 1979. A related goal of University Research Support is to improve and expedite the transfer of energy research concepts and findings from university laboratories to commercial and public use (the university institutional agreements program). Six awards were made in FY 1978 under this program. During FY 1979, support will be continued for these projects and one new award is planned. The Department of Energy has also been directed under Title VIII of P.L. 95-87 to establish regionally based university coal research laboratories to conduct research on problems of coal characterization and utilization specific to their regions, while at the same time increasing the number and enhancing the quality of professional manpower associated with coal research and development. This activity, as well as the university reactor fuel assistance activity, is carried out under the University Research Support program.

Technical Program and Policy Analysis provides the in-house staff necessary to advise the Secretary with the respect to the well-being and management of the multipurpose laboratories (excluding the weapons laboratories) and the staff to supervise or support research activities carried out by any of the Assistant Secretaries. The staff provides expert advice, policy analyses, determination of priorities, plans, strategies and coordination of a variety of activities which enhance the Department's capability to manage the energy research and development activities in an effective and efficient manner.

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

SUMMARY OF CHANGES BY AREA
Energy Supply Research and Development - Operating Expenses
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research
(In thousands of dollars)

FY 1979 budget authority	220,133
FY 1980 budget estimate	275,824
Net change	+ 55,691

	1979 Base	Change From Base
Increases:		
Program:		
Basic energy sciences		
Maintain current level and provide for selected expansions in basic research programs in:		
Materials sciences	77,690	+ 10,360
Chemical sciences	51,400	+ 11,700
Engineering	1,075	+ 1,075
Applied mathematical sciences	8,970	+ 2,730
Geosciences	6,455	+ 5,045
Biological energy	4,000	+ 3,200
Maintain current level of research in nuclear sciences	29,700	+ 2,300
Expand support of advanced energy projects	7,500	+ 9,300
Initiate construction of two new scientific research facilities	...	+ 8,700
Personnel-related expenses for the above programs	1,851	+ 719
Technical assessment projects		
Initiate new assessments as required to provide more comprehensive analysis of DOE's R&D programs	1,500	+ 1,500
Further study and identification of key problem areas related to the Solar Powered Satellite (SPS), including microwave bioeffects, communications effects and atmospheric effects	4,600	+ 2,900
Upgrade and modify experimental SPS systems required for studies of microwave effects on the ionosphere	...	+ 500
Personnel-related expenses for above programs	308	+ 158
University research support		
Award two new university institutional agreements	800[a/]	+ 1,500[a/]
Initiate coal research laboratories program by phasing in support for thirteen laboratories	...	+ 5,000
Personnel-related expenses for above program	122	+ 49
Technical program and policy analysis		
Personnel-related expenses for above program	1,662	+ 755
Total increases		+ 67,491

a/ Excludes $1.4 million budgeted under Fossil, Solar, and Fusion programs which will be used to support University institutional agreements.

	1979 Base	Change From Base
Decreases:		
Program:		
Basic energy sciences		
Complete constuction of three scientific research facilities	19,800	- 10,800
Technical assessment projects		
Deletion of policy and evaluation general systems studies funds designated for OER use in FY 1979	700	- 700
University research support		
Reduced support for university reactor fuel	2,000	- 300
Total decreases		- 11,800

Energy Supply Research and Development - Operating Expenses
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research
(Tabular dollars in thousands. Narrative material in whole dollars.)

	FY 1979 Estimated Budget Authority	FY 1980 Estimated Budget Authority
Basic energy sciences (ER)		
Nuclear sciences:		
Operating expenses	$ 28,400	$ 30,700
Capital equipment	1,300	1,300
Subtotal	29,700	32,000
Materials sciences:		
Operating expenses	71,520	81,300
Capital equipment	5,900	6,500
Construction	16,670	11,650
Subtotal	94,090	99,450
Chemical sciences:		
Operating expenses	48,000	58,800
Capital equipment	3,400	4,300
Construction	3,400	6,300
Subtotal	54,800	69,400
Engineering, mathematical and geosciences:		
Operating expenses	15,700	23,900
Capital equipment	800	1,450
Subtotal	16,500	25,350
Advanced energy projects:		
Operating expenses	7,300	16,600
Capital equipment	200	200
Subtotal	7,500	16,800
Biological energy research:		
Operating expenses	4,000	6,900
Capital equipment	0	300
Subtotal	4,000	7,200
Personnel resources	1,851	2,570
Total, basic energy sciences	$ 208,441	$ 252,770
Authorization: Sec. 209 , P.L. 95-91	$ 208,441	$ 252,770

Basic energy sciences

Basic Energy Sciences is the major Department of Energy program which plans, supports and administers basic research in the physical and biological sciences most important to the Nation's energy program. A balance among research areas and among research tasks is sought which will optimize the achievement of overall program objectives. Criteria used in deciding the proper balance among the activities within basic energy sciences include: the likelihood that research in a particular area will yield knowledge of phenomena important to energy technologies; the need to maintain interaction between the BES-supported scientists and engineers and those in other Department of Energy programs; prevention of unnecessary overlaps and avoiding serious gaps along the spectrum of activities from the most basic research to laboratory demonstrations of feasibility and in a manner which will enhance the probability of significant achievements; and the Department of Energy's responsibility for well-designed, scientifically excellent national programs using the arsenal of forefront research facilities.

In FY 1980, the Basic Energy Sciences request is for $252,770,000, an increase of $44,329,000 over FY 1979. Of this request, $218,200,000 is for operating expenses; $14,050,000 is for capital equipment; $17,950,000 is for construction; and $2,570,000 is for personnel resources. Highlights of the request include continuing a strong base research program needed to meet long-term energy needs; expanding research in areas where accomplishments have recently shown significant potential applications to the applied programs; and providing for three important initiatives. One of these initiatives would focus on the long-range aspects of nuclear waste management and would increase confidence in our ability to dispose safely of radioactive waste in the long term. Another would investigate advanced solar concepts and should impact on the longer-term prospects for solar energy. The third would expand the opportunities for university researchers to contribute to energy problems through upgrading university research capabilities. The request also provides for the last increment of funding for the National Synchrotron Light Source at Brookhaven National Laboratory (BNL) in New York, as well as new construction involving a Chemical and Materials Sciences Laboratory at Lawrence Berkeley Laboratory (LBL) in California, and expanded experimental capabilities at the Intense Pulsed Neutron Source-I at Argonne National Laboratory (ANL) in Illinois. These and other areas of emphasis in FY 1980 can be discussed in terms of the six major activities under basic energy sciences. These are: (1) nuclear science; (2) materials sciences; (3) chemical sciences; (4) engineering, mathematical and geosciences; (5) advanced energy projects; and (6) biological energy research.

Nuclear Sciences	$ 29,700	$ 32,000

Nuclear Sciences consists of two separate activities, one of which is research relevant to fission and fusion energy, while the other is a national service in support of a wide range of research studies. The first, Low Energy Nuclear Sciences, includes experimental research of both basic and applied nature, involving low energy particle accelerators, research reactors and radioactive sources. ("Low energy" includes research performed at accelerators which operate below 150 MeV and accelerate light ions. Nuclear research performed at accelerators operating at energies above 150 MeV is included under the Department of Energy's Nuclear Physics program, which is discussed in the Basic Sciences portion of the budget. The Nuclear Physics program also includes research at those accelerators which accelerate heavy ions, i.e. ions with a mass greater than an alpha particle, irrespective of the energy level.) Low Energy Nuclear Sciences also includes the measurement, compilation and evaluation of nuclear data. In addition, experimental research on the chemical and physical properties of the heavy elements (those with atomic number larger than 83) is supported under Low Energy Nuclear Science.

The second activity under Nuclear Sciences is isotope preparation. This activity includes the operation at Oak Ridge National Laboratory (ORNL) in Tennessee of the Calutron facility for the separation of isotopes, the High Flux Isotope Reactor (HFIR) for the production of heavy elements, and the Transuranium Processing Plant (TRU) for the processing of heavy element targets. These nuclear materials are made available through both loan and sales programs.

The FY 1980 request of $32,000,000 ($30,700,000 for operating expenses and $1,300,000 for capital equipment) is necessary to maintain Nuclear Sciences at the FY 1979 program level.

Operating Expenses

The FY 1980 request of $30,700,000 for operating expenses is an increase of $2,300,000 above the FY 1979 level. The following table illustrates the distribution of the request among the various activities within Nuclear Science.

Nuclear Sciences
Summary of Operating Expenses

	Budget Authority	
	FY 1979	FY 1980
Low energy nuclear sciences		
Nuclear research	$ 10,275	$ 10,945
Nuclear data measurements	4,345	4,785
Nuclear data compilation and evaluation	2,145	2,320
Heavy element chemistry	3,235	3,565
Subtotal, low energy nuclear science	$ 20,000	$ 21,615
Isotope preparation		
Electromagnetic isotope separation	$ 1,230	$ 1,335
Special isotope preparation	7,170	7,750
Subtotal, isotope preparation	$ 8,400	$ 9,085
Total, nuclear sciences	$ 28,400	$ 30,700

Low Energy Nuclear Sciences

The operating expenses request for FY 1980 for Low Energy Nuclear Sciences is $21,615,000, an increase of $1,615,000 above the FY 1979 level. The work supported under this heading can be discussed in terms of four specific areas of research: nuclear research, nuclear data measurements, nuclear data compilation and evaluation and heavy element chemistry.

The FY 1980 request for nuclear research is $10,945,000, an increase of $670,000 over the FY 1979 level. This request would support experimental research in basic low energy nuclear physics, using low energy particle accelerators, research reactors, and radioactive sources. These very fundamental studies in the low energy nuclear domain can provide information which is relevant to long-term development of fission and fusion energy systems. The studies, complementary to those carried out under the Nuclear Physics program, have as an objective the improvement of our understanding of the structure of the nucleus or the forces of nature which apply at the nuclear level. For example, at the LBL 88-inch cyclotron, using an on-line mass separator, nuclei are being produced at the limits of nuclear stability and their decay properties are being studied. These studies are performed using low energy, light ion nuclear reactions to produce nuclei having an unusual ratio of protons and neutrons compared to those stable nuclei found in ordinary matter. The studies permit investigation of detailed properties of individual nuclear states. At Argonne, low energy nuclear reactions are employed to produce radioactive nuclei of lithium and boron. Again, decay properties of these nuclides are studied to reveal information on the weak interaction force.

Several university accelerators will continue to be supported for basic low energy nuclear research studies. These include the cyclotron at the University of Colorado, the cyclograff at Duke University and the tandem Van de Graaff at the University of Wisconsin. It is planned to keep these machines at the forefront of low energy nuclear research. In particular, new developments on improving the polarized ion sources are underway at Duke and Wisconsin. A polarized ion source adds a new dimension in the study of nuclear reactions. In addition, light ion nuclear reactions are studied at the tandem Van de Graaff accelerators at Yale University and the University of Washington.

The request also provides for a large share of the operational support of the High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory (BNL), in New York. The TRISTAN II on-line isotope separator has been moved from the recently closed Ames Research Reactor to the HFBR. The new facility will be made available to university users as a national facility, and a number of university groups will be funded to study the nuclear properties of fission products, including delayed neutron emission, at the HFBR. Strong low energy nuclear sciences groups are supported at ANL, BNL, and ORNL. Smaller groups are supported at Ames Laboratory (for further nuclear spectroscopy studies at TRISTAN II) and at the Los Alamos Scientific Laboratory (LASL), in New Mexico, (for fundamental fission studies). Besides the university groups mentioned above, there are groups at the University of North Carolina and North Carolina State University (participants in the Triangle Universities Nuclear Laboratory at Duke), a small group at MIT (combining laser spectroscopy and nuclear spectroscopy to study properties of atomic nuclei) and another at Purdue University (working on nuclear spectroscopy). A small project devoted to solid state detector instrumentation is also underway at the University of Oklahoma. While much of nuclear research has moved into the user group mode at the national accelerator facilities, there is a continuing need for precision experiments at smaller scale facilities. Under nuclear research, an attempt is made to support a broad base of smaller facilities that can produce research results of significance to the program.

The budget request for nuclear data measurements is $4,785,000, an increase of $440,000 over the FY 1979 level. These funds would support measurements made mainly to provide nuclear data information needed by the Department's applied technologies. In many cases, of course, the data is also of interest to basic nuclear theory, particularly in the development of theoretical models to explain broad areas of nuclear phenomena. The measurement programs also interact synergistically with the more basic research programs in low energy nuclear physics, and each profits from the development of experimental instrumentation and techniques. The funding request is divided almost equally between measurements needed for the fission and for the fusion programs.

The activities devoted to satisfying the highest priority nuclear data needs of the fusion program are coordinated by a working group that includes representatives from three national laboratories (ORNL, LASL and Lawrence Livermore Laboratory (LLL)) and from two universities (Duke and Ohio University). The largest of these activities is that conducted at the Oak Ridge Electron Linear Accelerator (ORELA). The university groups and LASL use tandem Van de Graaff accelerators to provide pulsed neutron sources for measurements of elastic and inelastic scattering from nuclides that are contained in materials being considered in the design of fusion power reactors. LASL is also completing apparatus to be used in precise absolute measurements at the lowest possible energies of a number of light-ion reactions, such as tritium plus tritium and deuterium plus tritium, that are of great interest in fusion research, and perhaps also in the diagnostics of the performance of the Tokamak Fusion Test Reactor being built at Princeton.

The work supporting the fission program includes measurements at ORNL and Idaho National Energy Laboratory (INEL) of the average number of neutrons released during fission for Californium-252, the standard by which all other fissionable materials are measured and the most important parameter required in the design of fission reactors. Thus, any uncertainty or error will directly affect power reactor designs. A new, high precision determination of this standard was recently obtained at ORNL. At ANL, measurements will be continued on the yields of fast-neutron-induced fission products using nearly mono-energetic neutrons over an energy range of 0.1 to 8 MeV on the important fissile and fertile nuclides.

Measurements on Uranium-238 and Thorium-232 have recently been completed and a comparison of the data from the two experiments has made it possible to derive fundamental information relating to the "viscosity" of nuclear matter. At LLL the development of a fast chemistry system continues and measurements are being made of nuclear properties of short-lived fission products needed for reactor-fuel decay-heat predictions. At ORNL, the program of measurement of actinide cross sections is making good progress and contributing to the data base required for the calculation of the formation and burnup of actinide nuclides in reactors. Many of the measurements have required the development of new detection techniques to overcome the effects of the high-level background of alpha-particle emission. Projects in this area are also supported at several universities. For example, measurements of differential inelastic neutron scattering cross sections of thorium and uranium have been initiated at the University of Lowell in Massachusetts. Other programs contributing to nuclear data needs are located at the University of Michigan and the University of Washington.

The request for nuclear data compilation and evaluation is $2,320,000, an increase of $175,000 over the FY 1979 amount. These funds would support the major part of the United States effort in nuclear data compilation and evaluation. This effort is now coordinated by the National Nuclear Data Center (NNDC) at BNL, which receives the major portion of its funding from this program. Other contributors to NNDC are the programs of the Assistant Secretary for Energy Technology and the Electric Power Research Institute. NNDC has a major responsibility for the compilation of neutron data produced in the United States and Canada and coordinates a large United States effort in the evaluation of neutron data via its Cross Section Evaluation Working Group (CSEWG). The result is a massive computerized data base designated as ENDF (Evaluated Neutron Data File). This file is now internationally accepted; an updated version is almost ready for release. CSEWG is currently made up of scientists from 13 federal laboratories, 9 industrial firms, and 5 universities.

The Center has recently been assigned responsibility for the coordination of the United States effort in the compilation and evaluation of nuclear structure and decay data, as well as for selected charged-particle reaction data of interest for applied purposes. It coordinates this effort via a recently established National Data Network (NDN); which includes data centers at BNL, INEL, LBL, ORNL, the National Bureau of Standards (NBS), and the University of Pennsylvania. All but the NBS effort is funded by Nuclear Sciences. The United States effort is being supplemented by coordinated international participation in the nuclear structure and decay data effort which has been recently established with the cooperation of the IAEA (International Atomic Energy Agency). With this assistance, it is expected the desired 4-year update cycle can be achieved. The ORNL group, the originators of the Evaluated Nuclear Structure Data File (ENSDF) that has been adopted as the international format, will continue to provide the technical guidance for the program.

Recent products of these efforts include the issuance by the LBL group of an impressive (more than 1500 pages) new edition (the 7th) of the widely used "Table of Isotopes." The 6th edition included a printing of 10,000 copies which has been sold out. In the future, it is planned to provide a similar updated publication at approximately 4-year intervals that will be produced directly from the ENSDF data base, relieving the LBL group of its extensive parallel compilation and evaluation task.

