DEPARTMENT OF ENERGY

FISCAL YEAR 1982 CONGRESSIONAL BUDGET REQUEST

ENERGY SUPPLY RESEARCH AND DEVELOPMENT

VOLUME 3

SUPPORTING RESEARCH AND TECHNICAL ANALYSIS

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Department of Energy
FY 1982 CONGRESSIONAL BUDGET REQUEST

PROGRAM OVERVIEW

Supporting Research and Technical Analysis

The need to develop new and improved energy sources and to use energy more efficiently continues to be extremely important to the general welfare of the Nation. The role of basic (or supporting) energy research and technical analysis is to expand the scientific and engineering knowledge base on which the Nation's future energy options depend and to provide independent, objective analyses and assessments of research and technical needs relating to energy. Funding of basic research is an investment in the future. Through this investment, the applied technology efforts of industry and government will have a broader foundation of knowledge from which to discover new concepts, materials, processes and techniques important for energy production, conservation and utilization. Failure to strengthen our fundamental knowledge base of energy-related phenomena could result in limitations on productivity growth, erosion of the country's competitive position with foreign nations, additional pressure on the United States' balance of trade and continuation of inflationary trends.

The following five programs make up the Supporting Research and Technical Analysis category of the Department of Energy: (1) Basic Energy Sciences (BES); (2) Technical Assessment Projects (TAP); (3) University Research Support (URS); (4) Multi Program Facilities; and (5) Advisory and Oversight Program Direction. All five of these programs are under the Director of Energy Research.

The Basic Energy Sciences program is responsible for the long range, mission-oriented research of the Department of Energy. The chief purpose of the program is to provide the fundamental scientific and engineering base on which the Nation's future energy options depend. The major product of the BES program is increased knowledge. This knowledge is developed by sponsoring research in the traditional disciplines: the physical and biological sciences, geosciences, engineering and mathematics. The product of research in these disciplines then becomes a part of the body of data on which applied technologies rest. In addition to this focus on disciplinary research, there is also an emphasis on innovative applications of new knowledge to energy problems, and on the early application and, if possible, direct commercialization of the results.

Some examples of the BES research effort having immediate impact are: improvement of our capability to predict the consequences of nuclear reactor accidents and possible easing of nuclear plant siting restrictions as a result of research on fission product iodine; development of high strength steel alloys which could lead to significant savings in energy when used in automobiles; extended lifetimes of catalysts used in coal gasification through improved understanding of the mechanisms involved in their loss of activity and their regeneration; the application of titanium diboride coatings developed for erosion resistance in synfuel plant valves to the equally important function of cathode coatings in the manufacture of aluminum; and the use of a highly sensitive solid state device for identifying and locating geothermal resources.

Other examples of current BES research efforts that will likely enhance future energy alternatives are: the development of a fracture resistant steel for cryogenic applications through control of metallurgical structure; the production of hydrogen by a solar photochemical process which simultaneously lowers the production cost of an important oxygen containing industrial chemical; research on the way living systems attain high efficiency which has provided new thermodynamic insight to improve the efficiency of processes involving highly complex chemical systems; and the discovery that components of the cell walls of plants act as hormones which could lead to superior biomass production and environmentally benign herbicides.

The Technology Assessment Projects program provides the capability for independent, rigorous assessment of the base of research that underlies a variety of energy technologies. Assessments are consolidated under one organization, the Office of Energy Research, in fulfillment of legislated responsibility for the Director to advise the Secretary on the Department's research and development programs. In addition, TAP supports advanced technology projects in order to develop engineering and preliminary cost data and to accelerate the transition of technology, for which engineering feasibility has been proven, to the appropriate project organization within DOE for further development. These assessments and projects are very important to ensure that the Department's basic research effort contributes toward both the short-term and long-term objectives of the applied programs. A new subprogram under TAP is proposed in FY 1982, called Social and Economic Sciences. The intent of this effort will be to improve understanding of the basic social, economic and behavioral factors affecting energy-related activities. The assessment of the Solar Powered Satellite (SPS) concept, which was funded under TAP, was completed in FY 1980. No funds are being requested for SPS in this budget submittal.

The University Research Support Program includes five interrelated activities focused on the following three primary objectives: To strengthen university capability to do energy research, to strengthen the quality and increase the numbers of students interested in pursuing energy related professional careers; and to enhance technology transfer activities through cooperative research efforts between universities, the Department's national laboratories and private industry. The five program activities are: The University Institutional Agreements Program which provides modest support for seed-type exploratory research projects, workshops and seminars at a small number of universities with significant institutional strength and commitments in the energy field; and a related effort to the energy research and education capabilities at smaller, traditionally minority colleges and universities. The University Reactor Fuel Assistance Program which provides support to a small number of university nuclear research reactors for the actual fabrication costs of nuclear fuel and for a portion of the operating costs of these reactors when used by researchers at other, neighboring institutions. The University Laboratory Cooperative Program which supports the involvement and participation of university faculty and students in research and related programs are conducted at various Departmental national laboratories and contractor facilities. Special attention is paid to utilization of the unique research facilities and equipment at the national laboratories by university scientists. The Energy Manpower Assessment Program supports studies and analyses on the supply/demand of manpower at all levels for future energy programs. Finally, the Energy Graduate Traineeship Program, a new initiative proposed for FY 1982, will support on a competitive basis a small number of graduate level, predoctoral traineeships in energy-related disciplines where significant shortages of professional level personnel are predicted.

The purpose of the Multiprogram General Purpose Facility (GPF) program is to effect agency-wide support of these facilities at 12 multiprogram laboratories in order to assure the successful completion of assigned programs and missions. General purpose facilities include roads, site utilities and support buildings such as office and administrative buildings, maintenance facilities and garages. The GPF program provides formal recognition that systematic replacement and rehabilitation of aging facilities is a legitimate cost of doing business and that this problem area must be addressed on a continuing basis as long as the Department conducts major programs at the laboratories. Funding under the GPF program is restricted to projects where no one program uses more than approximately 60 percent of the facility. In addition, at defense multiprogram laboratories a multiprogram facility requirement results from expansion of nondefense program activities. The program approach is to systematically develop and execute construction projects in a prioritized manner to: 1) rehabilitate or replace deteriorated buildings; 2) replace trailers and other temporary facilities; 3) reduce overcrowding that is detrimental to safety and program effectiveness; 4) consolidate scattered operations; 5) rehabilitate or replace unreliable, inefficient and uneconomical utility systems, 6) correct deficiencies and maintain facilities to ensure that each site meets current environmental safety and health regulations and safeguards and securities requirements. The principal FY 1981 accomplishment is the start of design and construction of 13 projects at 8 separate locations. In addition, significant progress in structuring the program has been made in the establishment of a unified, multiyear approach to correcting facility deficiencies at the 12 multiprogram laboratories. The objective in FY 1982 to FY 1985 is to increase the program funding level to approximately $160,000,000 per year. This is the program level required to accomplish program goals given the size of the investment in the general purpose facilties at the 12 multiprogram laboratories, their age and the $2,000,000,000 backlog of deficiency-correcting projects.

Advisory and Oversight Program Direction provides funds for the personnel resources required by the Director of Energy Research to carry out his responsibilities specifically assigned by the Department of Energy Organization Act (P.L. 95-91) as well as those mandated by the Secretary in areas beyond the scope of the Energy Research programs. Included among these responsibilities are monitoring the Department's research and development program in order to advise the Secretary with respect to the well-being and management of the multiprogram laboratories; supervising or supporting research activities carried out by any of the Assistant Secretaries; and providing for program management of the Technical Assessment Projects, University Research Support, and Multiprogram General Purpose Facilities programs. The program provides funds only for the salaries and related personnel expenses for the personnel who carry out the studies, analyses, monitoring and coordination activities required to support the Director. It does not include any funds for outside contracts.

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

	FY 1980 Appropriation	FY 1981 Appropriation 2/	FY 1982 Base 2/	FY 1982 Request
Basic Energy Sciences				
Nuclear Science				
Operating expenses	30,500	32,400	32,400	37,800
Capital equipment	1,300	1,300	1,300	1,660
Subtotal	31,800	33,700	33,700	39,460
Materials Sciences				
Operating expenses	78,000	87,750	87,750	104,100
Capital equipment	6,300	7,100	7,100	9,630
Construction	11,650	300	300	4,500
Subtotal	95,950	95,150	95,150	118,230
Chemical Sciences				
Operating expenses	54,400	60,700	60,700	72,100
Capital equipment	3,700	4,140	4,140	5,960
Construction	4,300	3,200	3,200	6,100
Subtotal	62,400	68,040	68,040	84,160
Engineering, Mathematical and Geosciences				
Operating expenses	20,000	24,100	24,100	35,300
Capital Equipment	1,250	1,760	1,760	2,550
Subtotal	21,250	25,860	25,860	37,850
Advanced Energy Projects				
Operating expenses	5,000	6,350	6,350	9,000
Capital equipment	200	300	300	400
Subtotal	5,200	6,650	6,650	9,400
Biological Energy Research				
Operating expenses	6,000	7,250	7,250	9,500
Capital equipment	300	400	400	500
Subtotal	6,300	7,650	7,650	10,000
Inertial Plasma Physics Research 1/				
Operating expenses	6,400	5,400	5,400	7,400
Capital equipment	4,300	1,600	1,600	1,600
Subtotal	10,700	7,000	7,000	9,000
Program Direction				
Operating expenses	2,160	2,444	2,568	2,900
Subtotal	2,160	2,444	2,568	2,900
Total				
Operating expenses	202,460	226,394	226,518	278,100
Capital equipment	17,350	16,600	16,600	22,300
Construction	15,950	3,500	3,500	10,600
Basic Energy Sciences	235,760	246,494	246,618	311,000

1/Prior year funding provided through the Atomic Energy Defense Activities Appropriations.
2/Does not reflect general reduction of $508,000.

Authorization. Sec. 209. P. L. 95-91

Summary of Changes

FY 1981 Appropriation enacted	$ 246,494 1/
Built-in increases and decreases:	
Pay cost supplemental	124
FY 1982 Base	246,618
Program Increases and Decreases	
Basic Energy Sciences	
Maintain current level and provide for selected expansions in basic research programs in:	
Materials Sciences	+ 19,080
Chemical Sciences	+ 13,020
Engineering	+ 4,870
Applied Mathematical Sciences	+ 3,350
Geosciences	+ 3,770
Biological Energy Research	+ 2,350
Maintain current level of research in Nuclear Science and increase support of stable isotope program	+ 5,760
Expand support of Advanced Energy Projects	+ 2,750
Continue support of Inertial Plasma Physics Research	+ 2,000
Personnel-related increase for the above programs	+ 332
Increase support of accelerator improvement projects	+ 500
Complete construction of Chemical and Materials Sciences Laboratory	+ 3,100
Initiate construction of the High Temperature Materials Laboratory	+ 3,500
FY 1982 Budget Request	$ 311,000

1/Includes $7,000,000 for Inertial Plasma Physics Research provided through the Atomic Energy Defense Activities Appropriation

Basic Energy Sciences

Many of the Nation's current difficulties are due to reliance on an energy source, imported petroleum, that is both expensive and insecure. If this intolerable dependence is to end, it will be necessary for the United States to develop energy sources that are primarily of domestic origin and are acceptably priced. At the same time, means must be found to use all forms of energy more efficiently.

A variety of barriers impede rapid attainment of these objectives. Many of these barriers are due to inadequate technology. History has clearly shown that dramatic improvements in technology invariably come from the application of new scientific knowledge. The acquisition of such knowledge is the reason for the existence of the Basic Energy Sciences (BES) program.

The subprogram budget narratives that follow attempt to describe some of the research that has been done in previous years, and much that will be done with the requested funds. Such descriptions, due to the nature of BES' responsibilities, must try to convey the relevance and importance of over one thousand individual research projects, whose subject matter ranges over nearly all fields of modern science. There is, however, a common aspect of each of these projects: in some manner and in some time frame they can be expected to contribute to solution of the "energy problem". Each was selected with this in mind.

Ideally, in presenting the budget justification, all proposed tasks would be described sufficiently so that the reader could understand why the work is being done, what is hoped to be accomplished, and what would be the benefits. Equally important, a complete knowledge of all the components would make it clear that the total program is far more than a collection of separate projects. The sum of the parts is a research program with direction, coherence and priorities. Clearly, such a complete description is impossible.

Instead, we have tried to impart the essence of the BES program by a limited selection from the total.

The responsibility of BES is clear: the program managers must consider the merits of research on every aspect of energy, and select those topics that, when taken as a whole, comprise an optimum, balanced program of mission-oriented basic research. To carry out the program, BES plans, supports and administers energy related research in the physical and biological sciences, geosciences, engineering and applied mathematics. New scientific information in these areas will provide the fundamental scientific and engineering base on which the Nation's future energy options depend. The strategy is to:

- Provide critical knowledge and data and development of trained scientific talent through support of highly competent researchers in DOE mission areas;
- Provide for, and support operation of unique, specialized research facilities;
- Maintain liaison with other DOE programs, federal agencies and the scientific, academic and industrial communities;
- Use the scientific and industrial communities to identify needs and opportunities for research in energy relevant areas; and
- Promote early applications of the results of basic research.

Research carried out by the Basic Energy Sciences program cuts across the missions of all of the Department's technology development programs. The BES program management team provides a unique capability for marshalling scientific talent to attack problems that are critical to the Nation's energy needs. The cadre of scientists and engineers involved in the BES program includes professionals with years of experience, much of it stemming from the highly successful activities of BES and its predecessor organizations, in fostering and conducting creative basic research and in the management of major, complex research facilities. Several recent major accomplishments of the BES program were briefly discussed in the Program Overview portion of this budget request. In the much more detailed subprogram descriptions that follow, the program accomplishments will be expanded on further.

The Basic Energy Sciences program management has responded to the greatly increased requirements for research resulting from the formation of ERDA in 1975 to DOE in 1977. Each transition imposed new responsibilities for research. External advisory groups have repeatedly recommended increased funding for basic research support and have often called for BES to be given a larger role in developing the needed technology base for the different energy supply and conservation options. While BES is capable of increasing its scope of activities, it has not been able to do so to the extent recommended because of resource limitations.

In FY 1982, the Basic Energy Sciences request is for $311,000,000, an increase of $64,506,000 over FY 1981. Of this request, $275,200,000 is for operating expenses; $22,300,000 is for capital equipment; $10,600,000 is for construction; and $2,900,000 is for program direction. This budget request allows for significant enhancement of the newer subprograms of Biological Energy Research and Engineering, Mathematical and Geosciences, for expansion of the efforts to explore new concepts under the Advanced Energy Projects subprogram, and for Inertial Plasma Physics Research. It also includes continued increasing emphasis in:

- High temperature materials - corrosion, ceramics and coatings;
- Chemistry and physics of combustion processes;
- Chemical structure and behavior of coal;
- Catalytic mechanisms and surface phenomena; and
- Photochemistry for solar applications.

The request for construction funds allows for the completion of the Chemical and Materials Sciences Laboratory at Lawrence Berkeley Laboratory (LBL) in California and initiation of the High Temperature Materials Laboratory at Oak Ridge National Laboratory (ORNL) in Tennessee. These and other major areas of emphasis in FY 1982 are discussed in greater detail below in the seven major subprograms which make up Basic Energy Sciences. These are: 1) Nuclear Science; 2) Materials Sciences; 3) Chemical Sciences; 4) Engineering, Mathematical and Geosciences; 5) Advanced Energy Projects; 6) Biological Energy Research, and 7) Inertial Plasma Physics Research.

Nuclear Science

Objectives of the Nuclear Science subprogram are: 1) to expand our understanding of the properties and interactions of atomic nuclei; 2) to extend our knowledge of the chemical and physical properties of the actinide elements; and 3) to operate unique national facilities for nuclear research and for preparation of isotopes. These activities emphasize those areas most likely to be important for the nuclear fission and fusion energy technologies and related areas such as nuclear medicine.

Approximately one-quarter of the total Nuclear Science subprogram is a coordinated effort to establish a data base of nuclear information adequate to meet the long range needs of the fission and fusion energy technologies, nuclear regulatory activities, diagnostic and therapeutic uses of radioisotopes, nuclear waste management, and nuclear weapons research. This programmatic responsibility is discharged by direct measurement of nuclear data, by compilation of nuclear data into formats useful to applied scientists and engineers, and by evaluation of nuclear data into a single set of parameters which best describe experimental measurements. The evaluation work includes development of nuclear models which can be extrapolated to conditions that cannot be measured (for example, neutrons interacting with short-lived fission fragments in reactors).

Two-fifths of the Nuclear Science subprogram emphasizes fundamental research into the structure of nuclei and the interactions of nuclei with low energy protons, neutrons, deuterons, and helium nuclei. This work is conducted at university-based and national laboratory-based accelerator facilities and at BNL's High Flux Beam Reactor (HFBR). Approximately one-eighth of Nuclear Science supports research on the chemical and physical properties and the behavior of the actinide elements. A broadly-based understanding of these elements is essential because of their importance in understanding and developing nuclear waste management and fission reactor technologies and in medical and other uses.

The remaining portion is a service-oriented activity to provide special isotope samples for research, medical and industrial uses. In essentially all cases, this effort is the Free World's only source of isotopes in significant quantity. Three major isotope production facilities are supported at ORNL in Tennessee: the Calutron facility which separates stable isotopes, the High Flux Isotope Reactor (HFIR) which produces heavy actinide elements, and the Transuranium Processing Plant (TRU) which processes the HFIR targets.

The FY 1982 request of $39,460,000 for the Nuclear Science subprogram consists of $37,800,000 for operating expenses and $1,660,000 for capital equipment needs.

The major goals for FY 1982 are:

1) to reinstrument university-based and national laboratory-based nuclear research facilities so that they can meet the demands of frontier research. This is crucial to maintaining the overall United States position of leadership in nuclear research.

2) to establish programs at Oak Ridge Electron Linear Accelerator (ORELA) to measure systematic behavior of physical parameters which describe the interactions of neutrons with fission fragment and actinide nuclides. The technology related objective is significant improvement in our ability to extrapolate parameters to those nuclides which are long-lived enough to affect reactor operation but too short-lived for direct measurement.

3) to complete transfer to Brookhaven of responsibility for coordination of the Federal effort for storage and distribution of compiled and evaluated nuclear data. This transfer will produce operational efficiencies and improved service to users of nuclear data.

4) to establish systematic studies of those chemical properties of the actinide elements which jointly bear on nuclear waste storage or processing and on their purification for numerous uses.

5) to improve the efficiency and productivity of stable isotope production facilities. These facilities were constructed during World War II and are now in urgent need of modernization.

Operating Expenses

Nuclear Science
Summary of Operating Expenses

	Budget Authority	
	FY 1981	FY 1982
Low Energy Nuclear Science		
Nuclear Research	$12,565	$14,470
Nuclear Data Measurements	5,185	5,900
Nuclear Data Compilation and Evaluation	2,575	2,900
Heavy Element Chemistry	3,620	4,155
Subtotal, Low Energy Nuclear Science	$23,945	$27,425
Isotope Preparation		
Electromagnetic Isotope Separation	$ 1,320	$ 2,450
Special Isotope Preparation	7,135	7,925
Subtotal, Isotope Preparation	$ 8,455	$10,375
Total, Nuclear Science	$32,400	$37,800

Low Energy Nuclear Science

The operating expenses request for FY 1982 for Low Energy Nuclear Science is $27,425,000, an increase of $3,480,000 above the FY 1981 level. The work supported under this activity is carried out in four main subactivities: Nuclear Research; Nuclear Data Measurements;Nuclear Data Compilation and Evaluation; and Heavy Element Chemistry. Work under the Nuclear Research, Nuclear Data Measurements, and Nuclear Data Compilation and Evaluation subactivities is within the scope of the long-range National plan for basic nuclear research developed by the DOE/NSF Nuclear Science Advisory Committee (NSAC). The plan has been accepted by the Department of Energy, the National Science Foundation, and the Office of Science and Technology Policy as a framework for a coordinated Federal program in basic nuclear research. This FY 1982 budget request for Nuclear Science represents a major step toward full implementation of the NSAC plan. The plan establishes relative priorities among the competing subfields of basic nuclear research and is constructed as a delicate balance among the needs of basic nuclear research for: 1) new national facilities and major instrumentation; 2) efficient utilization of existing facilities; 3) long term viability of the smaller university-based accelerator facilities; and 4) adequate levels of scientific manpower.

The FY 1982 request for Nuclear Research is $14,470,000, an increase of $1,905,000 over the FY 1981 level. This request would support experimental research in low energy nuclear physics at FY 1981 levels of manpower and would permit initiation of major reinstrumentation projects at University of Colorado and Duke University. These very fundamental studies, particularly those involving neutrons, also provide information which is relevant to long-term development of fission and fusion energy systems including nuclear waste management.

Our long-term goal is a quantitative understanding of the structure of nuclei and the mechanisms by which nuclei interact with light ions and neutrons. Low energy studies now generally require high precision, high resolution, and other cabilities such as the ability to control the spins of both the projectile and target nuclei. Thus, development of electronics, nuclear radiation detectors, ion sources and other instruments is an important component of this activity.

A new facility that has been brought into operation is the TRISTAN II on-line isotope separator at the High Flux Beam Reactor (HFBR) at the Brookhaven National Laboratory. The most advanced in the world, TRISTAN II sorts by mass the fragments resulting from nuclear fission. This is done by a system of magnets. After such sorting, scientists study the nuclear properties of individual fission products. Important new programs (e.g., nuclear structure studies of neutron-rich nuclides and delayed neutron emission studies important to nuclear power development) are being conducted by a number of university user groups (Clark University, Cornell University, the Georgia Institute of Technology, University of Maryland, and the University of Oklahoma). Several of the national laboratories, notably Ames Laboratory, where the TRISTAN separator was originally developed, are also involved in the work at BNL. Experiments to study these mass-separated fission products by laser techniques are also being developed by scientists from Iowa State University and Texas A&M University. From these laser experiments, scientists will determine the shape or deformation of short-lived fission fragment nuclides and thus improve our understanding of how basic nuclear parameters change when neutrons are added to a stable core of protons and neutrons.

A powerful new technique has been developed at the BNL HFBR facility. This technique employs beams of neutrons filtered through particular materials to produce what is called "average resonance capture" in the target nuclei. Application of this technique recently provided the principal test of the new Interacting Boson Approximation (IBA) nuclear model. The IBA model represents a revolutionary new way of describing nuclear structure. IBA provides a unified framework within which apparently conflicting nuclear properties can be understood. Because of the importance of IBA to nuclear structure research, these "average resonance capture" experiments will be extended in FY 1982 to nuclides beyond the mass region studied so far.

Another long-term project at BNL, solar neutrino research, continues to excite the interest of astrophysicists and others interested in stars and how they burn. Neutrinos emitted in the course of nuclear reactions in the deep interior of the sun are our only direct source of information on physical processes occuring at the center of the sun. All other radiations are absorbed and re-emitted many, many times before the energy and/or particles escape the solar surface. Comparison of data from the BNL experiments with the best of present theoretical models of the sun shows an astounding discrepancy. Numerous attempts at modifying stellar models to fit the BNL data have failed in the sense that the required modifications are too drastic and/or are in conflict with other astronomical data to be credible without complete overhaul of our present understanding of stellar evolution. Steps to resolve this cosmological puzzle are in progress with a new detector system with unique, advanced capabilities.

The cyclograaff accelerator at Duke University (the major facility at the Triangle Universities Nuclear Laboratory (TUNL) that also includes the University of North Carolina and North Carolina State University) and the cyclotron at the University of Colorado continue to be very productive in research output. At TUNL, pulsed beams of monoenergetic polarized fast neutrons of intensities now adequate for important new reaction studies are now available as a result of the recent upgrading of the polarized ion source and associated apparatus there. In 1982, we plan to use these new capabilities to gain new knowledge of the mechanisms by which target nuclei capture and/or scatter projectile neutrons. At the University of Colorado, it has proved valuable to use their low energy cyclotron to complement reaction studies underway at higher energies at the Tri-Universities Meson Physics Facility (Canada) and the Clinton P. Anderson Meson Physics Facility (Los Alamos, New Mexico). The relative strength of competing mechanisms by which projectile protons interact with target nuclei varies with the energy of the proton. Thus experiments at a variety of energies are essential to understanding the competing reaction mechanisms. At the University of Wisconsin, a number of studies are underway that require the record performance of the new crossed-beam polarized ion source recently invented and constructed there. These include fundamental studies of the two nucleon system. Four other accelerators are jointly supported by the Nuclear Science subprogram and Nuclear Physics program (Office of High Energy and Nuclear Physics), since they are extensively used for both light- and heavy-ion research studies. These are the MP tandem Van de Graaff at Yale University, the University of Washington double FN tandem Van de Graaff, the 88-inch cyclotron at Lawrence Berkeley Laboratory, and the Texas A&M University cyclotron. Support for research groups with proven excellence will continue at these facilities. In general these four groups are conducting Low Energy Nuclear Science research on the mechanisms by which light projectile nuclei transfer mass and energy to target nuclei, basic structure of individual nuclear states and examination of fundamental physical symmetry laws as they apply to nuclei.

The budget request for Nuclear Data Measurements is $5,900,000, an increase of $715,000 over the FY 1981 level. These funds are required to support measurements to provide nuclear data information for the Department's applied technologies. In many cases, of course, the data are also of interest to basic nuclear theory, particularly in the development of theoretical models to explain broad areas of nuclear structure. The funding request is divided almost equally between measurements needed for fission and fusion energy technologies.

The measurements devoted to satisfying the highest priority nuclear data needs of the Office of Fusion Energy are coordinated by a working group that includes representatives from three national laboratories (ORNL, LANSL, and LLNL) and two universities (Duke University and Ohio University). The largest measurement program in support of the fusion program is that conducted at the Oak Ridge Electron Linear Accelerator (ORELA) where, for example, measurements have just been made of the total cross sections for 12 materials for neutron energies from thermal energies up to 80 MeV. These are data required for the shield design of the Fusion Materials Irradiation Test (FMIT) facility, under construction at Hanford. The LLNL group makes use of the world's most intense continuous source of 14-MeV fusion neutrons to make difficult measurements of the charged-particles (such as hydrogen and helium nuclei) produced when candidate fusion reactor materials are bombarded with neutrons, as they would be in a working fusion reactor. This information is especially needed for estimating radiation damage.

The Ohio University, Duke University, and LANSL tandem Van de Graaff accelerators are used 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. LANSL is also making precise absolute measurements at the lowest possible energies of reactions involving deuterium and tritium (fuels of the first generation of fusion reactors). This LANSL data is also needed for development of diagnostic techniques and instruments for the Tokamak Fusion Test Reactor being built at Princeton.

For the fission portion of the program, the Office of Nuclear Energy has recently identified long range reactor nuclear data needs which require the unique measurement capabilities of ORELA. These include several fission product capture cross-sections for isotopes that dominate the neutron absorption in fast reactors under long fuel burnups and the determination of systematics of reaction cross-sections in the actinide region. The work supporting the fission program also includes measurements just completed at ORNL of the average number of neutrons released during the spontaneous fission of californium-252, the standard by which the neutron emissions from all other fissionable materials are measured. At ANL, measurements of the yields of fast-neutron-induced fission products from the important fissile and fertile nuclides using nearly monoenergetic neutrons over an energy range of 0.1 to 8 MeV continue. These data permit accurate modeling of the fission products produced by any fission reactor neutron spectrum and are of special utility to the fast breeder reactor effort. At the National Bureau of Standards the activities relating to the measurement and development of neutron cross section standards are currently supported by Nuclear Science. At LLNL, 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. ORNL's measurement of actinide cross sections continues to contribute 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 ingenious new detection techniques to overcome the effects of the high-level background of alpha-particle emission. Other cross section measurements at the ORELA are performed by groups from Denison University in Ohio, the State University of New York at Albany, and Middle Tennessee State University. More precise measurements of the 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 Colorado School of Mines, the University of Michigan, the University of New Mexico, the University of Washington, and the Rensselaer Polytechnic Institute in New York.

The request for Nuclear Data Compilation and Evaluation is $2,900,000, an increase of $325,000 over the FY 1981 amount. These funds will support most of the Nation's effort in nuclear data compilation and evaluation. This effort is now coordinated by the National Nuclear Data Center (NNDC) at BNL, which receives the majority of its funding from the Nuclear Science subprogram. Other contributors to NNDC are the programs of the Assistant Secretary for Nuclear Energy, the Office of Fusion Energy, and the Electric Power Research Institute. NNDC has responsibility for the compilation of neutron data produced in the United States and Canada and coordinates a large national effort in the evaluation of neutron data via its Cross Section Evaluation Working Group (CSEWG).