The FY 1980 budget request for heavy element research is $3,565,000, an increase of $330,000 over the amount appropriated in FY 1979. This request is necessary to support a broadly-based research program for the study of the chemical and physical properties of the actinide elements. This program is needed to develop a thorough understanding of the behavior and interactions of these nuclear materials for the optimum development of fission nuclear power and for the intelligent implementation of effective nuclear waste management procedures. The research activities include studies of the behavior of actinides in aqueous and nonaqueous solutions, which are important to processing technology, as well as for the study of actinides in the environment. An entirely new data base is required to delineate the chemistry of the actinide elements under environmental conditions. Fundamental studies of the magnetic, spectroscopic, and thermodynamic properties and descriptive synthetic chemistry across the entire actinide series are underway to broaden our knowledge and understanding of these nuclear materials to provide a foundation for advancements in the more applied actinide-oriented research in the Department.

These research activities are carried out largely at the national laboratories because of the radiation hazard associated with the transuranium elements. At ORNL, a program to prepare and characterize pure samples of actinide metals has been established, and studies of crystal structure, solution thermodynamics, magnetic properties, and high temperature vaporization are underway. The vaporization studies are pursued in collaboration with LASL, and initial results on the volatility of californium metal have been obtained. This is the highest mass element for which these measurements have been made, and the expected high vapor pressure was confirmed. Further studies are planned for californium and other actinide metals to obtain more precise results for an accurate data base upon which to establish a comprehensive picture of actinide thermodynamics. Also, at ORNL a new study of the ability of geologic media to separate out and retain actinides from aqueous solutions is being pursued in collaboration with the Department of Energy programs in nuclear waste isolation.

At LBL, the study of the plutonium biological sequestering agents continues, and new compounds have been developed which show promise of being able to remove plutonium from living systems. The synthetic, organometallic chemistry investigations that produce these agents are supported under heavy element research; the biological evaluation is supported through programs of the Assistant Secretary for Environment. Other synthetic chemical studies of the preparation and characterization of research samples are being pursued to elucidate fundamental chemical and physical principles and properties of these elements and their compounds. A program to measure the reactions between actinide ions and environmentally important species such as carbonate, sulphate, and phosphate will expand and will develop the experimental methods necessary to obtain reliable data.

At ANL, a program of basic research in actinide nuclear materials is pursued in three areas: spectroscopic study of electronic energy levels where the fundamental mechanisms by which energy is transferred from one atom to another in a molecule are investigated; the study of the chemical behavior of actinide ions in aqueous solutions where equilibrium and time-dependent processes are explored; and the study of the inorganic chemistry of the actinides in pure compounds to elucidate structures, bonding characteristics, and thermodynamic stabilities. Experimental measurements of the light absorption and emission characteristics of certain plutonium, americium, and curium species will be nearing completion, and a systematic theoretical analysis of the energy level structures of the trivalent actinides uranium through einsteinium will be included in a final comprehensive report. This will constitute a significant increase in our knowledge of the energies of electrons in atoms as well as provide valuable data for the applied programs in laser development and isotope separation at LLL.

University-based heavy element research is expanding, and new work in the chemistry of actinides in saline solutions, spectroscopy and magnetic properties of actinide compounds in condensed phases, and the design of new agents for the separation of actinides from waste solutions will be started. Current studies in the inorganic chemistry of the very rare higher actinides, the investigations of the reactions of natural organic complexing agents with actinides, and the studies of actinide complex ion stability constants will continue.

Isotope Preparations

Isotope Preparations supports three major facilities at ORNL for the production, separation, and purification of a wide variety of isotopic and elemental research materials for sale and loan to Federal and non-Federal domestic and foreign customers for various kinds of studies. The FY 1980 budget request for Isotope Preparations is $9,085,000, an increase of $685,000 over the amount appropriated in FY 1979. This production effort is the only source of supply of this broad range of nuclear research samples in the Western world. Loans are also made from a select pool of samples for non-destructive measurements of nuclear data of importance to the Department of Energy's fission and fusion energy development programs and for long-range basic research problems. The electromagnetic isotope separation (calutron) facility separates and enriches many of the stable isotopes and has a limited capability for the separation of certain actinide isotopes having long half-lives. Certain of these isotopes are vitally needed for biomedical research and therapy and for many industrial applications.

At the High Flux Isotope Reactor (HFIR), certain isotopes of elements from plutonium to fermium (elements number 94 to 100) are produced by successive neutron capture. HFIR also provides irradiation services for non-routine isotope production, as well as ongoing user research programs on an "irradiation-unit recharge" basis. This is available to industry when similar services are not available commercially. This reactor has an isotope production, neutron irradiation and neutron beam research capability unique in the Western world. The third facility is the Transuranium Processing Plant (TRU), which processes the HFIR isotope-production targets and separates and purifies the very rare heavy actinide samples for allocation to scientists conducting research. These samples are the basis for studies in actinide chemistry and physics, for nuclear investigations into the limits of nuclear stability, and for the production of new nuclides.

Capital Equipment

The FY 1980 capital equipment request for nuclear sciences is $1,300,000, the same as the amount appropriated in FY 1979. Frequently, advances in our understanding of nuclear science are only achieved by the successful completion and interpretation of very complex experimental research. These activities require rather sophisticated items of equipment. Nuclear sciences research is based at a number of low energy light-ion nuclear particle accelerators, nuclear reactors, and radioactive research facilities, which are located primarily at the national laboratories and, to a lesser extent, at universities. To keep the research efforts at these facilities viable and up-to-date, it is imperative that modern scientific equipment be provided.

Equipment requirements in FY 1980 include fixed lasers and tunable dye laser heads and emission frequency scanning accessories; an interactive graphics system for nuclear data compilations at BNL; ion source equipment for a new on-line isotope separator at BNL; klystron power tube replacements for electron accelerators at ORNL; an x-ray generator for crystal structure studies; tank liners for the Calutron facility; high vacuum equipment; actinide element equipment processing racks; a radioactive waste carrier for the Transuranium Processing Plant at ORNL; and electronic components and power supplies.

Materials Sciences	$ 94,090	$ 99,450

Research sponsored under Materials Sciences is aimed at understanding materials properties and phenomena of importance to all energy systems. The objective is to provide the necessary base of materials knowledge required to advance the Nation's energy programs. Materials often are the key limiting factor in the development of new systems, the performance of present systems, and the evolution of advanced concepts. In Materials Sciences, emphasis is placed on areas where problems are known to exist or are anticipated, and where significant improvements in performance must depend on the selection of materials design based on improved understanding of the underlying mechanisms. The research program covers a very broad spectrum from which new solutions and new materials will be uncovered to apply to existing problems, insight will emerge to identify future materials trouble spots, and working models will be formulated to deal with unpredicted problems or phenomena when encountered.

Materials Sciences brings the disciplines of metallurgy, ceramics, engineering, solid state physics and chemistry to bear on problems relevant to energy systems. Some of the research conducted has as its objective the pursuit of goals which would be important primarily to one single energy technology (e.g., studies of catalytic materials of interest to coal conversion), whereas other research would be of interest to many technologies simultaneously (e.g., studies of brittle fracture of interest to every energy technology). In addition, there is research underway which has as its goal the long-term advancement of science, which can serve as the foundation for future technologies. This latter research often involves unique facilities available only at Department of Energy laboratories.

In addition to informal contacts, Materials Sciences research is coordinated with the Department of Energy applied technology programs through the Energy Materials Coordinating Committee and the Research Assistance Task Force. Interagency coordination is achieved through the Interagency Materials Group and the Committee on Materials (COMAT). To assist in establishing balance and a proper focus within the program, a series of workshops has been held on topics of importance to materials research. Similar workshops, which bring together scientists and engineers from industry, universities, Department of Energy and other government agencies, are being continued in FY 1979. These are only a few of the methods by which this program focuses its efforts and communicates information to interested parties. The FY 1980 request of $99,450,000 for Materials Sciences includes $81,300,000 for operating expenses, $6,500,000 for capital equipment, and $11,650,000 for construction.

Operating Expenses

The FY 1980 request for operating expenses for Materials Sciences is $81,300,000, an increase of $9,780,000 over the FY 1979 level. This level of activity is necessary to maintain the technical base of materials research underway, to meet the commitments arising from responsibilities associated with large facilities and to initiate selected new programs at universities and industrial laboratories.

In FY 1980, increased attention will be given to research areas related to welding, nondestructive evaluation, processing, solar energy, polymers, nuclear waste isolation, high voltage electron microscopy and surface studies. A new 1.2 MeV high voltage electron microscope at ANL is becoming operational in FY 1979 and will be used by ANL researchers and the rest of the scientific community to study energy-related materials behavior. Construction and concurrent R&D activities will continue at an increased rate at the National Synchrotron Light Source at BNL. Research and development activities related to the pulsed neutron sources at both

ANL and LASL will increase during FY 1980. Decreased efforts in certain Materials Sciences activities will be necessary to permit shifting emphases within the program. Among the areas where decreases will occur are: studies related to the Ames Research Reactor that was shut down in FY 1978, neutron related studies at the ANL CP-5 reactor which has been put on a reduced operational schedule, superconductivity studies, diffusion studies, certain aspects of the research on actinide materials and research on mechanical properties of refractory metals. These and other areas of research in Materials Sciences are discussed in more detail below.

The request can be discussed in terms of three major topics: metallurgy and ceramics, solid state physics, and materials chemistry, the requests for which are shown below.

Materials Sciences
Summary of Operating Expenses

	Budget Authority	
	Estimate FY 1979	Estimate FY 1980
Metallurgy & ceramics	$ 29,665	$ 34,300
Solid state physics	31,685	35,500
Materials chemistry	10,170	11,500
Total, materials sciences	$ 71,520	$ 81,300

Metallurgy and Ceramics

The objective of research under the Metallurgy and Ceramics category is to understand better the relationship between materials properties, structure (including chemical composition) and processing. Understanding the relation between the structure and properties of materials and the method (processing) of arriving at that structure is the key to improving present materials and creating new materials to meet the important needs of all energy systems. The FY 1980 request of $34,300,000 will support a level of activity necessary to take advantage of many of the new opportunities in the field. The request will permit the program to meet commitments related to new facilities, strengthen ongoing programs at universities and initiate some new research when coupled with the selected decreases referred to below. With new facilities such as the high voltage electron microscopes, analytical electron microscopes, pulsed neutron sources and surface analysis equipment, metallurgy and ceramics research will advance more rapidly to understand such properties of materials as fracture, corrosion, weldability, radiation resistance, superconductivity and transport phenomena, all of which depend on structure. The results of this research will ultimately enable the prediction of materials behavior and changes in material properties as a function of time, stress and a variety of environments. As our understanding of the relationships among properties, structure and processing and our ability to create new metal and ceramic structures increase, it will become possible to design materials to meet engineering requirements for emerging energy systems.

Significant progress was made during the past year in areas such as creep (slow deformation of materials), corrosion, fabrication of superconducting materials, hydrogen effects, hydride behavior, radiation effects and mechanical behavior of ceramics. During FY 1980, new metallurgy and ceramics research will emphasize in-situ studies using high voltage electron microscopes, work related to nuclear waste isolation including canister materials and glass and ceramics matrices, solar-related materials research, new activities designing and using pulsed neutron sources, structure and radiation damage studies, analytical and high resolution electron microscopy studies of materials, high temperature ceramics, mechanical properties at elevated temperatures, and corrosion. Research in nondestructive evaluation, welding and processing of materials will be strengthened, while areas such as diffusion, mechanical properties of refractory metals, electronic studies of actinide materials, powder metallurgy and superconductivity will receive decreasing emphases.

Under structure of materials, research is supported to enhance our understanding of the structure of materials at all levels that influence or control materials properties and behavior. The scope of this work includes atomic, electronic and defect structures as well as the morphology of complex materials. Representative accomplishments during the past year include: deposition of amorphous silicon containing atomic hydrogen, which results in a superior quality material for solar energy conversion applications, and the use of transmission electron microscopy to identify asbestos in air samples and to trace their origin to automobile brake drums. The increased availability of several new techniques to investigate the fine structure and microchemistry of bulk materials and surfaces requires special attention.

The FY 1980 request of $8,300,000 for structure of materials will provide for sustaining or expanding current work in such areas as the following: photo-excitation phenomena and technology for solar applications; behavior of refractory materials in hostile environments; sintering studies of complex technological ceramic materials to achieve control over the resulting structure and properties; fundamental atomic level studies on glasses containing heavy metal atoms which relate to material systems for radioactive waste containment; and improved conducting ceramics for magnetohydrodynamics (MHD), high temperature batteries, and other advanced energy technologies. Other areas of work which will be supported include atomic structure studies of hydrides for solar and other energy storage applications; electronic studies of superconductors with high transition temperatures; catalysis and surface studies for solar, fossil, and environmental applications; amorphous semiconductor thin films for solar energy conversion; the structure and deformation of polymers; impurity effects in materials for semiconductor-electrolyte junction cells for solar application; and photovoltaic devices for higher solar conversion efficiency. The request also provides for atomic resolution, high voltage, and analytical electron microscopy studies in solids in a manner which simulates operating conditions and processes of actual energy systems.

Research in mechanical properties is directed toward understanding mechanisms controlling strength and fracture in metals and ceramics, especially quantitative formulations of these properties. While a broad spectrum of research is supported on elastic and plastic behavior, current emphasis is placed on strength and constitutive equations (i.e. equations that relate materials properties to fundamental variables) for creep deformation, fracture toughness and alloy design, defect characterization and correlation with deformation and crack processes, and environmental effects. Substantive progess has been made in this research area. For example, deviation from the expected constitutive behavior of zircalloy-4, which is the fuel cladding in commercial nuclear power reactors, suggested that a type of defect, grain boundary cavitation, was occurring; this result, confirmed by microscopy, assists in explaining premature cladding failures during power ramping of the reactors and offers guidance to future alloy development. In the field of alloy design and fracture, studies of steels showed that brittle grain boundaries from a prior modification controlled fracture at low temperatures; based on this, effective alloy modification and thermomechanical treatments were utilized to inhibit this fracture mode, which may pave the way to future development of nickel-free alloys for liquid natural gas. With respect to environmental effects, careful examination of the fractures of a typical condenser tube brass, which failed by transgranular stress corrosion cracking, was found to show the mechanism by which the fracture occurred (cleavage as opposed to film rupture). Definitive hydrogen embrittlement results were obtained analyzing accelerated void growth along grain boundaries in carbon steels and observing changes in neutron scattering in niobium-hydrogen alloys. In addition to further emphasis in the above-noted areas, increased effort is planned on high temperature ceramics needed for turbines or heat exchangers, on in-situ testing of metal deformation and gas embrittlement using high voltage electron microscopes, and on corrosion-fatigue and sulfide cracking of steels simulating those considered in fossil or geothermal systems. Priority areas for new research include time dependent fracture at elevated temperatures, development of novel methods for measuring the strain at the tip of the crack, and the effect of protective coatings on failure modes and reliability of materials. $7,300,000 is required for mechanical properties research in FY 1980.

The area of physical properties includes research aimed at increasing the understanding of thermal, optical, transport and electrical properties of materials. The effect of various materials processing procedures, such as heat treatment and sintering in special environments, and the effect of external variables like temperature and pressure on such diverse phenomena as corrosion and electrical behavior, for example, are being investigated. Representative examples of advances made recently include: a positron annihilation measurement of the diffusion of sodium in alumina, which is important for battery development; a technique for fabricating refractory oxides of interest for MHD applications to nearly 100% of theoretical density; an identification of the chemical composition of the surface of catalysts vital to their hydrogenation activity; application of the recently developed "Internal Zone Growth" technique to fabricate composite materials that are important for several high temperature applications; and development of a new infiltration process for fabricating niobium-germanium-aluminum superconducting material.

The FY 1980 budget request of $9,000,000 for physical properties will sustain and expand current work in the following areas: basic ceramics studies, including long-term storage of radioactive wastes, mass transport in ceramics for MHD applications, and ion transport in solid electrolytes for high temperature battery applications; positron annihilation research for nondestructive studies of atomic and defect transport in metals; pulsed neutron scattering studies of the elasticity and electronic structure in superconductors; acoustic emission research for monitoring deformation and detecting seismic activity; investigations of heat transfer fluids used to transfer thermal energy from a solar collector to a heat exchanger, and of solar absorptivity of fluids for increased solar conversion efficiency; investigations of the kinetics and mechanisms of surface and solid state reactions for advanced energy technologies and catalytic applications, including solar, fossil, fusion, and energy storage materials systems; and studies of expanded ion implantation and defects in materials including implantation metallurgy, laser and electron beam annealing of ion-implanted materials, and defects in semiconductors and insulators for several advanced energy systems. Work involving sputter deposited surface metallurgy will be discontinued, and there will be a reduced level of effort in one of the fabrication development efforts on superconducting materials.