The Center also has 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, and the National Bureau of Standards (NBS), and the University of Pennsylvania. All but the NBS effort is funded by Nuclear Science. The United States program is being supplemented by coordinated international participation in the nuclear structure and decay data evaluation effort which has been established with the cooperation of the International Atomic Energy Agency (IAEA). With the IAEA's assistance, it is expected that our goal of a 4-year update cycle for all mass chain data sheets can be achieved. The maintenance of an up-to-date data file will make unnecessary, or much simpler, many of the special compilation and evaluation projects needed to meet specific information requirements for users such as the Nuclear Regulatory Commission and the biomedical community. The experienced group at LBL that produced the Table of Isotopes is now preparing specifications and formats for a Radioactivity Handbook that will derive most of its input from the computerized file of evaluated nuclear structure and decay data generated by the international network.

The FY 1982 budget request for the Heavy Element Chemistry subactivity is $4,155,000, an increase of $535,000 over the amount appropriated in FY 1981. These funds support a broadly based research program on the chemical and physical properties of the actinide elements and are needed to maintain approximately the same level of support as in FY 1981. This effort in heavy element chemistry comprises a close-knit group of projects which are building on painstakingly developed knowledge of the past thirty years and exploiting modern chemical techniques. The three principal objectives of heavy element chemistry research are: 1) to predict the chemical behavior and migration possibilities of actinide elements in anticipated environments of nuclear waste storage; 2) to lay the groundwork of understanding toward purer separations of the actinide elements and their isotopes for scientific, medical and industrial purposes and 3) to provide chemical knowledge on actinides necessary for a viable option of processing spent nuclear fuel in both economically and environmentally acceptable fashion.

A thorough understanding of the behavior and interactions of the actinide elements is important in the development of fission power systems and for the development of effective nuclear waste management methods. Therefore, fundamental studies of the magnetic, spectroscopic, and thermodynamic properties and chemistry of the formation of discrete compounds of most of the actinide elements have been underway for some time. Research includes studies of the chemistry of the actinide elements in solid compounds and gaseous states and the investigation of the behavior of actinides in aqueous and nonaqueous solutions. These latter studies are important to the separation of the freshly formed actinides from their production mixtures and from spent nuclear fuel, as well as to the study of actinides in the environment. An entirely new data base is required to understand the chemistry of actinide elements under various environmental conditions, and therefore a significant portion of this subactivity is being redirected toward research in this area.

The actinide elements are all radioactive. Most of this research is carried out at the national laboratories where the proper handling facilities are available for the more radioactive elements. Some studies of uranium, thorium and other actinides at lower levels of radiation are pursued at universities, but university-based scientists also pursue research at the laboratories in a user mode which fosters sound collaboration among scientists.

At the Lawrence Berkeley Laboratory substantial progress has been made in the search for agents capable of removing plutonium from biological systems. Preliminary tests with a new chemical, LICAM-C, show that when injected into mice and dogs this agent removes 70% to 90% of the in-vivo plutonium with minimum-to-no toxic side effects. This is significant because further work in this exciting project is planned in FY 1982 including the development of agents for the similar removal of americium and curium. This is important because of the possibility that nuclear workers might be accidentally contaminated with those very toxic substances.

At the Argonne National Laboratory this subactivity supports research in three general areas: spectroscopic studies of the manner in which light is absorbed and emitted by the actinide species under various chemical conditions; study of the chemistry of actinide-containing solid and gaseous compounds; and study of the behavior of actinides in aqueous solutions. The considerable expertise developed at ANL in actinide solution chemistry and spectroscopy has resulted in the development of three new research techniques for the determination of the chemical behavior of low concentrations of actinide elements which might occur near nuclear waste repositories. These techniques generate much needed data for shaping reliable predictions of the movement of nuclear wastes through the environment. Argonne's study of the chemistry of actinides in solid compounds has been recently redirected to an investigation of the synthesis and chemical and thermodynamic stability of types of materials of potential use as nuclear waste forms.

At the Oak Ridge National Laboratory this subactivity supports research in two general areas: the fundamental study of actinide reactions and properties, and the application of basic research techniques to the understanding of the behavior of actinides in nuclear waste management systems. The fundamental studies are done in collaboration with the actinide chemistry programs at LANSL and the University of Tennessee. These groups are expanding our understanding of the magnetic, electronic, structural, and thermodynamic properties and behavior of the heavier (less available) actinides where definitive data have heretofore been unavailable. A basis for an improved understanding of these nuclear materials is being provided by more information on the stabilities of actinide chemical compounds; an understanding of the unique behavior of the electrons in actinide elements and the consequences of this behavior in the properties of these materials; and new insight into the chemical effects of the radioactive decay of the actinides. In relation to nuclear waste management, basic research is underway to find host substances which will so strongly bind the actinides as to prevent their being leached out by natural waters. The inclusion of actinides in phosphate and titanate compounds is under study as these compounds have low ground-water leach rates and are known to be remarkably inert to chemical change over geologic time. This research is done in collaboration with research funded by the BES Division of Materials Sciences and is complementary to the work at ANL described above.

At the Los Alamos National Scientific Laboratory two projects are supported. The study of high temperature actinide thermodynamics will soon complete the vapor pressure measurements on einsteinium metal - the heaviest actinide for which these measurements can be made - and will turn to a study of the vaporization properties of compounds of potential interest to the high temperature processing of actinides. This is important to future possibilities for separating pure actinides or their isotopes from each other and from other chemical elements. This effort is unique in that it can make measurements on the very small existing amounts of some of the transplutonium materials. The second project deals principally with the chemistry of uranium and is expanding our knowledge of its higher oxidation states; this bears on the potential use of uranium as a catalyst, on advanced concepts for isotope separation technology, and on nuclear fuel reprocessing.

The university-based effort funded by this subactivity is particularly significant since it provides newly trained scientists, who are now in short supply, for the study and handling of actinides. These activities are largely conducted at the national laboratories by academic users who have access to the expensive specialized facilities. Some important recent advances by the university scientists include the characterization of chemical extractants of potential application in waste processing technology and an improved understanding of the reactions of actinides with environmental humic acid.

Isotope Preparations

A further activity supported under the Nuclear Science subprogram is the production, purification and allocation of special isotopes for investigations of the chemical and physical properties of the actinide elements and their compounds and of the nuclear properties and interactions of atomic nuclei. Thus this activity directly supports the DOE fission and fusion energy technology development programs. Cost-recovery sales are also made for necessary medical and industrial requirements which have no other practicable sources. The FY 1982 budget request for Isotope Preparations is $10,375,000, an increase of $1,920,000 over the amount appropriated in FY 1981. These funds are needed to maintain the operation of three major facilities at ORNL: the Electromagnetic Isotope Separation Facility (Calutrons), the High Flux Isotope Reactor (HFIR), and the Transuranium Processing Plant (TRU).

The Calutron operation produces multigram samples of various isotopes for loan to DOE researchers. This is referred to as the Research Materials Collections (RMC) program. The materials are available for non-destructive research and can be used where the experiments will not contaminate the sample. Each year loans are made whose total value exceeds $5,000,000, and approximately 50 percent of the Collection is on loan at all times. One of the primary uses of the RMC is in the determination of neutron cross-sections for fusion and fission reactors. Since the inception of the program in 1956, the Calutrons have enriched 233 stable and 26 radioactive isotopes of 60 elements including certain long-lived actinides. A recent enrichment of a plutonium sample resulted in 200 grams of high purity (greater than 99.9%) Pu-242 for DOE programs in safeguards, basic and environmental research, and neutron flux dosimeters. The Calutrons also produce samples for sale, on a production-cost-recovery basis, to the nuclear medical and industrial communities and to research groups where the material is destroyed or contaminated in experiments. Over 2000 shipments per year are made to domestic and foreign customers. This facility is a national resource and represents the major portion of the Western World's capacity for electromagnetic isotope enrichment.

The high atomic number, high mass transplutonium elements are produced in HFIR by neutron irradiation of curium-loaded targets which are processed and purified in the TRU facility. HFIR also provides irradiation services for non-routine isotope production, as well as ongoing user research programs on a cost-recovery 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 actinide samples from the HFIR/TRU complex are allocated largely to the investigators supported under the DOE programs in Nuclear Physics and Nuclear Science, but materials are also distributed to foreign institutions in which United States investigators are working.

Capital Equipment

The FY 1982 capital equipment request for Nuclear Science is $1,660,000, an increase of $360,000 over the amount appropriated in FY 1981. Of this total, $1,035,000 is needed for Nuclear Research, Nuclear Data Measurements, and Nuclear Data Compilation and Evaluation; and $625,000 is needed for Heavy Element Chemistry and Isotope Preparation. 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 sophisticated items of equipment. Nuclear Science research is conducted at a number of low energy, light-ion nuclear particle accelerators, nuclear reactors, and radioactivity-protected research facilities. These are located primarily at the national laboratories and, to a lesser extent, at universities. In order that these facilities conduct nuclear research at the frontiers of the field, it is imperative that modern scientific equipment continuously be provided.

At ANL, equipment is needed for the experiment being set up to measure the electric dipole moment of the neutron and also for new experiments planned to use lasers to measure isotope shifts and structure in radioactive atoms. Continued instrumentation of the TRISTAN II on-line isotope separator must proceed on schedule for optimal use of this new facility at BNL. Included are beam-line modifications, installation of the line for the laser experiments, completion of the helium-jet target system and the purchase of additional solid-state detectors. At ORNL the ORELA must soon obtain a new klystron (source of RF power for the accelerator) to ensure uninterrupted operation, and among the many smaller items needed is a xenon and helium gaseous scintillation system to measure sub-threshold fission cross sections.

Also at ORNL, a variety of equipment items is needed in support of the actinide chemistry research program. The collaborative effort with the University of Tennessee requires a larger-scale magnetic susceptometer to examine the chemical states of actinides trapped in more leach-resistant matrices for permanent waste storage. Structural studies of solid compounds of actinides require a modern x-ray generator, and thermodynamics and reaction studies of these materials require a differential scanning calorimeter. To realize a substantial increase in isotope separation efficiency, high-speed centrifuges are required at the Calutron facility to prepare "pre-enriched" feedstock. The actinide chemistry program at ANL needs a krypton-ion laser to extend the spectral region in which plutonium compounds can be examined.

Materials Sciences

The objective of the research effort in Materials Sciences is to increase our understanding of all materials related phenomena and properties underpinning the nation's energy development effort. It is well known that materials problems often are pace setting in the development of new systems, the performance of present systems and the evolution of advanced concepts. The nation cannot afford to fall behind in this field. In Materials Sciences, emphasis is placed where significant improvements in performance must depend on improved understanding of the underlying mechanisms that control materials properties. The subprogram covers a broad spectrum of research from which new solutions and new materials will be uncovered to apply to existing problems, insight will emerge to identify future materials problems, and working models can be formulated to deal with unpredicted phenomena when encountered. Some of the research is directed at a single energy technology (e.g., photovoltaic materials for direct conversion of solar energy into electricity), whereas other research is applicable to many technologies simultaneously (e.g., the embrittlement of structural materials due to the presence of hydrogen) and still other research has more fundamental implications underpinning all materials research (e.g., mechanisms of atomic transport in solids). Materials Sciences research is conducted primarily by personnel trained in the disciplines of metallurgy, ceramics, solid state physics, materials chemistry and engineering.

This subprogram is basic or long range in nature and is intended to provide the necessary base of materials knowledge that is needed to advanced our energy technologies. Emphasis is placed on areas where problems are known to exist or are anticipated and on generic areas of fundamental importance. Another aspect of the program is the development and utilization of unique facilities used not only by DOE contractors but also by other laboratory, university and industry scientists. Among these are facilities which will begin operation in mid-FY 1981 and will require full year operational costs in FY 1982, including the National Synchrotron Light Source (NSLS) at BNL, the Intense Pulsed Neutron Source at ANL and the nation's highest voltage electron microscope (1.5 MeV) at LBL. Research using these new facilities and other existing facilities is essential for this program to remain at the forefront of materials science.

The importance of basic materials research in the development of energy systems is clear when various examples of the problems and opportunities are considered: for solar photovoltaics - better processing techniques are needed to reduce cost, improved understanding of the mechanisms of degradation is needed to increase reliability and battery materials problems need to be solved for better energy storage; for synfuels production - corrosion, erosion and catalyst deterioration need to be fundamentally understood in order to improve efficiency; for nuclear waste isolation - improvements in glass/ceramic host materials are required and canister deterioration needs to be investigated; and for fusion - better superconducting materials need to be developed and the effects of high energy neutron radiation damage need to be understood.

At the DOE laboratories, technology and information transfer takes place between the basic and applied programs co-sited there. The Materials Sciences subprogram also supports research at universities and to a lesser extent industrial laboratories, taking advantage of the unique expertise of researchers at each of the different types of institutions. Coordination of DOE's applied materials development efforts with the Materials Sciences subprogram takes place primarily through the DOE Energy Materials Coordinating Committee (EMaCC). Materials Sciences Research Assistance Task Forces and less formal contacts among staff members round out the coordination efforts in DOE. The program utilizes workshops and reports of its Council on Materials Science (a non-governmental body with representatives from academia, industry and DOE laboratories) to help focus on critical issues. For example, in FY 1981, the Council reviewed research needs and opportunities in the areas of amorphous materials and nondestructive evaluation; in FY 1980, corrosion and novel materials were examined. Interagency communication and coordination are handled primarily through the Committee on Materials (COMAT), an interagency body comprised of senior representatives from appropriate governmental agencies, and through an Interagency Materials Group. The above are only a few examples of the mechanisms used for coordination, communication and operation within the materials sciences community.

During the past year significant progress has been achieved in a number of areas. A few examples include: the preparation of crystalline silicon photovoltaic materials with further improved efficiency using ion implantation techniques; the development of an amorphous silicon structure showing the role of hydrogen in photovoltaic response; the demonstration, using thermodynamic studies, of how radioactive iodine behaves under nuclear reactor conditions; the development of dual-phase steels for possible use in energy efficient cars; the preparation of hard coatings of titanium diboride which are extremely erosion resistant; the development of superconducting devices which can be used in the field to detect underground deposits of various types; the understanding of the kinetics of hydrogen permeation through thin coatings which enhance the permeation; the use of neutron scattering and x-ray scattering to detect oil droplets in shale; and the development of a new class of cryogenic steels. These and many other recent accomplishments are discussed in more detail below.