Radiation effects research focuses on materials phenomena relevant to the fission and fusion energy concepts. It involves application of theory and unique experimental facilities to the topics of radiation-induced nucleation and growth of defects in structural alloys, in superconductors, and in radioactive waste forms, as well as simulation of radiation damage and creep with heavy and light ions and electrons. The capability developed for these studies has also been directed toward hydrogen attack of steels and amorphization of silicon of interest to fossil and solar processes, respectively. There were a number of significant advances made last year in this area of research. Structural and dimensional changes were identified in crystalline oxides and other structures (spinels) exposed to alpha particle bombardment and hence helium gas generation. This is important baseline data if stable radioactive waste materials are to be designed on a scientific rather than empirical basis. Rate theories describing early stages of damage were improved by incorporating the important factors of the generation rate and concentration of point defects and their sites of disappearance. The causes of radiation induced changes in properties of niobium-titanium type II superconductors (used in fusion reactor magnets) were determined. Differential neutron damage cross sections for displaced atoms (interstitials) and damage functions in metals were evaluated, thus providing insight into the nature of radiation damage to be encountered in fission reactor cladding and fusion first wall materials. The controlling mechanisms of hydrogen attack of steels were determined and based on the data, inadequacies were found in the industrially-used methods for predicting safe operating ranges. These accomplishments lay the groundwork for future research.

The FY 1980 request includes $5,900,000 for radiation effects research. Major new efforts will relate to radioactive waste, including a project to evaluate alpha radiation damage in oxide ceramic waste hosts. Increased support for the high voltage electron microscope at ANL will provide for its availability to university and other users, and for its interfacing with an ion accelerator at ANL for in-situ experiments on ion-implantation, corrosion, and radiation effects. Both theoretical and experimental research will continue. Specific problems to be addressed include structural changes in possible nuclear waste forms (complex silicate glasses) and in radiation simulation and creep using light and heavy ion bombardment.

Engineering materials, for which $3,800,000 is required in FY 1980, includes basic research aimed at understanding more fully the fundamental materials science on which engineering systems should be based. It is intended that the efforts undertaken in this area will provide the link to engineering systems by studying the more complex materials and phenomena generally characteristic of actual operating systems. During FY 1978, the first year of funding for engineering materials, research was initiated on welding and nondestructive evaluation. These programs will be strengthened and some new research on corrosion and erosion will be initiated in FY 1979. In FY 1980, new programs emphasizing processing of metals and ceramics will be instituted. Although this program is very young, one interesting result has already occurred. In FY 1978, work performed at Sandia Laboratories resulted in the preparation of erosion resistant titanium diboride films which are now being tested for application in coal conversion plant valves.

Solid State Physics

The FY 1980 request for Solid State Physics is $35,500,000, an increase of $3,815,000 above the FY 1979 level. Solid State Physics is directed towards fundamental research on solids, liquids, and gases wherein the interactions of electrons, atoms, and defects are studied with the purpose of understanding how they influence solids. These interactions coupled with microscopic motions in solids are the ultimate source of material properties. Research in solid state physics includes a broad spectrum of theoretical and experimental efforts which contribute basic solid state knowledge important to all energy technologies. In FY 1980, expanded efforts in new material synthesis will be exploited through recently developed preparation techniques designed to help advance the efficiency and lifetime of energy-related materials. In addition, advanced pulsed neutron instrumentation will be designed to permit new kinds of analyses of solid and liquid materials of importance to energy technologies.

A number of important accomplishments have occurred in solid state physics during the past year. Preparation of amorphous silicon by heating silance at 2300 degrees centigrade with a tungsten source resulted in the production of high quality material for solar energy conversion. It was determined that atomic rather than molecular hydrogen was formed, and was responsible for the deactivation of imperfect bonds of silicon. A diamond point machining instrument was developed which allows the machining of metal surfaces to an exceptionally low roughness, the best reported to date. This development has important implications for laser, solar, and other technologies which require ultra smooth surfaces. Using electron microscopy, an in-situ measurement of crack propagation in stainless steel proved that a slip band precedes the crack, that this band contains an inverse pile-up of defects (screw dislocations), and the crack opening relates to the number of dislocations emitted from the crack tip. These microscopic observations were the first confirmation of existing theory in an important technological material. Fast ion conduction studies in lithium beta alumina by Raman scattering and model calculations revealed that high conductivity results from correlated motions of ion pairs which indirectly move lithium ions into the conducting plane. These results are important for advances in the area of solid electrolytes in energy systems. Two triple-axis superconducting quantum interference devices (SQUID), which are devices able to measure minute changes in the earth's magnetic field, were successfully deployed 4.8 kilometers apart near the San Andreas Fault in California. With this ultra-senstive apparatus, long-term monitoring of the earthquake zone can take place, with the possibility of predicting the onset of earthquakes at times much earlier than actual occurrences. This is an example of spin-off from basic research on SQUID devices.

The major research areas within Solid State Physics are neutron scattering, experimental research, theoretical research, particle-solid interactions, and engineering physics.

Neutron scattering supports research involving the use of the neutron as an analytical probe for the study of materials. The fundamental parameters and structures of superconductors, hydride storage materials, magnetic materials, polymeric substances, and many others are determined in a manner that cannot be accomplished by any other technique. At ANL, the IPNS-I is in the construction stage, and an existing prototype will be utilized to refine detection and analysis techniques for intense beams of intermediate energy (epithermal) neutrons. Additional new pulsed neutron activities will occur at the LASL Weapons Neutron Research (WNR) facility. A new small angle neutron scattering facility at ORNL, which was constructed by the NSF, will be heavily exploited in the study of new polymeric materials. The bulk of the Nation's efforts in this important area of neutron scattering research has historically been supported at Department of Energy laboratories, where the advanced steady-state and pulsed reactors are designed, constructed, and operated. Increasing costs, in part due to the advent of new pulsed systems, and the implementation of the user mode of operation are placing added burdens on this program to maintain efficient utilization of these facilities. The FY 1980 request for neutron scattering research is $10,470,000.

Experimental research is very broad in scope. It includes all fundamental experimental solid state physics investigations on liquids and solids of metals, alloys, semiconductors, insulators, and compounds. New high temperature materials of importance to advanced energy systems will receive increased attention. The studies of hydrogen and hydrides will be pursued through the most advanced spectroscopic, microscopic, and nuclear techniques. Synchrotron x-rays and light will be more prominently utilized in studying catalytic response, as well as in detecting trace impurities of importance to material behavior. Fast-ion conductivity research will enhance the search for new battery concepts with higher temperature and efficiency capabilities. The mobility and trapping of electrons in important solar materials will be pursued to determine optimum characteristics. Increased attention will be given to new classes of amorphous (structureless) materials, which hold promise for important advances in energy technologies where unusual temperature, electronic, and compatibility characteristics are required. The preparation and use of improved lasers for a variety of studies, including vapor deposition diagnostics and unusual coating characteristics, will be accelerated.

Highly advanced theoretical research is closely coupled with nearly all of these experimental areas. A large part of the theoretical effort is directed towards complex, dynamic processes in materials that require extensive use of the most sophisticated Department of Energy computer centers. Included in this research are theoretical predictions of film structures which are only one atom thick; low angle sputtering on fusion first wall surfaces; modeling of crack propagation in materials; and atomic collision cascades in solids. In advanced energy systems, material behavior is not easily predictable, so that a highly correlated experimental and theoretical research effort is important. To support the experimental and theoretical research efforts, $20,050,000 is requested for FY 1980.

Under particle-solid interactions, a major effort is underway which attempts to correlate the complex damage effects produced in solids by particles having various masses, energies and charges. The use of electrons, ions, and neutrons under closely controlled temperature conditions will be pursued. It is clear that correlation experiments are of considerable importance in reducing the need for tests that could extend for years. The area of low angle collision effects on surfaces will be expanded to aid in understanding sputtering processes. Research in this area, for which $2,230,000 is requested in FY 1980, continues to be of substantial importance to fission and fusion energy systems.

Engineering physics research will receive increased attention in several important new areas. Advanced instrumentation centering upon superconducting quantum interference devices (SQUID) will be expanded with new systems aimed at earthquake and geophysical monitoring. The instrumentation will be highly sensitive and transportable, and can be operated with newly developed closed-cycle refrigeration in remote areas. Novel material processing instrumentation will be advanced with increased use of electron beams, plasma sprays, chemical vapor deposition, and rapid cooling phenomena. New forms of nuclear waste materials will be prepared by solid state physics methods, with the goal of extended stability in hostile environments. Research of a different kind involves the extension of refrigeration techniques to new fluid systems which hold promise for the efficient utilization of low grade heat, which is usually lost or wasted as an energy source. Advanced grinding instrumentation will be pursued to allow the preparation of highly perfect flat, spherical and aspherical surfaces of importance to laser, solar, and other technologies. The FY 1980 request includes $2,750,000 for research in engineering physics.

Materials Chemistry

Materials Chemistry provides support for research directed toward developing our understanding of the chemical properties of materials as determined by their composition, structure and environment (pressure, temperature, etc.). This research also attempts to demonstrate how the laws of chemistry may be used to understand physical as well as chemical properties and phenomena. Included, for example, are studies of energy changes accompanying transformations, the influence of varying physical conditions on rates of transformations, and the manner in which the structure of atomic groupings influences both properties and reactivity.

Chemical concepts coupled with physical experimental techniques are used to study the kinetics of reactions of solids and liquids, the interaction and/or penetration of species in adjacent media, chemical corrosion and scaling, and the stability of materials of interest to fossil and geothermal technologies. The program also includes research on the chemical thermodynamics of high temperature materials phenomena. Electrochemical research important to storage batteries, fuel cells, and hydrogen generation is an important aspect of materials chemistry research, as is the study of elastomers and polymers, which will play a vital role in the development of various energy technologies.

A broad interdisciplinary approach to a wide variety of energy problems has yielded relevant contributions based on earlier studies of a fundamental nature. For example, knowledge of the crystal chemistry of sulfur oxide pollutants in the atmosphere has been extended to experimental tests of dolomite as an absorbent for sulfur oxides in coal combustion and gasification systems. Other examples are the use of neutron diffraction data to establish the chemical configuration of new complex compounds, and the use of x-ray diffraction data as a basis for the quantum mechanical analysis of the new organic salts which have unusually high electrical conductivities. The systematic study of surface chemical and physical properties has been applied to the catalytic conversion of hydrocarbon fuels, the interaction of energetic particles with refractory oxide walls and the catalytic processes related to poisonous pollutants in automotive exhausts. Studies of equilibria between tritium in liquid lithium and in low-melting fused salt mixtures have resulted in a procedure for the extraction of tritium from fusion blanket material which will be extended to the investigation of fused salts for solar energy storage.

Other recent accomplishments in materials chemistry can be cited. Studies of catalyst surfaces have shown that the role of adsorbed impurities is important in hydrocarbon reactions. Low oxygen coverage increases hydrogenation activity in platinum catalysts, while complete oxidation destroys catalytic activity. These studies reveal the importance of surface impurities in catalytic response. A new technique for analyzing stack plumes and aerosols has been developed. The technique is based on combining infra-red spectroscopy and inertially impacted particle collection that results in a lower limit detection of sulfates to 0.5 micrograms. Extension of this instrumentation to aircraft monitoring would result in rapid advances in pollution control, and in understanding atmospheric changes. Research on advanced battery electrode phenomena operating at temperatures as high as 450 degrees centigrade has resulted in improving charging-discharging characteristics. Utilizing iron disulfide as electrodes and molten lithium and potassium chlorides as electrolytes, harmful deposits occur which lead to battery failure. By adjusting the composition of the molten salt electrolyte, it has been found possible to prevent the formation of harmful deposits. These results are important to engineering scale-up for long-term battery tests.

The FY 1980 request for Materials Chemistry is $11,500,000, an increase of $1,330,000 above the FY 1979 level. It is planned in FY 1980 to expand significantly portions of materials chemistry research that is performed outside of the Department of Energy laboratories in order to utilize new forefront programs and skills in universities, as well as in private industry and not-for-profit organizations. The areas of research within Materials Chemistry are chemical structure, engineering chemistry, and high temperature and surface chemistry.

Research in <u>chemical structure</u> will be applied to a wide variety of problems where a knowledge of the relationship between the atomic structures of materials and their reactivity is required. An example of this effect is the influence of different chemical environments on the catalytic properties of metals. Changes in both the crystal and magnetic structure of Fischer-Tropsch (coal conversion) catalysts will be correlated with their roles in specific fossil fuel syntheses. The entire spectrum of structural analysis tools will be used to determine the chemical structural requirements of complex transition metal hydride compounds used in selective catalyzing processes important to fossil fuel conversion. Efforts to expand the scientific foundations of metal clusters and metal-cluster hydrides relating to their efforts in energy conversion schemes will be emphasized. The use of epithermal pulsed neutrons will be explored for the structural studies of molecular solids and fused salts. The preparation and structural studies of new polymers and elastomers important to many energy concepts will be expanded. The FY 1980 request includes $3,070,000 for structural chemistry.

Engineering chemistry includes those research activities bearing upon physical-chemical processes of mass transport, gas permeation, materials-related separation and removal schemes, and electrode interfaces. The FY 1980 request includes $3,990,000 for these research activities. An effort will be made to understand the bonding factors responsible for the decrease of solid cohesion (structural stability) of naturally occurring and synthetic compounds (dolomites) used in sulfur-scavenging in the combustion of coal. Studies will be initiated to investigate the structural and morphological changes that arise during the electrochemical incorporation of lithium into aluminum during charge-discharge cycles of high temperature batteries. Thermodynamic studies and kinetic measurements will be made of chemical systems concerned with the preparation of actinide compounds. Equilibria and kinetics of the exchange reactions will be measured to provide a foundation for the determination of the phase relationships in systems important to fuel preparation and waste materials.

In high temperature and surface chemistry, programs will be initiated on fundamental studies of the influence of surface properties on reactivity and for the correlation of mass transport and thermodynamic properties of molten salts in high temperature battery systems. Chemical studies of scale formation in geothermal environments include research for methods of inhibiting and removing the deposition of salts on the inner walls of pipes. The influence of micro-inclusions such as sulfides on the formation of pits and crevices will be examined to determine whether the presence of these inclusions plays a significant role in the initiation of chemical corrosion cracking. Both the theoretical and experimental aspects of new high temperature electrolyte cells will be investigated, and work will continue on the high temperature behavior of nuclear fuel materials. Molecular beam methods will be used for the study of the kinetics and mechanisms of the processes for the preparation of ultrapure silicon. The request for this area of research is $4,440,000 in FY 1980.

Capital Equipment

The FY 1980 capital equipment request for Materials Sciences is $6,500,000, an increase of $600,000 above the FY 1979 level. Materials sciences is continuing to direct its new research thrusts into areas relevant to the Department of Energy technologies and necessary for forefront research. Much of this research is by nature very equipment intensive. The equipment request takes into account major programmatic directions which provide insights into materials behavior and structural stability to increase the options for energy processes using conservation or solar, geothermal, fossil, fission, and fusion resources. Initiatives deemed particularly important are, among others: non-destructive evaluation, so that flaws can be found while subcritical to the size where catastrophic failure occurs, and corrosion, where surface spectroscopic analyses coupled with direct observation in environmental cells in advanced high voltage electron microscopes offer the potential for design of stable alloys or coatings.

Equipment is needed for research in a number of energy-related materials activities. The analysis of alloy surfaces and surface modification for advanced solar photovoltaics and fossil catalysts requires ion-implantation, electron scattering and diffraction equipment, as well as ion microprobes. The engineering materials and physics research areas of welding, nondestructive evaluation and deep underground surveying require power supplies, sophisticated photographic and thermographic instrumentation, superconducting devices, and various signal monitors. In-situ observation of corrosion and radiation damage requires linking up an ion beam accelerator and high voltage electron microscope at ANL. Equipment is needed for structural evaluation of complex materials, such as hydrides, for energy storage and oxide ceramics for MHD. Superconducting magnets and spectrometers are needed for exploiting the unique research reactor capabilities. Upgraded metallographic analyses related to several energy areas, particularly fusion and fission, require the purchase of a scanning transmission electron microscope for PNL.

Another area in Materials Sciences requiring advanced equipment is the forefront area of microscopic and quantitative microchemical analyses of surfaces and bulk structures. Examples of equipment needed for this research include low energy electron diffraction apparatus, scanning ion and Auger electron instruments, and combined scanning/transmission electron microscopes.

Two facility developments in Materials Sciences which will provide important new research capabilities will require equipment in FY 1980. These include the National Synchrotron Light Source at BNL (discussed below), and pulsed neutron source work at LASL and ANL, which will make use of a unique tool for evaluating critical steps in materials reactions or transport.

In addition to the above, high priority will be given to replacing small conventional items such as furnaces, vacuum pumps and x-ray power tubes, for which replacement is imperative to avoid unscheduled outages caused by malfunctioning antiquated equipment.

Construction

The FY 1980 construction request for Materials Sciences is $11,650,000. Of that amount, $9,000,000 is required in order to complete construction of the National Synchrotron Light Source at BNL in FY 1981 ($5,000,000 and $10,000,000 were provided in FY 1978 and FY 1979, respectively, for this $24,000,000 project). The $9,000,000 requested for this project in FY 1980 will be utilized for completion of construction of the housing, the storage rings, and associated laboratories and service buildings. In addition, it will permit the instrumentation of a small number of experimental beam lines. The stage of completion of the vacuum ultraviolet (VUV) ring complex will allow some experiments to be performed in FY 1980. Any reduction in the requested amount will adversely affect the procurement, construction and experimentation schedule.

The FY 1980 construction request also includes $2,400,000 for Expanded Experimental Capabilities for the Intense Pulsed Neutron Source-I (IPNS-I) at ANL. This project will permit expanded user facilities at this new pulsed neutron source. A large number of universities throughout the country have expressed interest in conducting experiments using pulsed neutrons to study the fundamental properties of materials. The FY 1980 funds will be utilized to double the number of research stations for neutron scattering at IPNS-I from five to ten and to double the capability at the radiation damage facility. It is essential that this construction be concurrent with the design and construction of the IPNS-I project in order to avoid retrofitting at a later date, which would entail much higher costs.

The remaining $250,000 in the construction request is for General Plant Projects for Ames Laboratory ($230,000) and the Notre Dame Radiation Laboratory ($20,000). These funds will permit minor additions and modifications to these facilities which will assist in maintaining them as safe and effective laboratories for the conduct of research and development.

Although its funding is requested in the Chemical Sciences portion of Basic Energy Science (and therefore discussed in more detail below under that portion of the budget), the $12,600,000 Chemical and Materials Sciences Laboratory at LBL will incorporate special structural features (e.g. vibration isolation) required to house an atomic resolution electron microscope (AREM) and its ancillary equipment. The microscope will be the first of its kind in the United States and will permit previously impossible materials sciences research involving the study of critical processes such as corrosion, grain boundary attack, and catalysis at the atomic level. This unique facility will be available for use by qualified researchers in the chemical and biological (environmental) sciences as well as the materials sciences.

Chemical sciences ....$ 54,800 $ 69,400

All kinds of energy systems, old and new, depend on chemical changes which, in many cases, are not well enough understood to be used to best advantage. The chemical details of different coals are not yet well enough known to guide the developers of liquefaction to the most economic and least hazardous processes. The chemical fundamentals of natural and artificial means of converting the energy of sunlight to useful and/or storable energy are only partly understood. Even combustion, on which we depend for most of our electricity, transportation, and heating, proceeds by chemical and physical sequences which we only partly comprehend, not well enough to achieve full advantage, economy and cleanliness from use of fuels. Chemical processes are the only means of recovering highly valuable metals from spent nuclear fuels, and of putting radioactive wastes into long-lasting forms for isolation; advanced knowledge of separative chemistry pertinent to these processes should enhance the choices and the public acceptability which are important to nuclear energy. The success of fusion energy will depend in part on still-to-come understanding of plasmas, extremely hot collections of positively charged ions and negatively charged electrons, and the interactions among those ions and impurity ions and atoms. Concerns about environmental effects of effluents from energy processes will be allayed or confirmed only by extending our basic understanding of the kinds of chemistry caused by and experienced by the effluent molecules, principally in the atmosphere.

The foregoing statements form one basis for the Chemical Sciences program. That is to provide the chemical and physical knowledge and understanding which will help to improve the economics, capabilities and cleanliness of energy processes. The other basis is to improve the state of the art and exploit new advanced techniques of chemistry and physics in order to raise the probability that new energy-process concepts will be discovered or invented. With respect to both of these bases, inadequately explored areas and gaps exist which must be addressed if we are not to lose further time in laying the scientific groundwork for future changes in energy processes which will inevitably become necessary.

To address these concerns, $69,400,000 is requested for Chemical Sciences in FY 1980. Of that amount, $58,800,000 is for operating funds; $4,300,000 is for capital equipment; and $6,300,000 is for construction.

Operating Expenses

The FY 1980 request of $58,800,000 for operating expenses for Chemical Sciences represents an increase of $10,800,000 above the FY 1979 level. In FY 1980, additional emphases will be placed on research critical to the solar and fossil technologies, to combustion processes, and to long-term nuclear waste isolation. A special effort will be made to increase further the involvement of university researchers in this important work.

The operating request for Chemical Sciences can be discussed in terms of two major activities: Fundamental Interactions and Processes and Techniques. The following table includes the estimates for these activities:

Chemical Sciences
Summary of Operating Expenses

	FY 1979 Estimated Budget Authority	FY 1980 Estimate Budget Authority
Fundamental interactions	$ 28,195	$ 33,625
Processes and techniques	19,805	25,175
Total, chemical sciences	$ 48,000	$ 58,800

Fundamental interactions

The Fundamental Interactions activity supports basic research concerning interactions of atoms, molecules, and ions (electrically charged atoms or molecules) with each other and with radiation. It involves the forces among these species which control the chemical bonding structure of a molecule or ion and its reactions, and the mechanisms by which they absorb energy, redistribute it (internally in a molecule, for example) and subsequently undergo chemical reaction. These data are important for our understanding of fuel combustion, solar photochemistry (including photosynthesis), nuclear fusion, magnetohydrodynamics (MHD) and other energy processes. In scientific terms, research in this task encompasses photochemical and radiation sciences, chemical physics and atomic physics. An increasingly important fraction of research in these areas is being carried on by university contractors.

The following recent accomplishments illustrate the kinds of impact scientific research in this activity can have on the energy technologies: The first (mentioned briefly in the Program Overview for Basic Research) involves a major new technique which has been devised for obtaining a highly important type of analytical data needed by large-scale users of coal. It is necessary for many such users to know the oxygen content of each coal batch, since that tells much about the available energy content. Previously, oxygen content had to be determined by difference, that is, by analyzing for contents of carbon, hydrogen, nitrogen, sulfur and minerals, and then subtracting these from the total weight and assuming the difference was oxygen. That was time consuming and grossly inaccurate. A Brookhaven chemist known for expertise in nuclear-initiated reactions has now shown how to obtain oxygen analyses of coal or other materials in an automated, fast (hundred of samples a day) and accurate manner. It can be done using any of numerous cyclotrons around the United States. It takes advantage of the fact that nuclei of helium atoms, accelerated to 10 million volts in the cyclotron, will convert oxygen atoms to a radioactive form of the chemical element fluorine, which soon releases gamma rays. The count of these rays measures the number of fluorine atoms and thus the original number of oxygen atoms.

The possibility exists of finding electrode-chemical combinations which would make electrochemical cells for converting the energy of sunlight into electricity and/or fuels, with sets of advantages and disadvantages different from those of dry photovoltaic converters. One obstacle to this development is the fact that silicon semiconductor electrodes are rapidly deactivated by layers of oxide which form on their surfaces when they are placed in water or other liquids of interest. A researcher at the Massachusetts Institute of Technology has succeeded doubly in one stroke: he has bonded a light-sensitive chemical to the silicon surface, which both protects the silicon from formation of oxide layers and enhances its light absorption. This has long-range promise for photoelectrochemical solar conversions.

Researchers at Sandia Laboratories in Livermore, California have used a laser technique on a tiny region in a flame to determine its temperature by inducing and measuring fluorescence of the highly reactive, short-lived chemical species in the flame called the hydroxyl radical. An excellent temperature measurement, it is the first based on any radical species. It is expected to be a strong tool in continuing research designed to better understand combustion in order to help attain greater fuel economies and reduce pollution.

The FY 1980 request for Fundamental Interactions is $33,625,000, an increase of $5,430,000 above the FY 1979 level. The request can best be discussed in terms of four major areas of research which are discussed below.

Approximately $6,525,000 of the requested funds is for solar photoconversion research, particularly at universities. Many different approaches can be taken to the conversion and storage of solar energy by photochemical means. They include photogalvanic reactions for producing electricity, photocatalytic reactions for decomposing water to give hydrogen, photocatalytic reactions to produce other fuels and valuable chemicals, and photochemical rearrangement reactions capable of storing and releasing heat. A promising approach involves "artificial photosynthesis", the mimicking of natural photosynthetic processes by collecting light in a manner which may ultimately allow production of hydrogen or electricity. All of these techniques are in the research stage.

Another major portion of the request ($4,900,000), will be devoted to combustion research. Of this amount, $2,100,000 will permit the necessary research and development to allow the Combustion Research Facility at Sandia Laboratory-Livermore, California, to open its doors in FY 1980 with a reasonable capability for serving users and in-house staff. These funds will be used for such necessary activities as the devising of needed new combustion diagnostic instruments, the preparation of standard systems for calibration of diagnostic tools, and the installation and testing of special equipment. The other $2,800,000 for combustion research will serve to continue to expand combustion research activities primarily at universities, including expanded work on combustion modeling. Modeling, intelligently coupled to experimental research, provides a powerful tool to aid the combustion scientist to understand the details of complex combustion processes.

A third major area within Fundamental Interactions is comprised of the long-term, very basic research underlying virtually all energy technologies. $16,500,000 is requested in FY 1980 for this type of research. Much of the money will be expended at universities in the fields of chemical and atomic physics and photochemisty. An important development in photochemistry and chemical physics will be the National Synchrotron Light Source, scheduled for completion in FY 1981. Construction of this facility is being funded under Materials Sciences, as discussed above. A large number of chemistry experiments are currently being planned for the facility, using both the x-ray source and the vacuum ultraviolet source. The x-ray source will provide the structural chemist with greatly improved capability for structural studies presently limited to conventional x-ray sources. Of special importance here will be the ability to study short-lived molecular and reactive species that cannot now be studied by conventional techniques. The ultraviolet source will provide new capability for studying molecules in the gas phase, the importance of which is twofold in a scientific sense. First, molecular reactions in the gas phase play important roles in combustion and many types of air pollution. Second, in the gas phase the molecule can be studied in its "true" state, unperturbed by anything other than collisions with its neighbor molecules, so that baseline knowledge of its characteristics can be obtained. About $500,000 of the request for long-term basic research will be used in preparing for use of the Light Source, to design and build the complex instrumentation needed for these chemistry experiments.

Other facets of the longer-range portion of fundamental interactions research to be expanded are chemical dynamics, emphasizing the study of the rates of elementary chemical reactions needed in modeling such complex phenomena as combustion, and theoretical chemistry, which provides the framework for the most basic understanding of almost all chemical problems. Similarly in spectroscopy, emphasis will continue on projects aimed at obtaining information about complex, energetically favorable processes. This information is used to identify and measure the amounts of important chemical species, many of which have extremely short lifetimes. In atomic physics, increased emphasis will be placed on atomic and ion structures, energy levels, excited state lifetimes, and energy transfer processes. Recent emphases in this area have involved studies of species with very high energy content, such as ions completely or almost completely stripped of electrons, and molecular ions so energetic that they undergo complete breakup. Other atomic and ionic systems are under investigation as potential laser sources in new regions of the electromagnetic spectrum. These studies take into account the influence of magnetic and electric fields on these systems, especially those unusual fields created by intense laser radiation.

Of the remaining $5,700,000 included in the request for Fundamental Interactions, about $2,300,000 will be devoted to fusion related research, largely in atomic physics. This research is centered around highly charged atomic ions - how they are formed, how they interact, how they are destroyed and the energy transfer involved in these processes. Large ions of this type are a potentially serious means by which the energy in a fusion plasma can be degraded and lost. Understanding of these processes is vital to the fusion program. The other $3,400,000 will be devoted to maintaining ongoing programs of research in chemical physics, which can be expected to help advance the understanding and opportunities for fossil conversions; studies related to isotopes and the nuclear fuel cycle; atmospheric chemistry; pollutants and the chemistry of various conservation techniques.

Processes and Techniques

The objective of the research sponsored under this activity is to promote the understanding of the basic chemical and physical processes which is fundamental to generating ideas for current and future energy technologies. New ideas are needed to ensure future energy process concepts for consideration. These research activities address the scientific problems which are barriers to such advances and, accordingly, increase the probability for providing creative solutions. The identification and development of new chemical process concepts are also important objectives served by this activity. A few of the major achievements of this work during the past year, briefly described below, illustrate the kinds of research which are supported under the Processes and Techniques activity.

The conversion of coal-derived carbon monoxide and hydrogen to liquid and gaseous hydrocarbon fuels is a well-known commercial process called the Fischer-Tropsch process. How to control this reaction to give the most desirable products is poorly understood. The conversion is accomplished by use of heterogeneous catalysts (metal particles on oxide pellets of high surface area) which cause the conversion to take place very rapidly and produce a wide variety of hydrocarbon fuel types from methane up to gasoline fraction molecules. Recently, a researcher at LBL has learned how the catalyst works to give specifically desired hydrocarbon types. In particular, he found that the size of the product hydrocarbon molecules could be controlled by the addition of very small quantities of ethylene and propylene (specific two- and three-carbon hydrocarbon molecules). This led to the realization that the catalytic process consists of a sequence of adsorption-reaction-desorption steps not known before. This advance in our understanding provides a key to catalytic reactor design and operation for obtaining more economically desirable products from carbon monoxide-hydrogen reaction.

Another catalysis scientist at Argonne has found a simple homogeneous (solution) catalyst which converts carbon monoxide and hydrogen directly to alcohols at considerably lower temperatures than is required for the known heterogeneously catalyzed reaction. This is interesting from purely a scientific point of view because it was previously believed not to be possible with the simple (one metal atom) catalysts. It is also important, however, for its potential to assist in the production of specific synthetic fuels from carbon monoxide and hydrogen.

Analytical chemists at Oak Ridge have solved a serious problem which has been plaguing experimenters in the simulation of extreme-condition rupture of nuclear fuel elements. Thermocouples, which measure high temperature by electrical means, were yielding very erratic results. The researchers found, by means of an Oak Ridge-developed technique (an ion micropobe mass analyzer), the surprising result that the thermocouple failure was caused by alloy formation of the thermocouple material at temperatures above 1100°C. The thermocouple metals, at these temperatures, were found to extract aluminum and magnesium from the electrical insulation made of aluminum oxide and magnesium oxide. This changed the composition and therefore the temperature-indicating electrical signal of the thermocouple metals. This knowledge led to corrective measures which resolved the problem.

The FY 1980 request for Processes and Techniques is for $25,175,000, an increase of $5,370,000 over the FY 1979 level. The increase will be used to maintain the current high priority efforts and to strengthen new efforts in organic chemistry and catalysis, which are important to new and advanced concepts in fossil energy, and nuclear waste separations research which is important to the concept of nuclear waste isolation. Processes and Techniques consists of four areas of research, namely chemical energy, separations, analysis, and chemical engineering sciences.

The request for chemical energy is $13,100,000. This research includes fundamental chemistry and process studies covering a broad spectrum of chemical disciplines, including organic, inorganic and physical chemistry, which focus particularly on chemical reaction process mechanisms and catalysis. Under chemical energy, studies of the chemistry of fossil resources will be conducted. Included here, for example, is work on the basic organic chemistry of coal constituents, their characterization and stability in reactive and atmospheric environments, the mechanisms of hydrogenation and dehydrogenation reactions and the chemistry of oxygen, nitrogen and sulfur atoms bonded in hydrocarbon systems. Thermochemistry and related correlations of thermodynamic data of importance to the fossil energy and other Department of Energy technology programs are also included. Catalysis research (homogeneous and heterogeneous) will also be carried out, including work to bridge our understanding of the relationship between those two separate, but very much related, fields of science. In addition, new efforts will be made to understand the effect of the particles which support the catalyst on the catalyst's ability to speed one reaction more than another, and the role of mixed clusters on the reactivity and selectivity of dissolved catalytic systems. Important research will also be supported to improve our understanding of the chemistry of converting cellulosic wastes to fuels and related enzyme catalytic processes. The chemistry of hydrogen production and storage will emphasize new thermochemical hydrogen cycles and understanding the limitations to combining hydrogen with metals for storage.