The FY 1982 request of $118,230,000 for Materials Sciences includes $104,100,000 for operating expenses, $9,630,000 for capital equipment and $4,500,000 for construction.

Operating Expenses

The FY 1982 request for operating expenses for Materials Sciences is $104,100,000, an increase of $16,350,000 over the FY 1981 level. This level is necessary to continue the Department's basic research program in materials which underpins all the energy technology programs. It will also permit commitments to be met arising from new equipment and facilities under development or recently completed. Two new facilities, the IPNS-I and the NSLS, will begin operation in mid-FY 1981 and will require full year operation costs in FY 1982. The increase required by Materials Sciences for NSLS operational costs alone is $2,500,000 (another $2,500,000 is being requested by Chemical Sciences). The high voltage electron microscope at LBL will also begin operation in mid-FY 1981 and require full year operation in FY 1982. Selected new initiatives will be undertaken at the expense of other programs being phased out. Increased efforts will be undertaken in high temperature materials, surfaces and surface modification, synfuel-related materials areas, and nuclear waste isolation research. The fraction of program funds designated for support of university-based research will be preserved (approximately 20%). In addition, funding will be allocated for university/industry/laboratory user groups to exploit the research capabilities of the new facilities.

The funding needs for the Materials Sciences subprogram will be discussed below for three major activities: Metallurgy and Ceramics, Solid State Physics and Materials Chemistry. The following table shows the funding for each of these three activities:

Materials Sciences
Summary of Operating Expenses

	Budget Authority	
	Estimate FY 1981	Estimate FY 1982
Metallurgy & Ceramics	$38,650	$ 44,620
Solid State Physics	37,715	46,930
Materials Chemistry	11,385	12,550
Total Materials Sciences	$87,750	$104,100

Metallurgy and Ceramics

The objective of research conducted under the Metallurgy and Ceramics activity is primarily to understand better how the behavior and properties of various metallic and ceramic materials are related and controlled by the structure of the materials and how they are processed (i.e., the methods and techniques used to prepare, form or fabricate materials). As a consequence of improved understanding, better materials and a greater ability to predict their behavior in energy systems are possible. An example illustrates this point: when it was known that a more efficient magnetic (property) material resulted from an amorphous (rather than crystalline) structure and that amorphous metallic structures could be produced by rapid quenching (processing), an entire new class of transformer core materials was created and is now under development in industry. Substitution of these amorphous steels for current transformer steels could save, it is estimated, about $200,000,000 in electrical energy losses per year. In the quest for new understanding, recent advances in techniques capable of observing types and arrangements of atoms on an ultra-microscale (down to the individual atom in some cases) have created research opportunities nonexistent just a few years ago. Advanced energy systems such as coal conversion or fusion will likewise challenge the present foundation of knowledge of materials performance, thus making even more important this fundamental research to develop new materials and to predict their behavior.

The FY 1982 request of $44,620,000 will support activity in Metallurgy and Ceramics at approximately the same level as in FY 1981 with some selected new projects and added emphasis for new facility-related research. Research at the new 1.5 MeV high voltage electron microscope at LBL will be initiated in mid-FY 1981 and will require additional funding for full operation in FY 1982. Radiation effects and neutron scattering research initiated at the IPNS-I in mid-FY 1981 will continue during the full year of FY 1982. The high voltage microscopes at ANL and ORNL will be operated in FY 1982 with about half of their operating time allocated to outside users. Increased support to build-up research groups utilizing the NSLS is included in this request. A modest increase is allowed for unsolicited proposals from universities and industry.

Research on high temperature alloys, ceramics and coatings will receive priority emphasis with particular attention to the environmental effects of sulfur, ceramics processing and the use of lasers for materials processing. The coupling of mechanical properties to nondestructive evaluation will be sought to further the quantitative predictive aspects of nondestructive evaluation. Research on corrosion will continue to receive emphasis as well as the structure and properties of amorphous and rapidly solidified materials. In addition, the following topics will continue to be emphasized: solar energy-related materials interface research; fusion-related work on radiation effects, both at high and low temperatures; synfuels-related research on erosion/corrosion phenomena in coal conversion-type atmospheres; and battery and fuel cell electrode/ electrolyte behavior.

Although much still remains to be done, by building on recent progress the research to be undertaken this next year will move the field closer to the ultimate goal of not only being able to predict materials behavior as a function of time, stress, temperature and a variety of other environments, but also being able to create new metal and ceramic structures to meet the severe engineering requirements for emerging energy systems. Research in metallurgy and ceramics is discussed in greater detail under the following five subactivities: Structure of Materials, Mechanical Properties, Physical Properties, Radiation Effects and Engineering Materials.

In the Structure of Materials subactivity, research is undertaken which encompasses electronic and atomic structure, crystallographic and morphological features and local chemistry. The criticality of this task reflects the intimate dependence of the mechanical, physical, radiation resistance, and engineering behavior of metals and ceramics on their structure. Structure of materials research includes the application of both forefront and standard techniques involving high voltage, analytical, atomic resolution, and scanning transmission electron microscopes, x-ray photoelectron spectroscopy, and extended x-ray absorption fine structure analysis. The electron microscope facilities at ANL, the University of Illinois, LBL and ORNL are widely used by scientists from other institutions that do not possess these unique instruments. These techniques are being used especially on problems concerning corrosion, coal, solar photovoltaics, and radioactive waste storage. In 1982 work will be expanded in high temperature structural ceramics, protective barriers and coatings for combustion materials, hot corrosion in weldments, and degradation of ceramics in coal-derived environments.

The FY 1982 request of $13,140,000 for Structure of Materials is required to sustain recently initiated research on topics such as behavior of refractory materials in hostile environments; sintering studies of complex ceramic materials to control their structures and properties; electrically conducting ceramics for fuel cells, high temperature batteries, and magnetohydrodynamic systems. University research utilizing the National Synchrotron Light Source will also be emphasized. Planned program reductions include rare earth metals preparation, surface studies and metal-insulator-semiconductor photovoltaics.

An improvement in the strength of steel was recently made under this program. The strength and fracture resistance of steels depend on the structure and distribution of the phases of iron present -- in this case, ferrite and martensite (this is termed dual-phase steel). The composition of these phases was studied using unique electron microscopy equipment at LBL, making it possible to optimize the structure of steel for strength, fracture resistance and fabricability. As a result, a new class of steel alloys having greater strength and fracture resistance per unit weight was developed. These dual-phase steel alloys can be fabricated using current commercial methods. The annual energy savings possible through weight reduction by using these dual-phase steels in cars, trucks and trains may approach 10 percent of the 20 quads currently consumed by the transportation sector.

In the solar energy area, a method has been developed to control the di- and tri-hydride content in amorphous silicon hydride. This modification results in increased photovoltaic efficiency. The defect structure of silicon and the nature of the alloyed hydrogen determine the alloy's optical and electrical behavior which in turn governs its photovoltaic efficiency. It has been found that initial introduction of hydrogen into the amorphous silicon matrix forms silicon monohydride, which has a good photovoltaic response. As more hydrogen is added, however, di- and tri-hydrides form which degrade the photovoltaic properties. Recent results following up on previously reported research have shown that the additional implantation of other elements (e.g., helium) can displace the hydrogen from the dihydride to the monohydride configuration, thus opening the possibility of tailoring alloys for optimum performance.

The Mechanical Properties subactivity supports research on the behavior of metals and ceramics subjected to various stress conditions and environments, particularly creep fatigue and stress corrosion cracking. These important phenomena affect the efficiency and reliability of components in various energy systems. The objective of this effort is to correlate macroscopic properties such as strength and fracture resistance with microscopic flow mechanisms and microstructural features. Understanding mechanical properties of metals and ceramics is crucial since plant safety and reliability depend on these properties, whether in nuclear reactor systems, synfuel plant systems, or transportation vehicles. The university community role is vital and as a consequence three fourths of the funds for mechanical properties research is spent in universities.

During the past year, progress was made in the development of steels for service at cryogenic temperatures. This development is relevant to energy applications such as liquid natural gas vessels and structural supports for superconducting magnets. The research culminated in the development of an attractive new class of nickel-free cryogenic steels. In order to obtain satisfactory strength and fracture toughness in these steels it was necessary to understand brittle fracture paths and process the metal to avoid these. In particular, boron was added to the alloy to suppress intergranular failure.

The failure of stressed components in coal liquefaction pressure vessels is often caused by hydrogen. High hydrogen pressures cause detrimental methane bubble formation in steels. The presence of these bubbles reduces strength. A model was derived to show the physical mechanisms controlling various states of bubble growth. An important practical implication of this work is that the bubbles can be removed by proper heat treatment.

In the development of constitutive equations to describe creep formation of metal alloys (e.g., in high temperature power plant components), pioneering work on zircalloy has elicited interest from the electric utilities' Electric Power Research Institute (EPRI). Specifically, EPRI provided material for determining the effects of crystallographic orientation on the behavior of fuel pin cladding in light water reactors, so that data needed to assess the validity of constitutive equations for design of reactor fuel pins could be gathered.

The above examples illustrate the need for and the contributions made by materials science to alloy development and component design for energy systems. In addition to the above research areas, which will continue, several new thrust areas are emerging. Two such areas are high temperature failure mechanisms in structural ceramics and metals (where grain boundary phases play a dominant role) and environment-assisted fracture (where synergistic interactions between an environmental contaminant and a grain boundary segregant control the local deformation and fracture). Research in these areas has recently been started which will continue to develop and exploit new techniques using small angle neutron scattering for examining cavity nucleation in creep and using scanning for detecting initiation of stress corrosion cracking. Two other areas where greater effort is needed are ductile fracture in materials with complex microstructures (such as weldments, where the assumption of fracture mechanics treating the alloy as a homogeneous continuum is not valid) and deformation and failure in amorphous metals (for which structure-property correlations have not been obtained). To support all of the above research on mechanical properties, $8,110,000 is required.

Physical Properties research is concerned with increasing the understanding of the thermal, optical, transport, and electrical properties and the behavior of materials, including the effect of processing treatments and exposure to in-service environments. Recent emphasis has been on corrosion, transport processes in radioactive waste containing ceramics and glasses, and the fabrication of fully densified ceramics of value in all energy technologies. The effort on fast-ion conductors for battery applications has been sustained, whereas work on superconductivity will be further reduced. Lower priority efforts on solar thermal energy materials, and ceramic-metal interfaces will be phased out.

A recent accomplishment of this research effort involves the kinetics of hydrogen permeation in metals. The properties of many materials are strongly affected by hydrogen on their surfaces or the diffusion of hydrogen into them. Recent experiments have led to a quantitative understanding of the rate at which hydrogen is dissolved in metals. It has been demonstrated that thin layers of palladium on niobium metal dramatically increase hydrogen absorption, with the significant result that every hydrogen molecule impinging on the surface splits into separate hydrogen atoms, which are subsequently absorbed. The experimental results show that the surface reaction steps of adsorption and dissociation are two hundred times greater on a palladium-coated niobium surface than on a clean, uncoated niobium surface, and that a similar enhancement of the permeation of the hydrogen atoms through the niobium also takes place with the palladium-coated niobium surface. This work is expected to provide guidance for new catalyst development where an increase of one or two hundred in hydrogenation catalyst reactivity would constitute a significant breakthrough. In addition, this research will impact on hydrogen storage technologies, in which rapid hydrogen permeation into and out of materials is required, yet limited by surface reactions.

The rate of oxidation-corrosion of many materials is controlled by the diffusion transport (rate at which atoms move through a substance) of the underlying metal through the oxide corrosion surface layer. Materials with improved oxidation-corrosion resistance would be of benefit to many energy technologies and this understanding is essential for the design of such materials. Recent measurements of diffusive transport of iron in iron oxide have lead to a detailed mechanistic understanding of this process, by which oxidation-corrosion proceeds. In order to sustain this research effort on physical properties, $10,220,000 is required for FY 1982.

Research on <u>Radiation Effects</u> provides increased understanding of the structure and properties of materials exposed to radiation, particularly neutrons and ions. Emphasis is placed on correlating changes which ultimately can be used to predict alloy behavior in fission and fusion reactors. This research is also relevant to non-nuclear technologies. For example, accelerator based ion-implantation can be used to modify near-surface structure and composition to improve materials wear or corrosion resistance for all technologies.

Radiation Effects research is highly dependent upon the development and use of unique facilities, such as high voltage electron and field ion microscopes, research reactors, and ion accelerators. These facilities constitute a national resource shared with university and industry staffs throughout the country.

The importance of developing realistic radiation simulation methods was demonstrated using a dual-ion beam facility to investigate void swelling behavior of a model stainless steel. In the experiment, the alloy was simultaneously bombarded with helium and heavy metal ions in order to simulate helium gas generation together with atom displacements in the alloy, as will occur in a fusion reactor first wall. In comparison with a different simulation method where helium was preinjected, this method showed that all aspects of void formation (the kinetics as well as size and spatial distributions) were much different.

An important need which this research effort is addressing is to simulate irradiation enhanced creep (a critical design property in both fission breeder and fusion reactors) on a time scale that is much shorter than can be achieved using reactor irradiation techniques. Major contributions to understanding the effects of cyclic irradiation on creep were achieved during the past year, e.g., it was shown that cyclic irradiation conditions can lead to greater creep than steady irradiation, and that the cyclic creep contribution can be avoided by operating at sufficiently high first wall temperatures in fusion reactors.

Underlying the above research on extended time swelling and creep properties is the detailed understanding of defect distributions generated in materials by a single neutron or primary recoil atom. During the past year, discrepancies between the actual radiation induced vacancy concentration in a damage zone versus that predicted by a widely accepted model were quantified. The differences were attributed to non-linear energy transfer effects. This result together with new information on radiation induced segregation will assist scientists to ultimately predict radiation effects with a minimum of experimentation.