The FY 1980 request for separations research is $6,375,000. In the chemistry of separations research, new concepts are studied to evaluate the chemical and physical complexities of the separation mechanisms and to synthesize and study new chemical separating agents. The FY 1980 request is required to permit a

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The FY 1980 request for the analysis portion of Processes and Techniques is $4,390,000. Analysis includes research basic to the enhanced understanding of chemical and physical techniques for analyzing substances important in energy processes. This research is closely connected to separations research. The development of analytical techniques often involves specialized separations to effect the removal of interfering impurities; it provides pure species for standards; or it makes quantitative analytical results more readily available. Likewise, new separation processes can and do arise from solutions to particular analytical problems, and analytical needs are frequently identified in separations research. The FY 1980 request for analysis will permit continuation of research to increase the sensitivity and precision of the quantitative detection of trace substances in various host materials. This activity includes the development of the analytical techniques necessary for the identification of trace pollutants. The analysis effort focuses on the problem areas which continually crop up in analytical systems and devices and obtains basic information which can be applied by others toward improving their own analytical capabilities. Research is also directed to developing entirely new concepts for such difficult analytical problems as the quantitative analysis of coal liquids.

The FY 1980 request for chemical engineering sciences is $1,310,000. In chemical engineering sciences, the scientific base of such phenomena as fluid dynamics (especially turbulence), gas-solid reactions, and solid phase catalysis of liquid or gaseous fuel-forming substances are studied to develop the chemical and mathematical relationships for more accurate process engineering. Engineering problems related to the Department of Energy technological efforts often are based on empiricism or trial-and-error. Research in chemical engineering sciences accordingly works to strengthen the scientific base of the engineering discipline, and thus facilitates reliable scale up and minimizes costly overdesign. The amount requested is necessary to address such difficult problems as gas-solid reaction modeling, which takes into account the transport of mass, heat and momentum, and development of thermodynamic models for establishing the properties of complex chemical substances including multicomponent mixtures. Emphasis will be given to improving and/or developing the scientific basis for engineering generalizations, unifying theories and innovative processes. Such efforts are expected to advance work in fluid mechanics, particle dynamics, mass and energy transport, engineering thermodynamics and the study of processes governed by physical and chemical rates of change. The ongoing research will be maintained on models for gas phase reactions in fluidized beds (solid particles caused to behave collectively like liquids by a stream of gas) of importance to the scale-up of conversion units for synthetic fuel.

Capital Equipment

The FY 1980 request for capital equipment for chemical sciences is $4,300,000, an increase of $900,000 above the FY 1979 level. The development of understanding of energy conversion processes often involves study of chemical reactions taking place on very short time scales (10^{-14} seconds) and involving species present in infinitesimal concentration whose lifetimes are equally short. The results of these reactions are important but very difficult to detect. These chemical and physical studies are just becoming possible because of recent developments in instrumentation which make it possible to detect events taking place on these time scales, to measure the times themselves, and to analyze the results of these interactions. Specialized small computers are needed in some cases just to conduct the chemical sciences experiments. Old, conventional equipment is just not capable of producing these needed results. Much of the proposed new research requires new types of lasers, spectrometers, minicomputers and other equipment not previously available. Of the total FY 1980 request for equipment, $3,185,000 is for the above-described kinds of need. An additional $665,000 is for advanced combustion research, and $350,000 is for equipment necessary to prepare for chemistry experiments at the National Synchrotron Light Source.

In addition, $100,000 is requested for general purpose equipment requirements at Ames Laboratory. This multipurpose equipment, which is essential to the proper, day-to-day operations at the laboratories, cannot be identified specifically with any one Department of Energy program. Included are the needs of the laboratories' service and support divisions, as well as equipment required to respond to health, safety, security and environmental considerations. It is important that obsolete and worn-out equipment be replaced in order to promote efficient laboratory operations, to increase productivity and to avoid high maintenance costs. FY 1980 general purpose equipment needs at Ames Laboratory include an x-ray fluorescence, programmable power supply, a disk drive for x-ray data analysis, a radiation counter, special fume hoods for toxic materials, a fork lift truck, and a front end loader.

Construction

The request for construction funding for Chemical Sciences is $6,300,000. The entire amount of the request is for initiating construction of the Chemical and Materials Sciences Laboratory at LBL. The project involves construction of an addition to an existing building at Berkeley which would provide approximately 50,000 square feet of laboratory and office space for chemical and materials research. In addition to providing for an expansion of research capabilities, the project will permit the integration of the ongoing programs which are presently conducted in overcrowded and widely dispersed quarters located throughout both LBL and the University of California-Berkeley campus, thus permitting major improvements in the efficiency and effectiveness of LBL research programs. The laboratory building would house an atomic resolution microscope and other ancillary equipment necessary to better understand the behavior of energy-related materials such as catalysts, coatings and thin film solar devices at the most fundamental (the atomic) level. This understanding will assist in the design and development of new and improved materials for energy systems. Areas of Chemical Sciences which will benefit from the project include photoelectron spectroscopy, coal conversion studies and photo-assisted surface reactions. The total estimated cost of constructing this facility is $12,600,000. The $6,300,000 required in FY 1980 will allow architect-engineering services to be conducted, the procurement of the atomic resolution microscope and related equipment and initial construction activities.

Engineering, Mathematics and Geosciences	$ 16,500	$ 25,350

The three disciplines which are grouped together under this activity bear directly on virtually every current or future energy technology, and research in these areas, therefore, is critical to the Department of Energy's mission. Two of these, applied mathematical sciences and geosciences, are well-established programs which need to be expanded to more effective levels. The third, basic research in engineering, is a long-neglected field of research for which a program has just been initiated in FY 1979.

The FY 1980 request for Engineering, Mathematics and Geosciences is $25,350,000 an increase of $8,850,000 above the FY 1979 level. While the amount of the increase is large relative to the FY 1979 base, the total amount requested in FY 1980 is small in view of the potential major contributions which this research holds in store for efficient and effective energy systems.

Operating Expenses

The FY 1980 request for operating expenses for Engineering, Mathematics and Geosciences is $23,900,000, compared to the FY 1979 level of $15,700,000. The distribution of the FY 1980 request among the three disciplines included in this activity is indicated in the following table:

Engineering, Mathematics and Geosciences
Summary of Operating Expenses

	FY 1979 Estimated Budget Authority	FY 1980 Estimated Budget Authority
Basic research in engineering	$ 1,000	$ 2,000
Applied mathematical sciences	8,600	11,100
Geosciences	6,100	10,800
Total, engineering, mathematics and geosciences	$15,700	$23,900

Basic Research in Engineering

Work under this heading was initiated in FY 1979 because of the recognition that many areas of engineering which are important to the success of many energy technologies lacked fundamental data and understanding upon which long-range advancements in energy processes and systems could be based.

As the program has been taking shape, efforts have been made to assure that important gaps in engineering knowledge bearing on energy would not be overlooked. A workshop was held which brought together experts drawn equally from university, government and industrial laboratories to review this field in the framework of the Department of Energy's responsibilities and programs. The workshop identified several areas which need to be emphasized because of their importance to energy technology developments. These areas include: (1) process and systems dynamics and control, including improved analytical techniques, computerized modeling of complex processes, and optimization techniques for minimum energy consumption; (2) fluid dynamics and thermal processes, including analysis of multiple phase flow, turbulent flow and flow-induced vibrations, understanding of heat transfer through and between various liquids, and processes for magnetic,centrifugal and filtrational separation of solids from liquids; (3) advanced industrial technology, including precision engineering to increase product life and minimize energy use, the basics of friction and lubrication to increase component lives and minimize energy use, and improvement of fabrication and production techniques to reduce energy use; (4) electric power technology, including solid state switches for high currents, basic processes involved in electrical insulation failure, improved instrumentation for monitoring critical points in electrical systems, and superconducting storage and transmission; (5) mechanics of solids, including structural design methodology for weldments, and mechanisms of failure of structures under dynamic loading; (6) geotechnical engineering, including development of better methods for determining stresses in shallow or deep earth locations, improvement in the ability to map fractures and faults at depths, increasing the effectiveness of drilling and excavation systems, understanding the basic mechanisms of rock movement in subsidence above underground mining and extraction of fluids; and (7) reliability and risk analyses including failure probability analysis and improved fault tree analysis.

All have the objectives, with different mixes of emphasis, of raising energy efficiencies, opening new technological possibilities, and improving reliabilities of energy systems.

The $1,000,000 appropriated in FY 1979 represents a very small start in addressing these needs. In particular, work was begun on heat pipe engineering, combustion engineering, nondestructive evaluation of flaws, and automated process dynamics and computerized control. In FY 1980, $2,000,000 in operating funds are requested for Basic Research in Engineering in order to continue the initial efforts started in FY 1979 and to enter a selected few new areas of great importance. These new efforts are to be selected with attention paid to the principal recommendations of the scoping workshop which has been held and to the results of followup workshops which are planned.

Applied Mathematical Sciences

The analysis of energy systems performance or energy supply-demand typically starts with the formulation of a conceptual model. Mathematics provides the language for expressing relations among concepts as equations among variables and parameters. Mathematics also provides the tools for obtaining general, qualitative understanding of the phenomenon under study. However, the phenomena of primary interest to Department of Energy mission programs are so complex that mathematical analysis alone is inadequate to obtain detailed quantitative understanding. Therefore, the mathematical models are transformed into computational models executed on digital computers to simulate the phenomenon's behavior. Typically, these models either require large quantities of data as input or yield large quantities of data as output. Moreover, larger quantities of data must often be assimilated to estimate parameters in these models. Statistics provides the tools for assimilating this data, while computer science provides the methodology for managing these collections of information. More generally, computer science contributes to understanding the process of organizing computer systems and developing the required computer programs not only to solve the computational models but also to display the required information in comprehensible forms.

Applied Mathematical Sciences provides the Department of Energy's central means for the continued systematic advancement of the mathematical, statistical and computer sciences in the ways needed for analyzing performance of present, developing and potentially new energy systems, as well as forecasting energy supply-demand relationships. Moreover, it is the only long-term research activity contributing to greater sharing and improved efficiency in the use of the Department of Energy's computer resources (approximately 2,400 computer systems with a purchase value exceeding $640,000,000).

One of the recent achievements, an automatic method of generating computer programs that fit specific needs with assured correctness, is an example of this program's important impact in the Department of Energy. This method, called TAMPR (Transformation Assisted Multiple Program Realization), was developed at ANL as a result of research to ascertain ways of reliably and automatically modifying computer programs, and, in particular, to transport programs from one computer to another.

In 1979, a planning effort has been initiated to develop a program in data management consistent with the Department of Energy's increasing use of information systems for energy, environmental, scientific, engineering and management concerns. A planning effort, together with specific projects, has been initiated to develop a program in high-performance computer systems. Many Department of Energy mission programs are dependent upon high-performance computer systems to accomplish their programmatic goals. Current Department of Energy research on issues relevant to the successful utilization of current and future generations of supercomputers is funded at a level which is miniscule when compared with the Department of Energy's capital investment in this class of computers and their annual operating costs.

The FY 1980 request for operating funds for Applied Mathematical Sciences is $11,100,000, an increase of $2,500,000 above the FY 1979 level. The specific categories of research for which this funding is needed are described in the following paragraphs.

Of the requested level, $975,000 is for projects in applied analysis, which address mathematical questions basic to the formulation and qualitative analysis of mathematical models, together with the analysis of the transition from mathematical models to computational models. These investigations of the mathematical analysis techniques are the foundation for the computer simulation of energy systems.

$1,755,000 is requested for computational mathematics. Computational mathematics emphasizes the synthesis and analysis of broadly applicable numerical methods and their implementation in quality software. These projects develop methods and software for numerical linear algebra, optimization, approximation, and differential equations. For example, numerical linear algebra projects focus upon the development of methods to solve systems of linear equations with several thousand variables. Potential applications range from computing economic equilibria in energy supply-demand models to assessing the structural integrity of nuclear reactor components. Although several laboratories and universities participate concurrently in this work, the following primary responsibilities have been established: numerical linear algebra (ORNL), optimization (ANL), differential equations (LLL and Sandia Laboratory-Albuquerque), and approximation (Sandia Laboratory-Livermore).

The request for data and systems analysis is $1,280,000. This supports statistical and operations research basic to the evaluation of data and models. A project on exploratory analysis of very large data collections will be expanded at PNL, while a joint project on evaluation of computational models will be initiated among BNL, LASL, and ORNL. These activities are closely coordinated with related shorter-term ventures in other parts of the Department of Energy, for example, the Energy Information Administration's (EIA's) Office of Information Validation.

$880,000 is required for software engineering. This program emphasizes techniques for the reliable synthesis of complex applications software from quality modules (for example, the output of the computational mathematics work described above), together with tools to increase the effectiveness of software implementers and users. This program builds upon the more theoretical studies supported by the NSF's mathematical and computer sciences program and, therefore,is closely coordinated with their software engineering program. In FY 1980, an increase will be committed to exploring the feasibility of a systemized collection of software tools, TOOLPACK, for the development of a mathematical software, an effort coordinated by ANL.

$710,000 is needed for data management projects, an area which was initiated in FY 1979. This initial effort is concentrated in areas of particular importance to the Department of Energy: the efficient storage and retrieval of very large data bases; the introduction of user interfaces for the individual who is not a computer specialist; and the integration of multiple data bases from diverse sources into a coherent system. This program, which will evolve into joint university-laboratory ventures, is primarily coordinated by LBL.

$1,040,000 is requested for work involving distributed systems. Based upon experience gained with previous experimental use of the ARPANET, an inter-site computer network, the program in distributed systems now focuses upon impediments in the use of distributed systems in the Department of Energy. Examples include research basic to the specification of network systems architecture, distributed applications structure, and user interface methodology, all aimed at greater resource sharing. This program, which involves participation by several laboratories and universities, is coordinated by LBL and LLL.

The request provides $1,175,000 for high performance systems, another program initiated in FY 1979. Various Department of Energy mission programs find the acquisition of the latest high performance computer systems necessary for the simulation of phenomena whose understanding is critical to their programmatic objectives. This new venture starts with two primary activities: the analysis of selected large-scale computational models from major Department of Energy mission programs to determine common structural characteristics and the evaluation of current and possible future designs of high performance numerical processors. Based upon these studies, matches between problem structures and computer structures will be identified and, therefore, will provide Department of Energy mission programs with guidance on optimal computer designs for their problems. Emphasis will be placed upon understanding how to determine and exploit the presence of parallelism in computations and computer structures. The initial planning for this program is the joint responsibility of LLL and LASL.

The previous activities are intrinsically multi-technology from an application perspective. Moreover, they build upon foundations which are sufficiently well understood or focus upon problems sufficiently well-defined that they can be pursued by research groups operating relatively independently from development or applications groups. Continuing communications among these groups are required. The following activities, which are also multi-technology from an applications perspective, require closer coordination with more applied groups. Moreover, because of the magnitude of the problem, they require joint funding with Applied Mathematical Sciences contributing a share directed toward the longer-term problems, while the Department of Energy technology program supports shorter-term objectives within the same team of researchers.

The FY 1980 request for work in computational modeling is $2,400,000. This activity investigates, jointly with other Department of Energy programs, innovative approaches to the formulation and solution of large-scale computational models. It examines methods best developed in the context of a specific model, but applicable to a broad class of models. Activities include projects in computational fluid dynamics, computational physics and chemistry, and econometric modeling. An example of how this task supports other Department of Energy programs can be found in the computer simulation of the combustion of fossil fuels. The Chemical Sciences activity discussed previously supports the modeling of fundamental flames to obtain better understanding of the interaction between chemical reaction processes and fluid flows. The fossil energy program supports the modeling of combustion engines to better understand impediments to reduced consumption and pollution. These programs support the development of computational models specific to their needs. Applied Mathematical Sciences does not support the development of combustion models, but rather supports the development of computational methods to be incorporated in these models. Innovative methods which show promise of major improvements in the reliability of the predictions of a model or of applicability to previously intractable problems are emphasized. Typically, these are unproven methods and, therefore, they represent high risk ventures. Support by Applied Mathematical Sciences of mathematicians collaborating with modelers and experimenters supported by other Department of Energy programs provides an opportunity to refine and test these methods on problems of continuing interest to the Department.

$590,000 is included in the request for information systems. Like computational modeling, this work consists of joint ventures with Department of Energy mission programs to develop and use information systems to manage very large collections of data. Initially, geographic information systems will be emphasized. Candidates for interaction include various EIA activities basic to the National Energy Information System or the Energy Emergency Management Information System. Another prime candidate is the Domestic Information Display System Project, an interagency venture organized by the Executive Office of the President. Each of these offers opportunities to explore innovative solutions to fundamental limitations in data management, communications, computer graphics, statistical analysis and user interfaces in the context of operational information systems.

The remaining $295,000 of the FY 1980 request is for support of special projects primarily related to the transfer of research results developed in computational mathematics and software engineering to the Department of energy computer user community. For example, "software clinics" are proposed at ANL, LASL and New York University's Courant Institute of Mathematical Sciences. These software clinics will augment the activities of traditional "user services groups" to exploit oportunities to utilize existing mathematical software libraries and automated programming aids.

Geosciences

The need for geosciences research is implicit in the fact that all energy resources are found in the earth and the sun and all waste products are returned to the earth and its atmosphere. The purpose of geosciences research is to develop an adequate information base and a sound understanding of the earth's crust and earth processes in research areas relevant to energy resources and the disposition and/or isolation of wastes. Included are studies in geology, geophysics and earth dynamics; geochemistry; energy resource recognition, evaluation and utilization; hydrologic and marine sciences; and solar-terrestrial-atmospheric interactions. The work is carried out primarily in Department of Energy laboratories and in universities, although some is conducted by other Federal agencies and by the National Academy of Sciences.

The FY 1980 request for operating expenses for Geosciences is $10,800,000, an increase of $4,700,000 above the FY 1979 level. Approximately $6,400,000 of the request is for continuing the existing base programs in geology, geophysics, geochemistry and the other research topics mentioned above. The remaining $4,400,000 is for four new programs which will impact numerous current and future energy processes and systems, but which will have particular significance for the isolation of radioactive wastes in geologic media. One of these programs, the study of the migration of chemical species in the earth's crust, is being started in FY 1979. The FY 1980 request for these programs, which is discussed below, will permit the other three to begin in FY 1980.

The program of chemical migration studies is a joint venture in cooperation with the National Science Foundation and the United States Geological Survey. This program involves the study of radioactive waste isolation, the concentration of hydrocarbon resources (oil and gas), and in-situ mining and rock-fluid interactions relating to geothermal energy. In FY 1980, $900,000 is required for this program and the radioactive waste isolation aspect of the work will be emphasized.

$2,000,000 is required in FY 1980 for a new program in continental drilling for scientific purposes. This will be an interagency program of drilling at scientifically selected sites for generation of information on the continent's underlying structure. The resulting knowledge will be important in predicting deposits of minerals and fuels and in establishing a scientific base of information relevant to nuclear waste problems.

Also in FY 1980, $1,100,000 will be required for the investigation of mineral hosts for element isolation. In this new program, the ability of different minerals to maintain their integrity under wide ranges of temperature and pressure will be compared. The most enduring will then be studied for their abilities to contain radioactive wastes without serious breakdown caused by radiation from the contained wastes.

Finally, $400,000 is requested in FY 1980 to launch studies of rock mechanics. It is important to all operations which withdraw materials or energy from, or emplace materials within, the earth to know the details and systematics of the mechanical behavior of rock substances. This work is intended to provide that kind of knowledge as a basis for conserving energy in drilling and excavating and for improving our ability to fracture rock hydraulically for geothermal energy systems and petroleum and gas recovery.

Capital Equipment

The FY 1980 request for capital equipment for Engineering, Mathematical and Geosciences is $1,450,000, an increase of $650,000 above the FY 1979 level.

Projects supported under Basic Research in Engineering will require $150,000 in equipment funds in FY 1980 to permit the acquisition of the modern instrumentation needed to launch new projects with reasonable chances of success. The needs include a wide variety of sensors for detecting and measuring optical, acoustic, magnetic, pressure, electrical and dynamic force signals.

Within Applied Mathematical Sciences, $600,000 is required for equipment. The availability of mini-computer systems with adequate precision for computational modeling and sufficiently large primary memories for computational modeling and information systems poses new alternatives for satisfying many, but not all Department of Energy computer requirements. During FY 1980, research systems will be acquired to explore innovative approaches to assure orderly acquisition of mini-computers for computational modeling and information systems by maximizing resource sharing and thus avoiding unnecessary duplication of computing capabilities. For example, one system, including necessary graphics terminals, will be dedicated to the analysis of large data sets at PNL, while existing systems at LBL and the Courant Institute of Mathematical Sciences at New York University will be enhanced. These systems will be linked by a high-capacity network to explore opportunities for resource sharing. They will also be interfaced to larger computer systems required, for example, for large-scale computational modeling. Interactive graphical and alpha-numeric terminals will be acquired for these and other sites.

For Geosciences, $700,000 is required for capital equipment in FY 1980. This request would provide valuable research equipment of vital importance to the base research program in Geosciences as well as to the new initiatives in the operating program. Major equipment needs at LASL include an internally heated pressure vessel, three microprocessor control/data acquisition systems, a prototype device for rock testing, and apparatus for superposed hydrostatic compression tests. At PNL, two Mobile Automatic Scanning Photometer (MASP) units for measuring solar radiation, a drum digitizer recorder and a high pressure, high temperature recirculating autoclave need to be acquired. The request will also provide for high pressure equipment for investigating the thermochemistry of geothermal-related materials, advanced electronics for an ultrasonic velocity measuring system, seismographic instruments and equipment for drilling experiments and data analyses.

Advanced Energy Projects .... $ 7,500 $ 16,800

Advanced Energy Projects includes two activities: Exploratory Energy Concepts (EEC) and Advanced Technology Projects (ATP). Exploratory Energy Concepts supports research on the scientific feasibility of novel concepts, while Advanced Technology Projects supports emerging technology systems which are beyond the proof of scientific feasibility but have yet to show technological viability. Thus, studies within Exploratory Energy Concepts entail high scientific risk, whereas projects within Advanced Technology Projects entail high technological risks. Projects supported by Exploratory Energy Concepts are generally smaller in scope compared to the projects supported by Advanced Technology Projects. In FY 1980, operating funds of $6,600,000 for Exploratory Energy Concepts and $10,000,000 for Advanced Technology Projects are requested. A small amount of capital equipment funds ($200,000) is requested to provide necessary equipment associated with projects funded within Exploratory Energy Concepts.

Operating Expenses

Exploratory Energy Concepts

The objective of Exploratory Energy Concepts is to explore the feasibility of novel, energy-related concepts which are at too early a stage of scientific definition to qualify for support by technology programs. Also included is exploratory research on concepts which are interdisciplinary in nature and hence do not easily fit into the existing Department of Energy program structure. The goal of exploratory energy concepts is to initiate support of about twenty new concepts during each year. This goal is a function of the number and quality of proposals received as well as the number of federal staff to operate and monitor this activity. Support is provided for a limited period only, typically not to exceed three years. After such a period, the concept is expected to either prove itself to a point where a source of further support can be identified, or else be dropped. Projects are considered on the basis of proposals submitted by researchers from universities, industry and national laboratories. Proposals from all sources are treated on an equal footing: all are subjected to a detailed technical peer review by individually selected panels of experts.

In FY 1978, the program's first year of operation, twenty-one projects were selected for support. The subject matter of those projects covered much of the total spectrum of energy-related research, including for example, new schemes for converting heat to electricity, a new approach to extracting oil from tar sands, new photovoltaic materials, research aimed at developing x-ray lasers and new methods of accelerating charged particles. Although the program is still very young, there has already been at least one significant accomplishment. A newly developed theory of solar concentrators has resulted in practical concentrator designs which will optimize the concentration of solar rays on heat receivers. The new approach is of particular significance for high performance solar collectors using heat receivers enclosed by evacuated tubes.

The following tables illustrate the distribution of FY 1978 funds among various sectors and among different technologies.

Exploratory Energy Concepts - Disposition of FY 1978 Funds

Distribution by Sector

	Number of Projects	FY 1978 Funding	Percentage of Total
Universities	11	$ 1,480	47%
Industry	7	1,316	42%
Department of Energy Labs	2	302	10%
Other Government Labs	1	54	1%
Total	21	$ 3,152	100%

Distribution by Technology

	Number of Projects	FY 1978 Funding	Percentage of Total
Solar	9	$ 1,422	45%
Nuclear	5	926	29%
Conservation	2	244	8%
Fossil	1	200	6%
Advanced Concepts	4	360	12%
Total	21	$ 3,152	100%

The distributions indicated in these tables resulted from the selection of the best of the many unsolicited proposals received. The annual funding level per project in FY 1978 varied between about $30,000 and $200,000, with an average of about $150,000.

Why is $6,600,000 in operating funds requested for FY 1980? New energy-related concepts are being born continuously. The amount requested would permit the achievement in FY 1980 of the goal of initiating about twenty new projects for support of exploratory research efforts (in addition to continuing the support of projects initiated in FY 1978 and FY 1979). Thus, about twenty new ideas generated by inventive minds throughout the country could be explored in depth in FY 1980 for their potential usefulness to energy applications.

Advanced Technology Projects

The FY 1980 budget request for Advanced Technology Projects is $10,000,000, an increase of $6,500,000 over the amount appropriated in FY 1979. The objective of this activity is to develop basic engineering data on energy technology projects which have potentially high-payoffs but which do not readily fit into existing Department of Energy programs. This program also serves as a mechanism for accelerating the transition of technology for which engineering feasibility has been proven, to the appropriate project organization within the Department of Energy for further development. Such projects might not be funded originally by an energy technology program for several reasons. For example, the potential high-payoff of these projects is usually accompanied by high risk, which makes them relatively unattractive funding choices for mainline program organizations. In addition, projects of this type typically fall outside of the main mission of most R&D organizations, and are therefore frequently not able to compete because available funds are all required for the pursuit of major ongoing programs. Projects selected for funding under Advanced Technology Projects are evaluated on the basis of their specific goals and milestones, are assessed on their potential impact on the energy problem concerned, and are reviewed by potential supporting program groups as to their predicted benefits.

The FY 1980 request would be used to initiate a number of new projects, as well as to continue the projects initiated in FY 1979, and would provide for both operational and analytic activities. The level requested is based on the funds required to support the second year of projects initiated in FY 1979, and provides for needed increases as projects reach the operational stage. In addition, an estimate of the amount required for new projects was made based on an extrapolation from the number of proposals received to date, the number accepted for funding, and their dollar value. Approximately two-thirds of the request is required for the continuation of ongoing projects and one-third is to permit initiation of new projects. Typically, the duration of these projects will be for no longer than three years, by which time the decision will be made whether to transfer the project to another Department of Energy organization for further funding and development, or to drop it. Frequent project review and timely transfer to technology programs are basic management principles. Several of the projects of particular interest to organizations under the Assistant Secretary for Energy Technology (ET) have been jointly funded with those organizations, and will be closely monitored by both ET and ATP to determine if performance goals acceptable to ET are being met, as a prelude to transfer of program management.

Within Basic Energy Sciences (BES), ATP will serve as a mechanism to provide rapid response to technological opportunities developed in the other BES programs. The role of ATP in such cases will be to act as an intermediate step in the further development of concepts evolving from other BES activities, after such concepts have shown scientific feasibility, whether initially studied in Exploratory Energy Concepts or in other BES activities. In this same capacity, ATP will also provide the Department of Energy interface with other government advanced technology groups, e.g. the Defense Advanced Research Projects Agency and the National Aeronautics and Space Administration, to explore the potential of non-Department of Energy funded research breakthroughs which might have a potential energy impact.

Several major new initiatives were begun in FY 1979, which are aimed at providing verification of technological feasibility, as well as the basic engineering data required in order to judge the potential impact of a new energy concept on the national energy situation. Specific projects funded, which are planned for continuation in FY 1980, include:

-- development of electrolytic cell - fuel cell solar energy systems for residences;
-- demonstration of the engineering feasibility of advanced catalytic systems, including synthesis of gasoline, and cogeneration of high-BTU gas and electricity;
-- advanced aerial geophysical exploration for geothermal resources;
-- computational concepts for very large (perhaps ten times) reduction in computer time for two-phase flow problems, particularly important in reactor safety problems;
-- in situ evaluation of radiofrequency heating of tar sands;
-- new combustion technology concepts.

One important effort would be in the development of a system for electromagnetic acceleration of macroparticles, including the fabrication of an accelerator test bed. If successful, this could lead to a potentially attractive method of initiating fusion in inertially confined systems.

The $10,000,000 requested would result in several major benefits. First, significant cost savings in design and implementation of second generation energy technologies including combustion, exploration, gasification, and product fabrication would be achieved by making it possible to advance conservative time schedules, and providing engineering data for pre-commercial design development. Second, multidisciplinary and interprogrammatic activities, such as the macroparticle acceleration project discussed above, would be verified to provide new program directions for further exploitation in other Department of Energy program organizations. Third, where unexpected technology problems are found, they would be redirected to other program divisions for further work in response to end-user requirements.

The funds typically would be spent in those geographic areas where significant supportive technology is available. Ordinarily, this implies that support would be provided close to the laboratory or facility where the basic concept was developed, unless necessary field experience or applications dictate specific sites, such as geothermal sources in Idaho or tar sand deposits in Utah.

Capital Equipment

Included in the request for Advanced Energy Projects is $200,000 for capital equipment for Exploratory Energy Concepts, the same level of support as in FY 1979. Some of the research efforts supported by Exploratory Energy Concepts require advanced instrumentation and other ancillary equipment. This request would provide these important equipment needs.

Biological Energy Research .... $ 4,000 $ 7,200

The Biological Energy Research (BER) program is a newly organized activity within Basic Energy Sciences designed to carry on a research program which explores ideas concerning [the use of biological systems for energy production and conservation.] The program derives from the FY 1979 transfer of projects, which are related more to the production and conservation of energy than to solving environmental problems, from the Assistant Secretary for Environment to the Director of the Office of Energy Research The major share of this work deals with research in plant and microbial sciences and focuses on the longer-term research aimed at understanding mechanisms which may lead to improved future strategies for taking advantage of biological processes in overcoming energy problems.

The principal objective of the Biological Energy Research activity is the following: to provide the biological foundation of information for the Department's efforts for biomass production for fuels and chemicals, bioconversion for conservation and bioprocessing for resource recovery. The direction of the research is toward developing a broad, intensive understanding of the biological factors involved with plant productivity as it bears on biomass and the biological conversion of biomass and other organic materials into fuel and chemicals, as well as ideas for using biological systems for sparing other energy resources.

Several FY 1978 accomplishments have resulted from the projects now supported under Biological Energy Research. These accomplishments are indicative of how research in this field can enhance our basic knowledge of biological systems and processes. Four of these accomplishments are discussed in the following paragraphs.

A biologically active material in plant host-parasite relations has been chemically characterized as a glucan (a type of sugar polymer). This material derives from fungal cell walls and is active in stimulating the production of antibiotic type compounds (phytoalexins) in plants which appear to protect the plant from damage by pathogens. These findings may lead to the development of a new concept in pesticides which has the advantages of effectiveness with diminished energy requirements, but without serious environmental concerns about toxicity. This concept is now under active investigation for application by several chemical firms.

A better definition of the function of photosynthetic "reaction centers" isolated from photosynthetic bacteria has been achieved. The study of these structures from the simpler bacterial systems provides models which are useful in understanding higher plant photosynthesis. Comparable reaction centers have not as yet been isolated from higher plant chloroplasts. In particular, newly derived information has allowed the development of a three dimensional picture of the orientation of the photosynthetic pigments, bacteriochlorophyll and bacteriopheophytin. This now permits the elucidation, in detail, of the architecture of the photosynthetic membrane.

Recent research has indicated that the concept of using elevated proline (an amino acid) content of plants as a measure of drought resistance is untenable. Some researchers had advocated that proline levels be used as a criterion for selecting drought-resistant plants.

The mechanism for regulation of gas and water exchanges of leaves has been further elaborated with the understanding of how the growth substance, abscisic acid (a messenger of stress), is triggered. These exchanges are crucial in determining how much dry matter (biomass) plants may produce.

Substantial segments of the program are performed at the Department of Energy Plant Research Laboratory, at Michigan State University in Lansing, the University of Tennessee-Comparative Animal Research Laboratory, BNL, LBL and at numerous university laboratories throughout the United States.

The FY 1980 request for Biological Energy Research is $7,200,000, of which $6,900,000 is for operating expenses and $300,000 is for capital equipment.

Operating Expenses

Biological Energy Research is expected to provide the fundamental information underlying future solar and conservation technologies and, in addition, provide a variety of ideas for future use of biological processes in energy matters.