This research on radiation effects warrants continuation to improve materials for advanced reactor systems as well as for radioactive waste management systems. With respect to the latter, more support will be given to ceramics and glasses. These projects will range from complex multiphase ceramics selected to identify the nature and kinetics of phase instabilities to less complex model materials which allow the role of specific defects to be assessed. Greater emphasis will also be given to the effects of radiation on mechanical properties, such as creep and embrittlement, which occurs in nuclear fuel cladding, pressure vessels, and other reactor components. Facility support is also required, primarily for the IPNS-I. In view of this facility's unique capability to study neutron induced damage independent of gamma ray effects, research is planned on non-metallic materials, (e.g., semiconductors potentially relevant to in-reactor radiation monitors and polymers and ceramics for insulators in fusion reactors). A 2 MeV ion accelerator coupled to the ANL high voltage electron microscope will be brought on-line in FY 1981 for in-situ observation of radiation damage. To permit the increased efforts noted above, decreases will occur in research on atomic defects and radiation effects in superconductors. Also, some work on analytical studies of neutron irradiation of metals and on electrical resistivity changes due to charged particle irradiation will be phased out. Reflecting the above, $7,800,000 is required for this radiation effects research.

Engineering Materials research is directed towards increasing our understanding and hence our ability to cope with or modify more complex phenomena and materials which approach "real" world material problem areas. This effort is still basic research, however, with model systems chosen and parameters controlled so that generalizations and extrapolations can be made. Some examples of research subjects under study include: welding, nondestructive evaluation, erosion, ceramics processing, and fracture under complex loading or environmental conditions.

The importance of the research contained in this subactivity lies in the fact that it provides an important interface to generic materials technology problems. For example, a common problem in welding stainless steel (used in many energy systems such as water cooled nuclear reactors) is cracking at high temperatures. A study during the past year, which resulted in a Welding Society award, showed how by altering various welding parameters, the weld structure can be modified so that it is less susceptible to cracking.

In the area of erosion, of great importance because of its detrimental effect on coal conversion plant components, considerable progress has been made both in understanding the phenomena of erosion and in developing methods for reducing the rate. A hard wear-resistant coating of titanium diboride has resulted from research supported by this program which shows promise for use in valves for coal liquefaction. Erosion of pressure letdown valves has been a limiting factor in the operation of coal liquefaction plants. A chemical vapor deposition technique was developed capable of depositing adherent, porous-free titanium diboride which exhibits excellent erosion resistance. Further tests are planned in pilot plants. In another coating program using the sputtering (electric field induced) technique, fabrication of a complex ceramic protective coating was shown to be possible. This particular program is aimed at understanding the relationship between sputter parameters and microstructure. This understanding permitted the coating of gas turbine components to be used as a protective barrier to combustion gases from coal derived liquid fuels. These coatings contain controlled chemical composition (graded from metallic to ceramic at the outer edge) and structure capable of withstanding the severe thermal cycling present in the utilization of gas turbines.

In the area of quantitative nondestructive evaluation, significant progress was made during the past year to improve the ability to identify and measure size and depth of surface and subsurface flaws. This improvement was made possible by advances in theory and the development of an experimental technique, called the dynamical photoelastic technique.

An FY 1982 budget of $5,350,000 is requested for this engineering materials research to strengthen the ongoing programs especially in ceramics processing and nondestructive evaluation.

Solid State Physics

Solid State Physics is directed towards fundamental research whereby the complex interactions of electrons, atoms, and defects are investigated with the goal of understanding how they influence solid behavior. Knowledge of these interactions is vital to the ultimate prediction and control of material properties. Research in solid state physics encompasses the broad spectrum of experimental and theoretical efforts which contributes basic solid state knowledge important to all energy technologies.

The activity in Solid State Physics exploits recent important discoveries made in the United States and the rest of the world. An example of this is the use of ions and laser beams (ion implantation-laser annealing) to alter and create new materials with improved properties for use in energy systems. The discovery of this technique by this program, has in a short time, resulted in substantial efforts by major corporate technologies in the United States, as well as greatly expanded efforts in western Europe and Japan. For example, these include photovoltaics for solar energy conversion and hardened surfaces that greatly resist wear. Techniques involving ultra-fast laser diagnostics have been used to measure and analyze melting phenomena as short as one-trillionth of a second. In addition, although superconductivity was first discovered nearly seventy years ago, advances continue to be made to use this fundamental phenomenon to improve energy and conservation systems. Moreover, the extension of superconducting phenomena to new discoveries of electron tunneling and the Josephson effect has resulted in the revolutionary development of SQUIDs (superconducting quantum interference devices), which exhibit unequaled properties of sensitivity. Systems using components with this electronic device can measure the smallest levels of voltage (10^{-15} volt) and magnetic fields ever achieved. The ability to make such sensitive measurements has greatly advanced diagnostics used for remote earth sensing, and is now being extended to areas of non-destructive evaluation and sophisticated biomedical applications such as nerve-pulse detection. Efforts in this program not only include applications of the devices but continued improvement in methods of fabrication and upper temperature stability. In FY 1982, increased efforts in new material synthesis and diagnostics are expected to further our insight into immobilization of nuclear waste forms, efficient solar photovoltaics, improved catalysts, oil shale exploitation, advanced instrumentation for geophysical prospecting and new heat engines, among many others.

A number of significant accomplishments occurred in the solid state physics program during the past year. Extended studies of new nuclear waste forms with an orthophosphate composition have included leach testing under various temperature, pressure and saline conditions. The tests were promising in that increased stability, by factors from 16 to 295, were found for these materials compared to the commonly studied borosilicate glass system. Advances in laser annealing and ion implanted material preparation have resulted in improved solar photovoltaic efficiencies beyond those previously reported by this program. Single crystal silicon implanted with arsenic and annealed with a single laser pulse resulted in a conversion efficiency of 15.1%. The much cheaper polycrystalline silicon exhibited an efficiency of 12.1%, primarily because of impurity profile control by the laser annealing method. Developments in new sophisticated instrumentation with SQUIDs have resulted in devices that operate above 16^{o}K, the highest yet reported. These devices are especially sensitive for deep earth exploration (more than 10 km) at low frequencies (less than 10 Hz). Actual field tests in a known geothermal area have revealed the correlation of a geological fault line sequence with the known source and have predicted new source areas which will soon be explored for confirmation. By combining the probes of small angle neutron and x-ray scattering, the size, shape, and pore distribution of oil contained in oil shale have been determined non-destructively for the first time.

These techniques will greatly assist extraction technology methods as well as enhance oil recovery schemes. In a complementary study, specific hydrocarbons in coal liquifaction solutions were identified spectroscopically. New diagnostics using photoemission have been applied to battery systems, especially electrolyte solutions, where as little as 2 ppb (parts per billion) iodine has been detected at the liquid surface. These same studies, which make use of the newly discovered Giant Raman Effect, have identified adsorbates under water, which is not possible to accomplish with usual spectroscopic techniques such as infra-red or electron energy loss spectroscopy. These are just a few examples of how research in solid state physics impacts a broad spectrum of energy technologies.

The FY 1982 request for Solid State Physics research is $46,930,000. These funds are required to maintain the current level of effort while accommodating the research efforts using the new, forefront facilities. The major research subactivities in Solid State Physics are: Neutron Scattering, Experimental Research, Theoretical Research, Particle-solid Interactions, and Engineering Physics.

Research involving <u>Neutron Scattering</u> uses the neutron as a probe for the study of materials in the condensed state. The neutron has a specific wavelength, nuclear interaction and magnetic moment, which allows us to learn about the microscopic properties of solids so we may more effectively utilize materials in energy systems. Fundamental phenomena such as superconductivity, magnetism, and crystalline structure are determined by using this technique of neutron scattering. Small angle neutron and x-ray scattering will be used in the investigation of oil shales, coal solutions, and polymeric structures. Catalysts and fast ion conductors will continue to be investigated. Pulsed neutron activity will also continue at the LANSL Weapons Neutron Research (WNR) facility and the Intense Pulsed Neutron Source-I at ANL. The major part of the national effort in the area of neutron scattering research has historically been supported at Department of Energy laboratories, where the advanced steady-state research reactors (HFIR and HFBR) and pulsed neutron systems are designed, constructed, and operated. Increased costs in FY 1982, due to added power costs, new pulsed systems, increased safeguards requirements, fuel increases, and added user instrumentation, place heavy burdens on this program in order to maintain efficient utilization of these important facilities. In preparation for the future, when it will be necessary to replace the aging High Flux Beam Reactor at BNL and the High Flux Isotope Reactor at ORNL, a small study effort on advanced neutron generator concepts will be initiated. To meet these added costs, the FY 1982 request for neutron scattering research is $11,400,000.

The Experimental Research subactivity is very broad in scope. It includes all fundamental solid state physics investigations of the solid and liquid state of metals, alloys, semiconductors, and compounds. Surfaces will receive increased attention through the use of the most advanced processing techniques and forefront diagnostic tools for analysis on the micro-scale. Chemical vapor deposition, molecular beam epitaxial growth and electron beam deposition will be combined with ion, electron, and laser pulses to create and modify entirely new materials which are expected to exhibit properties important to a host of energy technologies. Lasers will be increasingly used to modify surfaces to improve solar efficiency, corrosion resistance, and hardness, as well as to perform diagnostics of material preparation, degradation, and surface analysis. This latter effort involves the pulsed laser atom probe (PLAP) which allows isolated molecule identification and the real time analysis of catalytic adsorbates and intermediate reactions. High temperature materials such as carbides, nitrides and silicides will be synthesized and investigated for potential use in high temperature, efficient energy systems. The vacuum ultraviolet (VUV) ring of the National Synchrotron Light Source is scheduled for operation in the spring of 1981, and the x-ray ring is scheduled for completion later in the year. Extremely intense beams of x-rays, light, and infra-red radiation from the National Synchrotron Light Source will be used to investigate catalysts, solar material degradation, micro-impurity location, and unusual electronic effects resulting from monolayer-type coverages on solid surfaces. These latter include extremely high hydrogen absorption characteristics and increased catalytic response. A very broad spectrum of research at the National Synchrotron Light Source will result from a variety of laboratory, university and industry activities at this forefront facility. With the National Synchrotron Light Source becoming fully operational, $2,500,000 additional for facility operating costs alone is required in FY 1982. Efforts will continue in advancing our understanding of superconductivity and improving the characteristics of superconductors with regard to upper critical temperature and upper magnetic field. This class of materials continues to exhibit potential for several efficient energy systems. High pressure (above 1 Mbar) experiments on hydrogen will be conducted in attempts to produce a solid hydrogen in the metallic state. Theory indicates this material might exhibit unusual superconducting behavior. Fast ion conductivity will be investigated in both crystalline and amorphous materials in an attempt to learn how to improve battery performance. To support this broad effort within solid state physics, $24,700,000 is required in FY 1982.

The Theoretical Research subactivity is closely coupled with all of the other efforts within solid state physics. Unusual experimental observations such as very rapid laser melting and solidification phenomena and monolayer film electronic effects are examples of areas that require sophisticated theoretical analysis using high speed computers. Other important areas that require extensive computer modeling include dynamic processes such as crack propagation, particle damage phenomena in solids, and nucleation processes in material preparation systems. More generally, however, theoretical efforts are directed towards predicting material behavior in a variety of environments, a difficult but necessary task for nearly all advanced energy systems. To support this important theoretical effort, $4,280,000 is required for FY 1982.

Under Particle-solid Interactions the primary effort is directed toward correlating the complex damaging effects in solids resulting from particle bombardments with varying mass, energy and charge. Under closely controlled environmental conditions, especially temperature, experiments are conducted with neutrons, ions, and electrons. The correlations are necessary not only for understanding synergistic effects, but also for reducing exposure times to reasonable experimental limits. Although most of the research is directed toward effects on bulk materials, considerable effort is also given to surfaceglancing angle effects and sputtering phenomena. Research in this area, for which $2,290,000 is required in FY 1982, continues to be of prime importance to fission and fusion energy systems.

The Engineering Physics subactivity will receive increased emphasis in several important areas which are contributing to the applied efforts of the energy technology sectors. Instrumentation improvements for novel material processing will include the advancement of chemical vapor deposition, plasma sprays and electron beam deposition and wide-area epitaxial growth. Advances in the research on SQUIDs will be pursued with the construction and use of portable field instrumentation for testing for use in the exploration of oil deposits and geothermal sources and for earthquake detection. To facilitate this effort, multiple stations with closed-cycle refrigeration systems will be computer controlled. Scaled-up processing instrumentation for promising nuclear waste sequestering materials will be extended. Studies of fluids in novel engines that can efficiently use low grade heat will be conducted using liquid suspensions and the liquid alloy, sodium-potassium. These systems conceptually are capable of using diffuse solar energy which is usually lost as an energy source. New instrumentation for field ion microscope efforts will include PLAP (pulsed laser atom probe) which allows for the study of individual molecules on catalytic surfaces. This instrumentation coupled with a molecular imaging mass spectrometer allows for isolated molecule identification in real time. These important activities in engineering physics require $4,260,000 in FY 1982.

Materials Chemistry

Materials Chemistry research is directed toward improving our understanding of the chemical properties of materials by studying their chemical composition, structure, and bonding in varying environments of pressure, temperature and chemistry. Research in the materials chemistry area is closely coupled to other activities within materials sciences, including the use of the neutron as a probe for studying the chemical bonding in materials. X-rays, electrons, ions and lasers are also used in materials chemistry research in investigations of chemical properties of materials. These probes are heavily utilized in such studies as electrochemical corrosion and battery degradation processes during operation, the latter investigation being the first-of-a-kind. Additional closely coupled efforts include the synthesis of new nuclear waste materials in the Solid State Physics activity with the companion leaching investigations being done in Materials Chemistry.

An important part of this research on solids and liquids includes kinetic reaction studies of bulk and surface properties. The chemical thermodynamics of high temperature materials is also an important part of this effort. Chemical corrosion and scaling research are of interest to a broad range of energy technologies. Research centered upon the chemistry of surfaces includes forefront investigations of catalytic phenomena as well as the electrochemistry of advanced battery concepts. Chemical diffusion methods are used to study the retention of sulfur and nitrogen in solids, which is very important to improving the efficiency of absorbers and reducing environmental pollution.

A recent study in Materials Chemistry has significantly added to our knowledge of light water reactor safety. Thermodynamic studies of the chemical forms of fission product iodine species which are produced during irradiation of light water nuclear reactor fuel indicate these species are iodides (most notably cesium iodide) and are less mobile than molecular iodine (I_2) as previously assumed. Studies which extended earlier treatments to include tests with irradiated, commercial fuel rods (under the sponsorship of the U.S. Nuclear Regulatory Commission) have confirmed these observations. The results of these studies, indicating that the escape of radioiodine into the biosphere in a reactor accident depends very sensitively on the chemical environment, can have a significant impact on future reactor site safety analyses. These results are directly applicable to problems of predicting the dispersion of radioiodine that might be released as a result of fuel rod failures or meltdowns.

Other recent accomplishments in the Materials Chemistry activity include several related to surface chemistry investigations. Low energy ion deposition of a very small concentration of platinum (10^{12} platinum ions/cm^2) on the surface of titanium resulted in a two-dimensional array of platinum with a high surface area and an enhanced catalytic activity. The platinum later undergoes surface diffusion to form clusters with reduced surface areas and reduced catalytic activity. Since 10^{12} atoms/cm^2 represents less than one percent of full surface coverage, these results indicate the potential importance of using small amounts of ion-implanted platinum for surface catalytic control. Another example of catalytic research includes the discovery that two monolayers of ordered platinum on a gold surface cause a 30 percent increase in catalytic response in the dehydrogenation of cyclohexane. This again reveals the promise of using very small amounts of platinum in catalysis to cause very unusual surface chemistry effects. An additional surface study showed that a molybdenum surface covered with a potassium layer can be protected from a sputtering loss by using a negative voltage bias (-45V). This result is an important finding for control of sputtered contaminants from magnetic fusion first wall systems.

In cooperation with the Environmental Protection Agency, a real-time airborne analysis of the air space above a coal-fired power plant plume was conducted for the first time. This was made possible by the development, under the Materials Chemistry activity of a portable infra-red detection instrument. Very briefly, unusual sulfate particle distributions were found over short time periods, as small as thirty minutes after leaving the stack, and over considerable distance (tens of miles). Additional studies in the eastern United States revealed highly localized sulfate particle concentrations, thereby indicating the great importance of real-time rapid scanning, airborne instrumentation for the eventual advancement of plume chemistry and acid-rain control.

The FY 1982 request for Materials Chemistry is $12,550,000. These funds are to be used in support of subactivities in Materials Chemistry such as Chemical Structure, Engineering Chemistry, and High Temperature and Surface Chemistry.

Research in <u>Chemical Structure</u> will be directed towards those areas where a precise knowledge of the relationship between the structures of materials and their chemical reactivities is required. An example of this effect is the structural modifications in advanced zeolite catalysts and their effect on catalytic activity in specific fossil fuel conversion systems. Chemical structures are also important in understanding the bonding in hydrides and the storage of hydrogen in solids. Pulsed neutron experiments in the epithermal energy region will be exploited for new studies of elastomers, polymers, fused salts, and metal-cluster compounds for potential use in catalytic systems. The FY 1982 request includes $3,380,000 for structural chemistry.

<u>Engineering Chemistry</u> includes those research activities related to the physio-chemical processes of mass transport, materials-related separation and removal processes and electrode interface studies. The FY 1982 request includes $4,860,000 for these research activities. Recent studies of sulfur entrapment in solids for pollution control will be extended to nitrogen entrapment as well. Molten salt investigations will be extended to compositions of promise for potential energy storage systems. Airborne infra-red analysis of atmospheric solid particle pollution will be extended in an attempt to understand the complexities of local geographic disturbances, and, if possible, gain insights into regional effects. Research will continue on the temperature behavior of nuclear breeder fuel and the control of nuclear fuel cladding corrosion effects. Efforts more closely related to fossil energy conversion include new instrumental methods for removing small particles in fossil liquids through the use of vibratory and electric field methods of separation.

In <u>High Temperature and Surface Chemistry</u> efforts will be expanded in the study of surface modifications related to enhanced catalytic activity, particularly to the mechanisms involved in efficient material usage. The use of ions to modify surfaces will also be extended to weldments where corrosion-protecting coatings would be important. This research will also include the analysis of impurities important in chemical corrosion processes. Thermodynamic studies of controlled geothermal liquids will be conducted in an effort to understand the complex parameters affecting deleterious geothermal scaling processes. Thermodynamic studies will also be extended to high temperature battery concepts and advanced nuclear fuel materials in order to better predict their behavior. The request for this important area of research is $4,310,000 in FY 1982.

Capital Equipment

The FY 1982 capital equipment request of $9,630,000 reflects the direction of the Materials Sciences subprogram into energy-related and pioneering research areas such as surface science related to catalysts and corrosion resistant coatings for synthetic fossil fuel development, structural ceramics for high temperature turbines and heat exchangers, geologically stable nuclear waste hosts, and thin films for photovoltaic and photothermal systems. Pre-eminent science in these areas depends on advanced specialized equipment. For example, computer controlled nuclear magnetic resonance apparatus is proposed for evaluation of the structure of catalysts, particularly at active catalytic sites. Analytical electron microscopes are needed to detect and analyze complex phases and trace impurities, and their distributions in metals and ceramics to aid in designing stronger alloys and improved processing methods; ancillary apparatus such as in-microscope specimen stages, detectors, and spectrometers are also requested. Equipment is required to allow controlled fabrication of new materials, such as plasma deposition of amorphous silicon and an ion accelerator coupled with a laser for producing metastable alloys and compounds, which may open new vistas for materials reliability under harsh operating conditions.

Major facilities are being brought on line which promise to advance dramatically this research program. These include the National Synchrotron Light Source, the Intense Pulsed Neutron Source, and electron microscopes with unique capabilities for atomic resolution, analytical chemistry, in-situ testing, and high voltage operation. Efficient operation of these facilities requires computer interfacing to allow timely data analysis and feedback for improved experimental design; this is particularly important and costly for the NSLS beam lines. Also for the NSLS, instrumentation has been proposed for preliminary experiments which must precede full-scale equipping of beam lines in order to optimize the design of equipment. In a parallel manner, a feeder transmission electron microscope is essential for the atomic resolution microscope facility to permit optimization and extension of this landmark facility.

For an effective research program, outmoded general laboratory as well as specialty equipment must be replaced. Needed equipment includes crystal growth apparatus, vacuum pumps and mechanical testing machines. The failure of even mundane apparatus leads to costly and unproductive periods of research.

Construction

Of the $4,500,000 request for construction funding for Materials Sciences, $3,500,000 is for initiating work on the High Temperature Materials Laboratory at ORNL, $700,000 is for Accelerator Improvements and Modifications and $300,000 is for General Plant Projects.

The proposed High Temperature Materials Laboratory (HTML), has a TEC of $17,000,000. The purpose of the HTML is to provide appropriate space and equipment to conduct research designed to provide an understanding and useful application of the relationships between a material's properties at elevated temperatures and its structure, composition, and environment. Although this facility will be used predominately for basic research it will provide space for the co-location of applied materials efforts, thus enhancing the process of technology transfer. Materials limitations dominate virtually all of our advanced concepts for energy conversion and use. These limitations are most commonly associated with mechanical or chemical stability at elevated temperatures in more aggressive environments. The efficiency of energy producing and conversion systems could be significantly increased if materials were available to operate at higher temperatures. Also, the reliability of components and in some cases the feasibility of new systems are dependent on high temperature mechanical properties, erosion/corrosion resistance and thermal conductivity and stability. For example, turbine generators would be more efficient if the mechanical properties of materials could be retained at higher temperatures; battery electrodes in advanced high temperature systems could continue to operate if the accelerated diffusion and chemical attack did not deteriorate these materials at elevated temperatures; and more efficient solar systems would be possible if inexpensive coatings would retain their optical properties at high temperatures. In addition to long range research which would help create new materials and approaches for the high temperature materials areas, the concentration of expertise at the HTML would assist in the solution of short-range complex elevated temperature materials problems such as those evident in synfuel plants and other advanced energy systems. This facility will be established as a national center which will accommodate researchers from universities and industry in addition to those from DOE national laboratories.

The $700,000 for Accelerator Improvement and Modification would be used to maintain and improve reliability and efficiency of operations of the High Flux Beam Reactor and the National Synchrotron Light Source at BNL and the Intense Pulsed Neutron Source at ANL. The $300,000 for General Plant Projects would be used to provide for minor new construction, other capital alterations and additions, and for buildings and utility systems at Ames Laboratory ($275,000) and Notre Dame Radiation Laboratory ($25,000).

Chemical Sciences

The objective of the Chemical Sciences subprogram is to expand our knowledge base in the chemical and related sciences, especially in those areas likely to lead to new and improved processes for the development and use of domestic energy resources.

Research performed covers an array of topics ranging from energy-related phenomena involving liquids, gases and plasmas, to the chemical properties of solids such as coal, chlorophyll and catalysts, and to phenomena and behavior of submicroscopic particles such as molecules, atoms, ions and electrons. The research results can be critical to decisions on the economic viability of both existing and new technology concepts. For example, much remains unknown about the basic factors governing such things as automobile engine combustion efficiencies and about optimum conditions for converting coal to liquid fuels. Scientific knowledge enhances our ability to discern good ideas from impractical ones.

Research in the Chemical Sciences has both short and long term applications. Research on chemical catalysis is providing insights which already can be used in industrial processes to improve efficiencies in areas such as coal liquefaction. Other research, such as on photochemical splitting of water to produce hydrogen, is yielding results likely to contribute to solar energy technology a decade or so from now. Still other research, such as on the radiation emitted by ions moving very fast through thin foils, is producing new information with a high probability of usefulness in future energy applications; in advanced areas such as this, however, it is too early to specify likely applications.

Typical of the advances achieved by Chemical Sciences' researchers is the recent discovery of a catalyst which allows the direct use of carbon monoxide and hydrogen derived from coal for industrially important chemical reduction reactions; heretofore, hydrogen alone was required and had to be prepared in suitable purity at much greater expense. In the combustion research area single unaggregated carbon atoms have been generated for the first time by a laser-based technique. Since such atoms figure significantly in some combustion systems, their behavior must be studied if combustion is to be fully understood for fuel efficiency. This technique gives researchers a tool for such studies. A third example is the preparation of a remarkable solid formed when a germanium-fluorine substance slips between the submicroscopic sheet-like layers which make up graphite. The properties observed thus far for this solid suggest it may provide a basis for the development of batteries having very high energy densities in the future.

In 1980 we noted the objective of opening the new Combustion Research Facility for use of its advanced diagnostic techniques by Sandia Laboratories' in-house scientific staff and by visitors from industry and universities. This has been done, with great enthusiasm shown by scientists from the automotive industry. Plans were also described for strengthened efforts toward better understanding of the chemical effects of catalysts, for deeper knowledge of coal chemistry and for insights into photochemistry which may be put to use in capturing solar energy. Evidence that the catalyst and photochemistry work has been making strong progress is seen in numerous accomplishments, examples of which are cited herein. Progress in the difficult subject of coal chemistry has also been made, exemplified by two groups at Oak Ridge National Laboratory who have opened new understandings in organic chemistry of coal-related substances and in the chemical physics of coal constituents under temperature and pressure conditions used in coal conversion plants.

It is also worth noting that the experimental National Resource for Computation in Chemistry (NRCC) is being closed down after thorough consultation with our colleagues in the National Science Foundation and after review by an eminent committee and other members of the chemistry community. Though a valuable pioneer in software standardization, the NRCC gave way to more urgent needs for chemical research.

The Chemical Sciences subprogram is organized along disciplinary lines into two basic research activities. The Fundamental Interaction activity is mostly longer-term in nature and slanted toward the chemistry-physics interface, while the Processes and Techniques activity is mostly targeted to generic needs identified for the energy technologies.

Coordination of the Chemical Sciences research with other DOE activities occurs at two levels: in the laboratories on a scientist-to-scientist basis, and in DOE headquarters (and with other agencies) on both a conference or committee basis and by individual interactions. Research information is exchanged so that newly recognized technological needs are made known to basic researchers and new insights in the chemical sciences are brought to the attention of applied researchers. Chemical Sciences headquarters' staff and senior scientists in its program also serve as advisors and resource people to DOE's energy technology staffs.

Within the FY 1982 request for $84,160,000 for Chemical Sciences, $72,100,000 is for operating expenses, $5,960,000 is for capital equipment and $6,100,000 is for construction. Each is discussed in turn below.

Operating Expenses

The $72,100,000 request in FY 1982 for Chemical Sciences' operating expenses is $11,400,000 above the funding in FY 1981. This increase is needed for two purposes: meeting costs of operating and using major new facilities, principally the National Synchrotron Light Source and the Combustion Research Facility; and maintaining advanced energy-related chemical research at the FY 1981 level. The increase needed for facility-related expenses is $4,740,000, so that the rest of the subprogram will be increased by only $6,660,000. The few new and strengthened efforts described below will therefore come at the expense of valuable but less urgent ongoing efforts.

A large share of the Chemical Sciences effort is carried out in DOE's national laboratories. Roughly two-thirds of the funds are for these laboratories, while most of the remaining funds are for university projects. The national laboratories are staffed with leaders in chemical research and have advanced, often unique equipment. They offer opportunities for basic researchers to interact with energy R&D teams as well as with visiting scientists from universities and industrial laboratories. The planned funding pattern is the following:

Research Sites	Operating Expenses FY 1981	Operating Expenses FY 1982
DOE laboratories	$42,300	$51,250
Universities	16,760	19,250
Other	1,640	1,600
Total	$60,700	$72,100

These figures include the effects of the new, specialized facilities coming on line. This subprogram's share in operating the National Synchrotron Light Source increases from zero to $2,500,000 in FY 1982. Support of the Combustion Research Facility increases by $900,000 as research use of this new facility nears the planned level. Inflation consumes most of the increase and therefore support of the facilities will require the termination of some activities of less priority with the resultant loss of some highly trained people.

Five areas of chemistry will receive added emphasis in FY 1982. They are: 1) combustion, to exploit advanced techniques to study complex, very fast chemical reaction sequences; 2) photochemistry, to extend research on water photolysis; 3) chemistry of coal, especially the makeup of the organic constituents and their behavior under processing conditions; 4) catalysis, where despite wide application, our understanding is fundamentally poor, making the shift of the use of catalysis from petroleum processing to coal processing, for example, difficult; and 5) separations methods, with particular concern for improved possibilities for resolving nuclear wastes isolation issues, including such goals as recovery of valuable non-radioactive metals and cleanup of treatment waters.