The FY 1980 request of $6,900,000 in operating expenses for Biological Energy Research represents an increase of $2,900,000 over the FY 1979 level of funding. This increased funding is essential to cover numerous research gaps in the current program. For example, while considerable emphasis is now given to the more immediate application of technologies such as biomass and fermentation of wastes, there is little attention paid to research designed to provide a fundamental understanding of many of the processes which will shape the future scientific complexion of these technologies. Biological Energy Research is designed to generate such information, which is necessary to provide a foundation upon which future strategies for the development of these and other technologies can be based. About 50 percent of the current programs is conducted at universities throughout the United States and the major part of the increase in funds requested in FY 1980 is expected to be used for support of university programs.

Of the $6,900,000 requested in FY 1980, $4,700,000 is planned for research involving the production, characterization and adaptation of plants for fuels and chemicals. In particular, work involving two currently neglected but nevertheless very important activities in plant research would be expanded in FY 1980. One is research designed to comprehend the physiological and biochemical adaptation of plants for productivity in less than optimal environments including the prospects of the genetic transfer of adaptive characteristics. The other is how the plants partition energy once it is trapped. The synthesis by plants of chemicals (hydrocarbons, for example) of potential use as fuel or chemicals will be another topic which will be emphasized, including the biochemical and genetic control mechanisms for determining the nature and quantity of such synthesis. Investigations will continue into biological photosynthetic mechanisms with a view to overcoming the limitations of productivity by plants. Increased knowledge in this area would also provide information for modeling artificial photosynthesis devices, which would complement research on photochemistry sponsored within the Chemical Sciences activity discussed earlier.

The Biological Energy Research activity will also include research involving the microbial conversion of biomass (including wastes) into useful fuels and chemicals and evaluation of other biological energy concepts. In FY 1980, $2,200,000 in operating funds would go toward this work. A considerable increase is expected in the research effort involving the fermentation reactions of microorganisms, which offer numerous possibilities for the conversion of various organic residues into useful fuels and chemicals. The mechanism of methane generation, the breakdown pathways of cellulose and lignin, the sequential or cooperative reactions of conversion, plus the potentialities of genetic and physiological manipulation of these processes fall within this research effort. The production of hydrogen by algae and other microorganisms will be explored. The biochemical derivation of the hydrogen, the enzymes involved and the energy requirements for the process are intended areas of research. New biological energy studies will be carried out with an attempt to identify systems which might have utility in the accumulation of dilute metal ions for recovery of resources from low grade ores, and reduction of energy inputs into industrial and cropping activities. Thus, this research is designed to look for imaginative uses of organisms which relate to a wide variety of energy matters.

Capital Equipment

The request for Biological Energy Research for capital equipment is $300,000 in FY 1980. This funding would provide important tools for research including a computerized gas chromatograph-mass spectrometer used for chemical characterization of complex mixtures in plants and microorganisms. Other equipment needs include analytical centrifuges, other spectrophotometric equipment, gas analyzers and liquid scintillation counters. These equipment funds are necessary to support the important biological research discussed above.

Personnel resources	$ 1,851	$ 2,570

The FY 1980 request for personnel resources for the Basic Energy Sciences program is $1,133,000, an increase of $354,000 above the FY 1979 level. The request is necessary to provide for the salaries, benefits, travel and related expenses associated with the 66 staff years of effort which have been assigned for budgetary purposes to the Basic Energy Sciences program. These include 54 staff years from the Associate Director of the Office of Energy Research for Basic Energy Sciences as well as the allocation of 12 staff years from the Director of Energy Research's administrative staff. The request provides an increase of one staff year in FY 1980, which is necessary to provide for additional workload resulting from the growth in the research programs supported under Basic Energy Sciences in FY 1980.

Basic Energy Sciences is the major Department of Energy program which plans, supports and administers basic research in the physical and biological sciences most important to the Nation's energy programs. It supports construction and operation of unique scientific research facilities and the conduct of research programs at these and other Department of Energy facilities. In addition, it is estimated that approximately 400 off-site contracts will be supported (primarily at universities throughout the United States, although there are some with industrial firms and other governmental bodies). This represents only a fraction of the total number of proposals that must be reviewed and evaluated annually.

Basic Energy Sciences is a broadly diversified program requiring staff with expertise in scientific areas such as chemistry, physics, engineering, metallurgy, geosciences, biology, mathematics and computer science, as well as in administrative and financial management. Basic Energy Sciences staff are responsible for program direction and management of complex technical programs in these scientific areas. Their activities include assessing scientific needs and priorities of the program, developing long-range program plans, technical review of proposals from laboratories and universities, and monitoring the progress of ongoing university contracts, laboratory programs and construction projects. Very close coordination is required with the Department's applied technology programs to assure that their long-term needs can be identified and provided for in a timely manner. Coordination is also required with Department of Energy field installations and contractors, other Federal agencies, the Congress, and industry.

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

CONSTRUCTION PROJECT DATA SHEETS
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research

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

Brookhaven National Laboratory

Basic Energy Sciences

1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

3. Date A-E work initiated: 2nd Qtr. FY 1978

3a. Date physical construction starts: 4th Qtr. FY 1978

4. Date construction ends: 2nd Qtr. FY 1982

5. Previous cost estimate: $24,000
Date: 12/76

6. Current cost estimate: $24,000
Less amount for PE&D: 0
Net cost estimate: $24,000
Date: 1/79

7. Financial schedule

Fiscal Year	Authorization	Appropriation	Obligations	Costs
1978	$ 24,000	$ 5,000	$ 4,713	$ 1,196
1979	0	10,000	10,287	5,100
1980	0	9,000	9,000	9,500
1981	0	0	0	6,700
1982	0	0	0	1,504

8. Brief physical description of project
This project provides for the design and construction of an electron storage ring complex for dedicated use as a high intensity synchrotron radiation source; for the design and construction of new building space to house the storage rings and associated experimental, laboratory and office areas; and for the design and fabrication of experimental equipment required to serve the basic initial needs of the scientific users.

CONSTRUCTION PROJECT DATA SHEETS

Brookhaven National Laboratory

1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York	2. Project No. 78-13-a

8. Brief physical description of project (cont'd)

The basic approach of the complex is for two storage rings designed for flexible operation over electron energies extending up to 2.5 GeV for the x-ray ring, and up to 0.7 GeV for the ultraviolet ring. Each ring is designed for operation with circulating currents approaching 1 ampere, and the two rings will be served by a common injector, specially designed to accommodate the high current objectives. Some of the large storage ring sectors will operate at moderate magnetic fields, primarily providing photon beams in the x-ray wavelength region. Other sectors will incorporate high magnetic field "wigglers" to simultaneously generate radiation with short x-ray wavelengths. Each wiggler will consist of a tripole superconducting dipole capable of attaining about 40 kilogauss at the center. The x-ray ring will be about 170 meters in circumference, and will provide as many as 40 photon source ports, some with small source size and exceptionally high brightness. Most of these ports can be equipped to serve more than one experiment. The high current proposed will require an injection energy of about 650 MeV, obtainable from a ring booster equipped with either a linac or a 50 MeV microtron as its injector. A second smaller ring, having a mean diameter of about 14 meters and a circumference of about 44 meters, will operate at 700 MeV with a circulating current of up to 1 ampere. It will be utilized in the long wavelength region and have 16 ports for experimental stations.

The project includes a building of approximately 77,000 sq. ft. gross area, of insulated panel construction on steel frame with reinforced concrete slab and shielding. It will house the two storage rings, booster linac and injector, experimental areas, supporting office and laboratories and mechanical and electrical equipment including necessary to building electrical needs, controlled environment air handling systems, standard laboratory service piping, and fire protection systems, as well as electric power and cryogenic equipment essential to operation of the storage rings and experimental apparatus. The building materials handling system will include two, two-ton bridge cranes. Supporting utilities and drainage systems will be extended from existing plant distribution systems. Standard laboratory and office furniture will be provided.

9. Purpose, justification of need for, and scope of project

The National Synchrotron Light Source is proposed as a national, user-oriented, dedicated facility for advanced multidisciplinary research with synchrotron radiation, a powerful investigative tool which will be of major importance for the materials, chemical, and life sciences. Although the facility is proposed because of its value for fundamental research in these broad areas, the work which would be done at such a facility is clearly relevant to the practical energy and environmental concerns of the Nation. Both in this country and abroad, researchers using synchrotron radiation have been limited by the characteristics of existing sources. The few facilities which are dedicated to this research are small and

CONSTRUCTION PROJECT DATA SHEETS

Brookhaven National Laboratory

1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

9. Purpose, justification of need for, and scope of project (cont'd)

provide spectra extending from long wavelengths only to the far ultraviolet. Those sources which can furnish photons at limited wavelengths were designed for high energy physics, so that synchrotron radiation utilization is parasitic, with serious attendant shortcomings. Moreover, most of the latter sources are synchrotrons and do not have the beam stabilities provided by a storage ring. Thus it has been recognized in the U.S. and elsewhere that there is a need for specially designed facilities intended exclusively for the production and utilization of synchrotron radiation in pure and applied research over the entire range of wavelengths starting from the infrared to the x-ray region.

It is evident from what has already been accomplished with the limited capabilities of existing facilities that a dedicated, specially designed facility for synchrotron radiation research would have a strong impact on a broad range of scientific and technical fields, because it would make feasible types of experiments otherwise impracticable. Among the many specific areas involved are: solid state, atomic and chemical spectroscopy over the entire spectrum; photo and radiation chemistry; crystal structure by diffraction; lattice defect structure studies, including microscopic strain field analysis of both intrinsic and extrinsic defects; the physics, chemistry, and structure of surfaces and thin films; amorphous and ordered x-ray microscopy; optics, including non-linear optics and holography; and a variety of possible technological applications, such as the writing of compact integrated microelectronics and systematic investigation of processes related to solar energy applications.

Although innovative in design, the state-of-the-art presently available will permit an assured construction. The report of the National Academy of Sciences Panel entitled "An Assessment of the National Need for Facilties Dedicated to the Production of Synchrotron Radiation" makes a prime recommendation that: As a response to the national synchrotron radiation needs, the U.S. make an immediate commitment to construct a new dedicated national facility or facilities. The proposed construction project at BNL responds to this recommendation.

The $9,000,000 requested for appropriation in FY 1980 will provide for completion of the engineering and design, procurement and construction. The request includes funds required for improvements to land, the laboratory-office building and special facilities.

CONSTRUCTION PROJECT DATA SHEETS

Brookhaven National Laboratory

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1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

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10. Details of cost estimate*

a. Engineering, design and inspection at approximately 25% of construction costs, item b			$ 4,100
b. Construction costs			16,400
(1) Improvements to land, including site preparation, curbs, walks, paving, and special compaction		$ 140	
(2) Accelerator and laboratory building		5,600	
(3) Special facilities		10,300	
(a) 2.5 GeV storage ring	$ 3,735		
(b) 700 MeV storage ring	1,864		
(c) Injector system	945		
(d) Associated apparatus	1,906		
(e) Experimental equipment	1,850		
(4) Utilities		360	
c. Standard equipment			500
Subtotal			21,000
d. Contingency at 14% of above costs			3,000
Total project cost			$24,000

11. Method of performance

Design of the conventional facilities is on the basis of a negotiated fixed price architect-engineer contract, with design of the special facilities (magnet sectors, main vacuum chamber, rf cavities, etc.) by Brookhaven National Laboratory. Conventional construction is being accomplished by fixed price contracts awarded on the basis of competitive bid. Fabrication of special facilities, as well as the provision of magnet and rf power supplies, cryogenics, control equipment, etc., is by commercial vendors where possible on the basis of fixed price contracts awarded on the basis of competitive bidding. Assembly and testing is being performed by Brookhaven National Laboratory.

*The above estimates are based on Title I and partial Title II.

CONSTRUCTION PROJECT DATA SHEETS

Brookhaven National Laboratory

1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

12. Funding schedule of project funding and other related funding requirements

	Prior Yrs.	FY 1980	FY 1981	FY 1982	Total
a. Total project funding					
1. Total facility costs					
a) Construction line item	$ 6,296	$ 9,500	$ 6,700	$ 1,504	$24,000
b) Expense funded equipment	130	0	0	0	130
c) Inventories	100	200	200	0	500
Total Facility Costs	$ 6,526	$ 9,700	$ 6,900	$ 1,504	$24,630
2. Other project funding					
a) R&D necessary to complete construction	$ 3,120	$ 1,177	$ 1,260	$ 100	$ 5,657
Total other project funding	$ 3,120	$ 1,177	$ 1,260	$ 100	$ 5,657
Total Project Funding (item 1 & 2)	$ 9,646	$10,877	$ 8,160	$ 1,604	$30,287

b. Total related funding requirements (estimated life of project: 20 years)

1. Facility operating costs	$ 3,500
2. Programmatic operating expenses directly related to the facility	3,370
3. Capital equipment not related to construction but related to the programmatic effort in the facility	1,120
Total other related annual funding requirements	$ 7,990

13. Narrative explanation of total project funding and other related funding requirements

a. Total project funding
   1. Total facility costs
      a) Construction line item - explained in items 8, 9 and 10.
      b) Expense funded equipment - This includes a linac, ultra-vacuum system, and fast valve safety systems for beam levels.
      c) Inventories - This includes high voltage capacitor systems and rf cavity models.

CONSTRUCTION PROJECT DATA SHEETS

Brookhaven National Laboratory

1. Title and location of project: National synchrotron light source, Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

13. Narrative explanation of total project funding and other related funding requirements (cont'd)

2. Other project funding
   a) R&D necessary to complete the project totals $5,657,000, including $3,120,000 expended in prior years. This R&D is related to computer calculation of electron orbits, magnet configurations, injector upgrading, preliminary beam line and wiggler design, vacuum system preliminary design, building criteria, machine cooling and power criteria, and rf system and cavity work.

b. Total related funding requirements

1. Facility operating costs
   The major operating costs include power, water, and facility operational maintenance, equipment and machine development, and technical support for users.

2. Programmatic operating expenses directly related to the facility
   The programmatic operating expenses are associated with the (a) scientific manpower, (b) material handling and preparation, (c) data acquisition and analysis, and (d) experimental beam line preparation.

3. Capital equipment not related to construction but related to the programmatic effort in the facility.
   These equipment funds will provide continual utilization growth of the facility through the acquisition of: beam lines, vacuum and magnetic shutters, x-ray and ultra-violet spectrometers, computer interfacing, mirrors and reflectors, and detectors for a full range of photon energies.

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

CONSTRUCTION PROJECT DATA SHEETS
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research

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

Argonne National Laboratory — Basic Energy Sciences

1. Title and location of project: Intense pulsed neutron source-I (IPNS-I), Expanded Experimental Capabilities, Argonne National Laboratory, Argonne, Illinois

2. Project No. 80-ES-9

3. Date A-E work initiated: 1st Qtr. FY 1980

3a. Date physical construction starts: 3rd Qtr. FY 1980

4. Date construction ends: 2nd Qtr. FY 1982

5. Previous cost estimate: None
Date:

6. Current cost estimate: $2,400
Less amount for PE&D: 0
Net cost estimate: $2,400
Date: 1/79

7. Financial schedule

Fiscal Year	Authorization	Appropriation	Obligations	Costs
1980	$ 2,400	$ 2,400	$ 2,400	$ 500
1981	0	0	0	1,400
1982	0	0	0	500

8. Brief physical description of project

This project will provide nearly a doubling of research stations and associated instrumentation to take better advantage of the capabilities in IPNS-I. Installations and operation of these research stations in IPNS-I will permit the generation of new scientific data and will allow in situ operational experience essential to the study and development for potential higher flux development.

This project will also provide two cryogenic systems for use with low temperature irradiations in two of the four thimbles of the radiation effects facility in IPNS-I. Existing buildings and services will be used to the maximum extent practical to contain and support the primary equipment for the cryogenic systems.

Argonne National Laboratory

1. Title and location of project: Intense pulsed neutron source-I, Expanded Experimental Capabilities, Argonne National Laboratory, Argonne, Illinois

2. Project No. 80-ES-9

9. Purpose, justification of need for, and scope of project

Neutron Scattering

By expanding the experimental capabiltity of IPNS-I research stations in the manner described herein the following effects will be realized:

- Acceleration of the rate at which the entire scientific community can utilize this unique facility
- Broaden the range of experimental capability so that a wider selection of qualitatively new scientific problems can be attacked
- Significantly enlarge the experimental area throughout so a larger number of experiments can be conducted in the crucial early years of operation
- Expedite the process of gaining experience essential to advance optimization of sources and instruments

The doubled experimental capability at the pulsed neutron source resulting from this project will provide first of a kind capabilities for a much larger number of experiments in the material, chemical and biological sciences. Examples of some of these which are closely related to energy technologies are studies of:

- Proton binding and diffusion in metal hydrides related to hydrogen storage;
- Surface-adsorbed and intercalated molecules in systems related to catalysts;
- Structure of amorphous semiconductor materials and metallic glasses.

Examples of fundamental scientific studies are:

- Structure of biological molecules and materials complexes, especially exploiting differential (deuterium vs. hydrogen) labeling;
- High-frequency excitations in magnetic materials;
- Structure and dynamics of molten salts, liquid metals and aqueous solutions.

CONSTRUCTION PROJECT DATA SHEETS

Argonne National Laboratory

1. Title and location of project: Intense pulsed neutron source-I (IPNS-I), Expanded Experimental Capabilities, Argonne National Laboratory, Argonne, Illinois

2. Project No. 80-ES-9

9. Purpose, justification of need for, and scope of project (cont'd)

Radiation Effects Research

Cold radiation effects experiments will be made possible by the addition of cryogenic systems for two of the four irradiation thimbles.

The cryogenic experimental stations to be acquired will provide unprecendented research capability for in situ radiation damage measurements coupled with the capability to exploit the nearby array of other experimental facilities, of which the high voltage electron microscope is a prime example.

10. Details of cost estimate*

a. Engineering design and inspection at 20% of construction costs, item b		$ 350
b. Construction costs		1,750
(1) Special facilities		
(a) Experimental stations	$ 1,270	
(b) Cryogenic systems	480	
Subtotal		2,100
c. Contingency at approximately 14% of above costs		300
Total project cost		$ 2,400

11. Method of performance
Design and assembly of the experimental stations will be accomplished by the operating contractor (ANL) because of the unique nature of the facilities required, the close coupling between the experimental facilities, the accelerator and the neutron source, and the specially-applicable knowledge and skills of the laboratory staff.

*Based upon completed conceptual design.

CONSTRUCTION PROJECT DATA SHEETS

Argonne National Laboratory

1. Title and location of project: Intense pulsed neutron source–I (IPNS–I), Expanded Experimental Capabilities, Argonne National Laboratory, Argonne, Illinois

2. Project No. 80-ES-9

12. Funding schedule of project funding and other related funding requirements

a. Total project funding

	Prior Yrs.	FY 1980	FY 1981	FY 1982	Total
1. Total facility costs					
(a) Construction line item	$ 0	$ 500	$ 1,400	$ 500	$ 2,400
(b) Inventories	0	150	200	200	550
Total facility costs	$ 0	$ 650	$ 1,600	$ 700	$ 2,950

b. Total related funding requirements (estimated life of project: 20 years)

1. Facility operating costs	$ 190
2. Programmatic operating expenses directly related to the facility	380
3. Accelerator improvements and modifications	200
Total other related annual funding requirements	$ 770

13. Narrative explanation of total project funding and other related funding requirements

a. Total project funding

1. Total facility

(a) Construction line item – explained in items 8, 9 and 10.

(b) Inventories

An inventory of critical spare parts is needed to insure replacement and repair capability in the event of failure of system components. Component failures could lead to shutdown operations which would delay or possibly abort research programs. The optimization of operation would be enhanced by the immediate availability of parts so that repair or replacement could be accomplished in as short a time as practicable.

b. Total related funding requirements

The potential lifetime of IPNS–I is estimated at 20 years.

1. Facility operating costs

Neutron Scattering and Radiation Effects	Dollars ($1,000's)
1 Staff	$ 60
3 Hourly	100
Materials & Services	30
Total	$ 190

CONSTRUCTION PROJECT DATA SHEETS

Argonne National Laboratory

1. Title and location of project: Intense pulsed neutron source-I (IPNS-I), Expanded Experimental Capabilities, Argonne National Laboratory, Argonne, Illinois

2. Project No. 80-ES-9

13. Narrative explanation of total project funding and other related funding requirements (cont'd)

2. Programmatic operating expenses directly related to the facility
A group consisting of 6 additional staff and technical support personnel will be assigned to the IPNS-I upgraded facilities for effective use of instruments by experimenters outside the host laboratory, for maintenance and operation of instruments, instrument improvement, provision of special capabilities and instruction of users in measurement and data handling. This cost is therefore shown as a component of research costs.

	Dollars ($1,000's)
Support of IPNS-I Technical Staff	
6 Staff and Technical Support	350
Materials and Services	30
Total	380

The effort related costs of the above include general laboratory expenses (indirect costs) as well as program direction and direct allocation expense.

3. Accelerator improvements and modifications
The capital costs required to improve the Booster-II accelerator system to enhance and expand the efficient and effective operations are estimated at $200,000 per year.

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

CONSTRUCTION PROJECT DATA SHEETS
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research

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

Lawrence Berkeley Laboratory (LBL) — Basic Energy Sciences

1. Title and location of project: Chemical and materials sciences laboratory, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No. 80-ES-10

3. Date A-E work initiated: 2nd Qtr. FY 1980

5. Previous cost estimate: None
Date:

6. Current cost estimate: $12,600
Less amount for PE&D: 0
Net cost estimate: $12,600
Date: 1/79

3a. Date physical construction starts: 1st Qtr. FY 1981

4. Date construction ends: 4th Qtr. FY 1982

7. Financial schedule

Fiscal Year	Authorization	Appropriation	Obligations	Costs
1980	$ 12,600	$ 6,300	$ 6,300	$ 2,100
1981	0	6,300	6,300	8,000
1982	0	0	0	2,500

8. Brief physical description of project

This project will provide a laboratory-office addition to Building 62 of approximately 50,000 gross square feet for chemical and material sciences research. As presently conceived, it will be a three-story concrete and steel framed building with partial basement and high bay area. The latter will house a 500 kV Atomic Resolution Microscope (ARM). Other major equipment will include a 200 kV High Resolution Electron Microscope (HREM) with scanning transmission capability, microdensitometer, beam scattering chamber, environmental chamber, auger microprobe with field transmission source, x-ray and kv spectroscopy systems, computer control system, a bridge crane, and a glove-box closed hood system. The building will be equipped with an elevator and ramps to accommodate the handicapped, standard laboratory piping and fire protection systems, and environmentally controlled air in specific equipment areas. Utility systems will be extended from existing plant services. Toxic effluents will be contained within the facility through high efficiency particulate (HEPA) filters for airborne effluent,

1. Title and location of project: Chemical and materials sciences laboratory, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No. 80-ES-10

8. Brief physical description of project (cont'd)
and a liquid collection system integral to the glove box system.

9. Purpose, justification of need for, and scope of project
This facility will house research groups and provide support facilities for programs in basic research in chemical and material sciences. It will provide space for energy-related research that has been identified as high priority programs by DOE.

An atomic resolution microscopy program at LBL will provide unique capabilities necessary for:

A. The real space determination of localized crystal structure in complex structural and electronic materials, overcoming both the phase problem and low spatial resolution of conventional diffraction techniques;

B. The imaging of individual point defects and impurity atoms in the close-packed crystal structures which characterize advanced energy materials, allowing the direct observation of grain boundary segregates and their effects to corrosion, embrittlement and solid state transformations, and

C. The indentification of atomic mechanisms associated with catalysis, abrasive wear, and the crystallization of polymers and glasses.

Each of these problems is critical to the progress of materials design in energy research, yet there is no instrumentation available in the U.S. for investigating possible solutions. Success in achieving atomic resolution images has already been demonstrated on a prototype 500 kV microscope at the University of Kyoto, Japan, while similar instruments are being developed in the large integrated microscope laboratories of several foreign countries. The acquisition of such a microscope, designed for 1.7 A point-to-point resolution, will allow LBL to establish the capability for atomic resolution in this country.

The Atomic Resolution Microscope (ARM) must also include an energy-loss spectrometer attachment for high resolution chemical analysis in order to complement its detailed morphological information. Feeder microscopes are essential to screen specimens and determine optimum candidates for imaging in the ARM, and experimental microscopes will be utilized to test component modifications which assure state-of-the-art performance for the 500 kV machine. These facilities will also require laboratory space, instrumentation and staff for specimem preparation, image interpretation and instrument development. LBL's effort will be undertaken jointly with scientists at other institutions, notably Arizona State University, and provide for maximum interaction among researchers with widely different fields of expertise in the energy sciences.

The problem areas requiring immediate application of atomic resolution microscopy are those associated with free surfaces and internal interfaces in energy-related materials. Emphasis will be placed on the detection and identification of amorphous

CONSTRUCTION PROJECT DATA SHEETS

Lawrence Berkeley Laboratory (LBL)

1. Title and location of project: Chemical and material sciences laboratory, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No. 80-ES-10

9. Purpose, justification of need for, and scope of project (cont'd)

phases in ceramics, the atomic variations responsible for intergranular failures, e.g., stress corrosion cracking and hydrogen embrittlement in steels, the effect of grain boundary structure on phase transformations in alloys, the atomic events associated with the development and poisoning of catalysis, and the defect structures responsible for the breakdown of electronic junction devices.

With the insight that atomic resolution microscopy will give to these areas of urgent concern, the long range development of materials for advanced energy systems can proceed on a sound fundamental understanding of atomic structure. This project supports the continuing leadership capability at LBL in electron microscopy within the United States.

In addition this facility will provide a better focus of ongoing programs presently being conducted under unsatisfactory space conditions and dispersed over twelve different locations within LBL and on the University of California Berkeley campus, with only 150 of the total 500 Divison staff members located in the Division headquarters, Building 62. The unique combination of multi-disciplinary talent at the Laboratory will be used to bring to bear the most advanced experimental and theoretical techniques on problems relating to structural features and reaction mechanisms of chemical processes for energy technologies, such as the catalytic conversion of fossil fuels and combustion processes. New insights into the dynamics of chemical processes at the atomic level, required to further the understanding of chemical processes in advanced energy technologies, will be generated where present understanding of crucial chemical reactions is not satisfactory.

In addition to atomic resolution microscopy, the following topics of investigation are planned to be conducted in the facility.

A. Photoelectron Spectroscopy:

Of particular interest are: the structure of high-temperature species and their interaction with radiation and surfaces, properties of clean and adsorbate-bonded surfaces, energy transfer and lifetimes in high-energy excimers.

B. Conversion of Coal:

Mechanisms and kinetics of coal liquefaction and gasification reactions will be studied together with the interactions of homogeneous and heterogeneous catalysts with coal. Of particular interest is the elucidation of factors which control catalyst activity, selectivity and resistance to poisoning.

CONSTRUCTION PROJECT DATA SHEETS

Lawrence Berkeley Laboratory (LBL)

1. Title and location of project: Chemical and materials sciences laboratory, Lawrence Berkeley Laboratory, Berkeley, California	2. Project No. 80-ES-10

9. Purpose, justification of need for, and scope of project (cont'd)

C. Molecules on Surfaces:

Ultraviolet, visible and infrared ellipsometry will be used as a new technique to follow the transition between physically and chemically adsorbed states of molecules on solid surfaces and to establish pathways of catalytic reactions.

D. Metal Clusters:

Surface displacement reactions, modeled on established molecular coordination chemistry, will be used to obtain structural, bonding and chemical information about chemisorbed molecules. A more precise comparison between homogeneous and heterogeneous catalysis will be devised from molecular research with metal clusters.

E. Photon-Assisted Surface Reactions:

Light that forms photoelectrons of reasonable lifetimes at solid surfaces is to be used to conduct chemical reactions which are otherwise thermodynamically not possible. In particular, the role of photoelectrons will be investigated in the reactions of water and carbon dioxide to produce hydrogen and hydrocarbons.

Integration of ongoing programs presently being conducted in different locations and under overcrowded conditions will allow the more efficient use of shared facilities and provide for improved interdisciplinary interaction in the conduct of collaborative efforts.

10. Details of cost estimate*

a. Engineering, design and inspection at about 15% of construction costs, item b		$ 920
b. Construction costs		6,140
1. Improvements to land	$ 200	
2. Building 50,000 sq. ft. gross at about $115/sq. ft.	5,750	
3. Utilities	190	

*Based upon a completed conceptual design.

CONSTRUCTION PROJECT DATA SHEETS

Lawrence Berkeley Laboratory (LBL)

1. Title and location of project: Chemical and materials sciences laboratory, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No. 80-ES-10

10. Details of cost estimate (cont'd)

c. Standard equipment		4,450
1. ARM & Associated equipment	$ 3,500	
2. Chemical sciences equipment	900	
3. Bridge crane, laboratory furniture	140	
Subtotal		$11,600
d. Contingencies @ approximately 14% of items a & b above		1,000
Total project costs		$12,600

11. Method of performance

Design will be on the basis of a negotiated architect/engineer contract. To the extent feasible, construction and procurement will be accomplished by a fixed price sub-contract awarded on the basis of competitive bidding.

12. Funding schedule of project funding and other related funding requirements

	Prior Yrs.	FY 1980	FY 1981	FY 1982	FY 1983	Total
A. Total project funding						
1. Total facility costs						
a. Construction line item	$ 0	$ 2,100	$ 8,000	$ 2,500	$ 0	$12,600
Total facility costs	$ 0	$ 2,100	$ 8,000	$ 2,500	$ 0	$12,600

B. Total related funding requirements (estimated life of project: 50 years)

1. Facility operating costs	$ 125
2. Programmatic operating expenses directly related to the facility	5,000
Total other related annual funding requirements	$ 5,125

13. Narrative explanation of total project funding and other related funding requirements

A. Total project funding

1. Total facility

CONSTRUCTION PROJECT DATA SHEETS

Lawrence Berkeley Laboratory (LBL)

1. Title and location of project: Chemical and materials sciences laboratories, Lawrence Berkeley Laboratory, Berkeley, California

2. Project No. 80-ES-10

13. Narrative explanation of total project funding and other related funding requirements (cont'd)

a. Construction line item
no narrative required

B. Total related funding requirements

1. Facility operating costs: inlcudes estimated cost for janitoral service, and facilities such as light, heat, water, telephone.
2. Programmatic operation expenses related to this facility. The program activities to be conducted in the facility are described in Section 9 above.

Department of Energy
FY 1980 CONGRESSIONAL BUDGET REQUEST

CONSTRUCTION PROJECT DATA SHEETS
Energy Supply Research and Development - Plant and Capital Equipment
Basic Research

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

Office of Basic Energy Sciences — Basic Energy Sciences

1. Title and location of projects: General plant projects, various locations

2. Project No. 80-GPP-1

3. Date A-E work initiated: 1st Qtr. FY 1980

3a. Date physical construction starts: 2nd Qtr. FY 1980

4. Date construction ends: 2nd Qtr. FY 1982

5. Previous cost estimate: None
Date:

6. Current cost estimate: $ 250
Less amount for PE&D: 0
Net cost estimate: $ 250
Date: 1/79

7. Financial schedule

		Costs			
Fiscal Year	Obligations	FY 1978	FY 1979	FY 1980	After FY 1980
Prior Year Projects	xxx	$ 279	$ 154	$ 0	$ 0
FY 1978 Projects	270	65	105	100	0
FY 1979 Projects	270	0	75	195	0
FY 1980 Projects	250	0	0	60	190
		$ 344	$ 334	$ 355	$ 190

8. Brief physical description of project

This project is required to provide for minor new construction, other capital alterations and additions, and for retirements to land, buildings and utility systems. Where applicable, the request also includes the cost of installed capital equipment

CONSTRUCTION PROJECT DATA SHEETS

Office of Basic Energy Sciences

1. Title and location of project: General plant projects, various locations · 2. Project No. 80-GPP-1

8. Brief physical description of project (cont'd)
of the requirements. No significant R&D program is anticipated as a prerequisite for design and construction of the sub-projects under consideration.

The currently estimated distribution of FY 1980 funds by office is as follows:

Ames Laboratory	$	230
Notre Dame Radiation Laboratory		20
Total project cost	$	250

9. Purpose, justification of need for, and scope of project
The following are examples of the major items of work to be performed at the various locations:

Ames Laboratory .... $ 230
Requirements include: expansion of the plant protection system ($50,000); upgrade of the metallurgy building electrical system ($60,000); energy conservation modifications to building systems ($60,000); and an equipment cooling system for the metallurgy building ($60,000).

Notre Dame Radiation Laboratory .... $ 20
This project provides for modifications to the Radiation Research Building at the University of Notre Dame. Changes in the method of pursuing the research program necessitate some minor modifications and improvements for smooth and efficient operations.

10. Details of cost estimates
See description, item 8. The estimated costs are preliminary and, in general, indicate the magnitude of each program. These costs include engineering, design and inspection.

11. Method of performance
Design will be on the basis of negotiated architect-engineer contracts. To the extend feasible, construction and procurement will be accomplished by firm fixed-price contracts and subcontracts awarded on the basis of competitive bidding.