The estimated funding for the two principal activities, Fundamental Interactions and Processes and Techniques, is shown in the following table:

Chemical Sciences
Summary of Operating Expenses

	FY 1981 Estimated Budget Authority	FY 1982 Estimated Budget Authority
Fundamental Interactions	$ 36,277	$ 44,450
Processes and Techniques	24,423	27,650
Total Chemical Sciences	$ 60,700	$ 72,100

Fundamental Interactions

The Fundamental Interactions research activities deal with the most basic physical and chemical characteristics of matter at the level of molecules, atoms, ions and electrons. The forces between such particles determine whether they will chemically react with each other, whether energy will be liberated or absorbed during such interaction, and whether any other phenomena will occur. Knowledge of these fundamental interactions is central to the successful conversion, storage and conservation of energy; this knowledge is also critical to understanding the environmental effects of these processes. The research is divided into three subactivities: Photochemical and Radiation Sciences, Chemical Physics and Atomic Physics.

The Fundamental Interactions activity is broadly scoped in its advanced research, as can be seen in some of its recent accomplishments. At the Lawrence Berkeley Laboratory, a light-induced process to split water has been discovered, yielding gaseous hydrogen while trapping the active oxygen, simultaneously produced, in a stable form of interest for an important industrial application. Photolytic reactions induced by sunlight in water normally yield atomic hydrogen and oxygen-containing species, but gaseous oxygen is not normally an immediately removeable co-product. The LBL discovery solves that problem and holds the simultaneous promise of very significant energy and dollar savings in the large-volume chemical business of making propylene oxide, a major industrial chemical.

At Stanford University, research on the mechanism of an important biochemical process has provided new thermodynamic insight into the possibility of attaining greater efficiency of energy utilization in complex chemical systems. Living systems derive their energy supply from the conversion of ATP (adenosine triphosphate) to ADP (adenosine diphosphate). ADP is converted back to ATP during the process which converts sugars to oxidized chemicals via a multi-step reaction pathway. The quantities of the intermediates in the process are observed to oscillate, with frequencies on the order of 1 minute, with definite relationships among the different intermediates' oscillations. A description of the thermodynamics of oscillating reactions has been developed, which demonstrates that the oscillations cause an increase of 10-15% in overall efficiency over that which would be observed in their absence. Essentially, this comes about because some of the energy which would be dissipated is instead intercepted at peaks in the oscillation, so that it appears as useful work. Beyond biochemistry, the description has been recast in terms of a heat (Stirling) engine to demonstrate the generality of this concept.

The study of highly charged ions (atoms which have been stripped of most of their electrons) is important in the development of fusion energy because these ions may occur in fusion plasmas and dramatically sap their energy. Until now, obtaining such highly charged stripped ions for isolated basic study could only be done in energy ranges far above that typical of fusion plasmas. A new method has been devised at Kansas State University in which a beam of particles at millions of electron volts strikes a gas target, stripping the gas molecules of most of their electrons. The resulting highly charged ions emerge from the target at relatively low energies heretofore not attainable for such highly charged ions. The ions are then accelerated to a few hundred electron volts for the fusion-related experiments. This technique is being adopted by several laboratories.

The FY 1982 request for Fundamental Interactions is $44,450,000, an increase of $8,173,000 over FY 1981. Within this total, $20,760,000 will be devoted to research in Photochemical and Radiation Sciences, an increase of $4,875,000 over the FY 1981 funding. A large share (over one-third) will be used for research in solar-related photochemistry. The most promising work in artificial photosynthesis, homogeneous and heterogeneous photochemistry, photoelectrochemistry and molecular energy storage will be continued and supplemented by new projects at universities, national laboratories and industry. Particular emphasis will be placed on studies of the effects of catalysts on light-induced chemical changes which would be useful in production of chemicals other than fuels. This has great potential for energy conservation.

Also figuring very prominently in the area of Photochemical and Radiation Science is the National Synchrotron Light Source (NSLS). Chemical Sciences will provide $2,500,000 as its share of the costs of operating this new facility (up from zero in FY 1981) as well as $1,400,000 (up by $800,000) in support of research using it. The NSLS will place our national chemical research in the forefront of several areas, all highly important in future energy capabilities. One of these is the study of gas phase chemical reactions by combining the molecular beam technique with photoionization caused by high-intensity narrow-frequency light from the NSLS, and with mass spectrometry. By this means, two important national needs will be served: a better understanding of combustion and a better understanding of the chemistry of gases such as coal-derived synthesis gas will be developed. The chemical behavior of clusters of molecules will also be studied with the unique capability of NSLS to understand certain phenomena in the atmosphere linking together global solar energy gain and loss, atmospheric pollutants and the growth of carbon dioxide in the atmosphere. Cluster studies will also shed light on soot formation, a subject of central importance concerning wider use of fuel-saving diesel engines. Another exceptionally important use of the NSLS is the strong insight it offers into the behavior of catalysts, wherein lie great possibilities for making liquid fuels from coal or coal-derived substances more economically. The most important research of all at NSLS, however, will in all probability result from the highly advanced studies of energy-related phenomena not now identified with any specific energy technology.

Nearly 40% of the Photochemical and Radiation Science effort is long-term fundamental research seeking to understand the very basic interactions of light and other radiation with matter. Sited at sophisticated facilities such as ANL's electron linear accelerator and the Notre Dame Radiation Laboratory, as well as in university chemistry departments, this kind of research often opens up totally new concepts and techniques for energy technologies and for other parts of the discipline of chemistry. An example of this is the highly advanced technique of picosecond spectroscopy, in which chemical species are measured and characterized in lifetimes of a few trillionths of a second. Too varied to list individually, these projects are carried out by highly skilled and imaginative leaders in their fields, who are at the same time likely sources of new energy ideas.

A smaller part, about 7%, of this subactivity supports important research in nonsolar-related photochemistry and radiation chemistry related to the environment and to combustion chemistry. Photochemical studies have strong possibilities of achieving sufficient understanding of some problems of energy-related atmospheric pollution so that solutions may be identified. In the related area of combustion chemistry, important new research possibilities are provided by the photochemical and radiation chemical formation of short-lived species known or suspected to have significant roles in combustion.

For the second part of Fundamental Interactions, Chemical Physics, the funding required is $17,380,000, an increase of $2,708,000 over FY 1981. This subactivity is the best overall example of combining science at the very fundamental level with long-term practical possibilities. One example of this is seen in the advanced laser techniques of the new Combustion Research Facility (CRF). These advanced techniques should ultimately lead to a better understanding of combustion to make more efficient use of each gallon of fuel. The university and automotive industry scientists who regularly visit the Facility share this expectation. Another example is in the advanced mass spectroscopy and ion beam research at BNL, whose researchers have pointed to a completely new possible approach to relatively inexpensive fusion energy.

The Chemical Physics subactivity includes combustion research not only at the CRF but also at universities. Over 45% of this subactivity is for the combustion research effort, especially to bring the new CRF to a level of effective use. Funding is required to operate the facility, including state-of-the-art lasers which will be steadily improved as diagnostic tools for probing further into the still dimly understood details of combustion behavior. This subactivity provides the entire support for operating and maintaining the CRF, as well as the largest part of the expenses for research using it. In-house researchers and users from universities, national laboratories and industry will use the advanced lasers and other diagnostic equipment on scientific problems of fundamental combustion kinetics, engine chamber phenomena and coal combustion. The remainder of the combustion funds will support research at universities and other laboratories on other important combustion questions, including the mechanisms of forming soot pollution in diesel engines.

Also within the Chemical Physics subactivity is long-term research which is basic to progress in not only the technologies of energy production and use but also to most of the other Chemical Sciences activities. This research explores the basic causes of chemical interactions in order to systematize our knowledge of them and give us the predictive power needed in designing efficient new systems for energy conversion, storage and conservation. It consists of theoretical and experimental studies of reaction rates and reaction mechanisms, with leading scientists using and improving sophisticated techniques such as molecular beams, laser saturation and variational transition state theory. The request for this group of projects is nearly one-third of the Chemical Physics subactivity.

About 15% of the Chemical Physics subactivity bears on needs for knowledge in fossil energy technologies. This consists largely of theoretical and spectroscopic studies designed to contribute basic understanding of catalytic phenomena. The kinds of information sought by advanced techniques include the need to determine precise distances of molecules from the catalytic surfaces on which they sit. This would allow us to predict the type and strength of attachment to the surfaces, a key insight into the surfaces' catalytic activities, which can help in designing future fuel conversion systems efficiently and economically.

The remaining part, nearly 5% of the request for Chemical Physics, is for research which is related to technologies for energy conservation. This includes studying the chemical structures of hydrides, substances which can store hydrogen. Hydrogen is a potentially useful fuel which would have more widespread use if it were easily storable when produced by solar or other means, and releasable on demand, as is potentially the case with the use of hydrides.

The third part of Fundamental Interactions is the area of Atomic Physics, for which $6,310,000 is requested, an increase of $590,000 over the FY 1981 funding. This research effort is concerned with the behavior of molecules, atoms and, following their loss of electrons, their corresponding ions. The electrons may be dislodged by collisions with other molecules and atoms of sufficient energy, by collisions with other ions, bombardment by other electrons, or by light absorption. All of the processes obviously involve energy transfers, so that better knowledge of them contributes in a general way to understanding, devising and controlling a wide spectrum of energy processes. Thus a principal portion, nearly two-thirds, of the atomic physics projects is considered to be long-term fundamental energy research, emphasizing the forces between small particles and similar phenomena on a submicroscopic scale. The other one-third is for fusion-related research. In particular, these studies examine, both experimentally and theoretically, the formation probabilities and lifetimes of highly charged ions of heavier elements. The need for this kind of information in fusion research and development is strong because such ions may arise from container walls and enter fusion plasmas as impurities. When this happens, the ions may absorb energy from the plasma for times long enough to diminish or extinguish the desired burn. The choice of method for preventing this will depend heavily on the kind of information being generated here.

Processes and Techniques

The Processes and Techniques activity supports basic research in those chemical and physical sciences that are concerned with chemical reactions, catalysis, thermochemical properties, analytical techniques, chemical and physical separations, and mass and momentum transport phenomena including turbulence. These basic research activities address the areas where scientific problems have been encountered by teams engaged in energy technology pursuits, or where scientific barriers to technological advances can be expected to arise. Some of these problems bear on liquid fuels from fossil and biomass resources, nuclear waste processing and isolation, fusion, hydrogen, engineering aspects of combustion and other energy processes.

The Processes and Techniques activity can be expected to produce new knowledge which will help not only with solving practical energy problems using imaginative ideas but almost surely with generating new ideas and even providing early warning of possible future problems. At Oak Ridge National Laboratory, chemists have devised an ingenious new spectrometric technique of broad applicability for chemical analyses in energy research and development. Potentially portable and rugged for use in remote locations, an already demonstrated prototype showed how, through direct use of the speed of light by way of fiber optics, substances are identified and their quantities measured by their absorption of light (i.e., absorptive strengths across a spectrum of light frequencies). Unlike other techniques, however, it does so essentially instantaneously. The system can be tailor-made to monitor the particular spectral range of interest in specific analytical applications.

The catalyst referred to above which allows use of a cheaper coal-derived synthesis gas in place of energy-intensive hydrogen is also scientifically remarkable for showing that two different chemical reactions can be made to proceed at equal rates by one catalyst. The practical potential of the catalyst is the promise of savings of energy and money in important industrial processes such as those used to synthesize intermediates for certain plastics. Producing pure hydrogen in volume is energy-consuming and expensive. On the other hand the principal initial product of gasifying coal or char is a mixture of carbon monoxide and hydrogen (synthesis gas) in proportions which vary according to process conditions. The catalytic reduction discovered consumes the carbon monoxide and hydrogen equally well, thus allowing use of synthesis gas from any source.

Researchers at ORNL discovered a technique for recovery of stable palladium during the reprocessing of spent nuclear fuel elements. Its implementation could ease our current heavy dependence on Soviet and South African palladium as a catalyst for automobile exhaust cleanup. Palladium is also being considered for possible future use as a coal conversion catalyst. The technique depends on quick separation of unwanted radioactive palladium from another radioactive metal, ruthenium, which will decay to the desired nonradioactive palladium. The key is having a strongly radiation-resistant system which can process the spent nuclear fuel after a minimum of cooling time. The object of the new technique is to remove the ruthenium as soon as possible, before its nonradioactive daughter palladium forms and becomes mixed irretrievably with the already-present radioactive palladium. It has been demonstrated that the required separation of ruthenium from the radioactive palladium with a separation factor greater than ten thousand can be done using molten uranium and magnesium. The U.S. production of palladium has never exceeded 1,000 kg per year, while our consumption has reached 46,000 kg./yr. It is estimated that additional production of about 1,000 kg./yr is possible from the spent fuel of reactors already operating and under construction.

At Argonne National Laboratory, chemists who have been measuring oxygen isotope ratios in the carbon monoxide (CO) present in the atmosphere have uncovered a possibly serious energy-related problem. They can distinguish natural CO from automotive and wood-burning CO and they find that the amount of wood/automotive CO increased in the eight years from 1971 to 1979 by an amount greater than that attributable to those sources. A possible explanation: a drop in the atmospheric content of the hydroxyl radical (OH), which is the principal remover of CO. A drop in atmospheric OH would be expected when sulfur dioxide and nitrogen oxides increase. If this possibility is borne out, it would pose a significant problem to be solved for energy sources which generate large amounts of SO_2 and NO_x.

The FY 1982 request for Processes and Techniques operating funds is $27,650,000, an increase of $3,227,000 over the FY 1981 level. The increase is necessary if the most technologically pertinent areas of coal chemistry, nuclear waste separations, catalysis, biomass conversion chemistry and combustion-related turbulence research are to be strengthened. The Processes and Techniques activity comprises three subactivities called Chemical Energy Separations and Analysis, and Chemical Engineering Sciences.

The FY 1982 requirement for Chemical Energy research is $13,560,000, an increase of $1,307,000 over the FY 1981 funding. This effort includes basic organic chemistry research related to the conversion of coal and other fossil resources to gaseous and liquid fuels, where the emphasis is on understanding the chemical structure and interactions of the chemical constituents in coal. It will also provide basic understanding which could lead to alternative paths for accomplishing such goals as removal of heteroatoms (e.g., sulfur,nitrogen) at less severe processing conditions to circumvent difficult materials problems and unnecessary hydrogen consumption. This subactivity also includes catalysis research, both liquid phase (homogeneous) and solid phase (heterogeneous), to understand the principles which govern catalytic activity, selectivity, and poisoning/regeneration. As is evident from the accomplishments described earlier, these basic studies can contribute to very significant savings and efficiencies in energy-consuming technologies and can lay the foundations for future catalyst systems widely applicable in making synthetic fuels. This work includes fundamental organometallic chemistry which provides a basic understanding of the transformations of small molecules like carbon monoxide and hydrogen to produce bulk chemicals and synthetic fuels. In addition, research in inorganic chemistry and thermochemistry will be carried on to address questions bearing on devising and refining new thermochemical cycles with the potential of obtaining hydrogen fuel from water. Related research on the chemical and molecular-transport properties of systems is aimed at understanding the effects of chemical structure and surface properties to determine how extensively metals and metal salts store hydrogen as metal hydrides, and the rates at which they take up and release hydrogen. The chemistry of converting cellulosic materials to fuels and related enzyme catalysis is studied in order to increase our understanding of how these resources can be more efficiently converted to usable fuels. The Chemical Energy research also includes long range basic and multitechnology-related science.

The request for Separations and Analysis research is $11,910,000, an increase of $1,177,000 over FY 1981. In this area of chemistry the theoretical basis for the design of new molecules for selective separations is investigated, the basic mechanisms of separations are determined and new methods for effecting separations are studied. It also includes research on the basic aspects of analytical techniques to increase precision, lower detection limits and decrease the costs of analysis. The increase is primarily for research to study the chemical stability and selectivity of complex molecular groupings, in order to enhance the separation of components of spent nuclear fuel to provide options for the isolation of potentially hazardous components. Research on the mechanisms of transport involved in separation devices is conducted to increase the efficiency of separation and to reduce the volume of radioactive waste handled. Study of the chemistry of molten salt and liquid metal solvent extraction systems is carried out to provide radiation-resistant options for processing of nuclear fuels with little or no prior "cooling" and to enable the recovery of very valuable metals, like palladium in nonradioactive form. Separations research also includes the chemistry underlying the recycling of materials such as uranium and the extraction of metals from low grade sources and noxious waste materials. An important aspect of this subactivity is research, primarily at universities, on the fundamentals of isotope chemistry, synthesis of new separation reagents and the study of isotopic complexes such as helium in hydrides, a problem of interest to both fusion and fission programs.

The requested funding will provide for continuation of nearly the same level of analytical research as in FY 1981. Seizing on new advances in chemistry and physics, modifying existing techniques and inventing new ones, all provide expanded capabilities which are of significant benefit to many technologies. Sensitive analyses of molecular species, especially organic ones, are studied to provide more effective and more efficient means of detection of species likely to occur in fossil fuel conversion facilities. This area also includes multitechnology-related research or basic science considering the physical and chemical properties of atoms, ions and molecules for various detection methods to advance separation concepts and analytical techniques.

For Chemical Engineering Sciences in FY 1982 the requested amount is $2,180,000, an increase of $743,000 over the FY 1981 funding. This subactivity includes research on single and multiphase fluid dynamics (especially turbulence), reaction modeling of gas-solid reactions, transport in porous media and development of thermodynamic models for establishing the properties of complex chemical substances including multicomponent mixtures, (e.g., a range of hydrocarbons plus nitrogen-containing organics, as in shale oil) which are frequently encountered in energy processes. The resulting developments of more physically precise models provide the information needed to design more efficient fuel conversion plants. Most of the increase is for new turbulence research to improve the capability for modeling complex combustion processes. Throughout the chemical engineering sciences effort, emphasis will be given to improving and/or developing the scientific basis for engineering generalizations, unifying theories and innovative processes.

Capital Equipment

The FY 1982 request for capital equipment for Chemical Sciences is $5,960,000, an increase of $1,820,000 above the FY 1981 level. This increase is important to the health of the Chemical Sciences effort in four ways: 1) to continue the introduction of state-of-the-art lasers and other diagnostic instruments for in-house and visitor researchers at the recently opened Combustion Research Facility; 2) to advance in a timely way the return on the construction investment by equipping the beam lines at the new National Synchrotron Light Source; 3) to maintain world competitiveness of our researchers by replacing equipment which has become increasingly outdated; and 4) to replace or repair worn out items, also a pressing problem stemming from equipment budgets which in recent years have proven to be inadequate in relationship to the needs.

The Combustion Research Facility at Sandia National Laboratories (Livermore) begins operation in FY 1981. It must be well equipped with specialized forefront instruments designed for its needs, if it is to fulfill its purpose of providing to the Nation's combustion research effort an efficient, centralized facility for collaboration of scientists from DOE laboratories, industrial laboratories and universities for fundamental combustion research. The request includes $1,190,000 for the Facility to acquire a special high-energy laser system, smaller lasers for diagnostic and excitation purposes, equipment for the turbulent diffusion flame facility, gas handling equipment and general electronic equipment for combustion experiments. A large fraction of the funds provided will permit outfitting a suitable number of users' laboratories at the facility and the establishment of a vigorous users' program. In addition, equipment will be used to strengthen the capabilities of the in-house Sandia combustion diagnostics research program, which studies flame processes in order to discover ways of promoting more efficient combustion.

The National Synchrotron Light Source (NSLS) at BNL begins operations in mid-FY 1981. This facility will add significantly to this country's capabilities in chemical research using intense, narrow-spectrum ultraviolet and x-ray light. The kinds of chemistry which will benefit from the NSLS include many energy-related fields: combustion, catalysis, surface effects in general, gas kinetics, and atmospheric chemistry of energy-generated substances. Beam line instrumentation is the heart of the NSLS buildup; it includes molecular beam chambers with associated equipment, mass spectrometers and extraordinarily effective vacuum pumping. Approximately $550,000 of the equipment request will be required for these purposes. These funds will help assure a vigorous in-house and user program of research in chemistry.

Meeting the third and fourth requirements noted above is the purpose of $4,070,000 of this request. It is vitally important that we reverse the deterioration of recent years in the two dimensions of scientific competitiveness: using state-of-the-art equipment and doing so across the whole advancing front of chemical science. Recent advances in instrumentation technology permit study of chemical processes involved in energy capture, conversion, storage, and release which earlier were entirely impossible, because they took place in too short a time, or involved inaccessible regions of the wavelength spectrum. Processes involved in photosynthesis taking place in less than a trillionth of a second can now be observed. Photochemical studies which impact the use of solar energy and the explanation of complex combustion processes require the use of newly developed lasers which are more powerful and can reach wider regions of the spectrum. New studies on coal chemistry and catalysts have increased the need for instruments capable of rapid, accurate analysis of complex, heterogeneous substances. Large quantities of accurate laboratory data have brought about the need for small special purpose computers, which have become available only in the last few years, to handle and present the information, and to allow researchers to interact dynamically with the displayed information. Other specific needs include: electron spin resonance spectrometers, a neutron data acquisition and control spectrometer, an angle-resolved photoemission electron chamber, a crossed molecular beam system, a Fourier-transform nuclear magnetic resonance spectrometer, streak cameras for billionth-second light detection and a cobalt-60 gamma ray source for radiolysis studies.

In addition, $150,000 will be provided to Ames Laboratory for general purpose equipment. The multipurpose equipment, which is essential to the proper day-to-day operations at the laboratory, is used for all Department of Energy programs at the Laboratory. Included are the needs of the laboratory service and support divisions, as well as equipment required to respond to health, safety, security and environmental considerations.

Construction

The request of $6,100,000 for construction funds in the Chemical Sciences subprogram is for completion of the Chemical and Materials Sciences Laboratory at LBL. This project, which was started in FY 1980, provides for approximately 49,000 square feet of laboratory and office space for chemical and materials sciences research as an addition to an existing laboratory building. The purposes of this project are two-fold: expanded materials research capabilities and improved efficiency and effectiveness of ongoing chemical programs. The capabilities being expanded will include an atomic resolution microscope with the extraordinary power to resolve and image individual atoms. This microscope, with ancillary facilities, will permit better understanding of the behavior of materials such as catalysts, coatings and thin-film solar devices at the very fundamental atomic level. In Chemical Sciences, the new laboratory space will bring greater effectiveness to research in photoelectron spectroscopy to elucidate surface chemical phenomena such as catalysis, in coal conversion fundamentals and in photochemistry of surfaces, a promising field for future solar energy devices.

As originally presented to Congress in the FY 1980 Presidential Budget, the project had a TEC of $12,600,000, for which $6,300,000 in appropriations was requested for each of FY 1980 and FY 1981. Since then, two major developments have affected the project: $2,000,000 of the $6,300,000 originally appropriated in FY 1980 was rescinded, and final Congressional action on FY 1981 appropriations reduced the project's FY 1981 funding to $3,000,000. The $4,300,000 available in FY 1980 has been obligated for acquisition and housing of the atomic resolution microscope. The $3,000,000 appropriated in FY 1981 is being used to continue work beyond preliminary design for the portion of the project which would provide laboratory facilities for chemical and materials research and support facilities for the atomic resolution microscope. Because the reduced funding has lengthened the duration of the project's construction, the TEC has been revised to $13,400,000 so that $6,100,000 is required in FY 1982 to complete the fully scoped project. Without this funding, the Department would be in the position of having a foundation for the laboratory addition, but without funding for the building itself.

Engineering, Mathematical and Geosciences

This subprogram conjoins three largely distinct activities central to fulfilling the responsibilities of the Office of Basic Energy Sciences. The Engineering Research activity was created in FY 1979 to fill a void in the Department's energy research programs. The Mathematical activity is applied mathematics and focuses strongly on the equations, computer algorithms, information analysis methods and advanced computer concepts undergirding every aspect of energy technology development. The research in the Geosciences activity addresses basic research problems associated with locating, defining and extracting energy resources and disposing of wastes from energy production processes.

Together these activities produce new insights, data, instruments, models and techniques important in solving the many key energy problems susceptible to attack through research in their respective disciplines. The objectives are, first of all, to help our nation meet its energy needs, and second, to enable the Department to meet its specifically mandated responsibilities in the areas of national security, environmental protection, and basic research.

The Engineering Research activity first funded in FY 1979 is focused along two lines: the advancement of engineering sciences needed for energy production facilities, and engineering for increased energy efficiency. Currently, over 40 mid-to-long term projects are underway at universities, industrial firms and national laboratories throughout the country. The needs have been heavily documented in DOE's comprehensive review of its technology base activities, in studies of the Energy Research Advisory Board, and elsewhere. The priorities have been carefully formulated. Initial emphasis was placed on engineering aspects of conservation. A major increase is requested for new initiatives in engineering research important to energy production.

In this context it is planned in the near term for Engineering Research to increase emphasis on adequate data bases for synfuel production and geothermal resource exploitation, as well as on new instrumentation and measurements methodology for applications in future energy systems. In the longer term, given the multitude of overwhelming engineering problems arising from the nation's energy needs, it is expected that this activity will engage the efforts of more than 500 leading research engineers and other applied scientists in the United States.

The Applied Mathematical Sciences activity continues to feature internationally recognized research in applied analysis, computational mathematics and numerical methods for partial differential equations. This work is centered at the national laboratories and the Courant Institute of New York University and is tightly coupled with ongoing work elsewhere in DOE. Largely through careful restructuring of this activity over the last four years, two additional lines of work have been solidly established. An outstanding university-DOE laboratory consortium has been set up in the area of information analysis techniques and is already making major contributions to solving problems arising not only in physical research but also in DOE's health and environmental research and Energy Information Administration. Major efforts are also underway in the area of advanced computer concepts which are achieving solutions to problems - such as three dimensional modeling of combustion chambers - previously considered intractable. This latter area requires new and expanded programs and the potential payoffs are enormous.

The Geosciences activity, like Engineering Research, started from a very small base relative to the associated, and extensively documented, needs. It is concentrated on work central to the exploitation of geothermal, fossil fuel and nuclear fuel resources and to the prediction of the long-term consequences of disposal of nuclear and other wastes from energy production. A strong base has been established in geology, geophysics and geochemistry with over 60 projects underway including work, for example, in geothermal reservoir modeling and studies of microcracks in rocks and the properties of ground waters and magmas. Additional emphasis is required in the areas of geochemical migration, rock mechanics, regional geologic studies, and the DOE portion of the National Continental Scientific Drilling program. The work in this last area is focused on studies of magma-hydrothermal systems and on maximizing the energy-related geologic information obtainable from holes drilled primarily for other purposes. Funds are requested for initiation of studies in organic chemistry important for the efficient discovery and utilization of fossil fuels.

Operating Expenses

The FY 1982 request for operating expenses for Engineering, Mathematical and Geosciences is $35,300,000 compared to the FY 1981 level of $24,100,000. The distribution of the FY 1982 request among the three activities is shown in the following table:

Engineering, Mathematical and Geosciences
Summary of Operating Expenses

	FY 1981 Estimated Budget Authority	FY 1982 Estimated Budget Authority
Engineering Research	$ 3,400	$ 8,000
Applied Mathematical Sciences	11,400	14,500
Geosciences	9,300	12,800
Total Engineering, Mathematical and Geosciences	$ 24,100	$ 35,300

Engineering Research

The objectives of the Engineering Research activity are 1) to extend the body of knowledge underlying current engineering practice in order to open new ways for enhancing energy savings and production, prolonging useful equipment life, and reducing costs while maintaining output and performance quality; and 2) to broaden the technical and conceptual base for solving future engineering problems in the energy technolgies. In FY 1982, $8,000,000, an increase of $4,600,000, is requested for Engineeering Research.

This activity seeks solutions to a broad class of fundamental energy related engineering problems. The present program concentrates on six high priority engineering research areas: 1) tribology (basic nature of friction reduction phenomena); 2) automation and process control; 3) heat transfer and heat exchange; 4) engineering mechanics of solids; 5) modeling of engineering aspects of combustion processes; and 6) non-linear systems dynamics. These areas of emphasis were selected after extensive review and consultation with industrial representatives (including Engineering Societies Commission on Energy, American Society of Mechanical Engineers, Society of Automotive Engineers and Joint Society for Computer Control) as well as leading research engineers from universities and DOE laboratories.

Examples of specific problems which this research is designed to solve include the reduction of energy losses and wear due to friction in machinery, including automobiles. Support is provided for research on reduction of rolling friction in car tires and friction losses in piston rings. Both of these represent significant inefficiencies in present car designs. Another important problem area is that of improvements in heat exchanger performance while minimizing noise and vibrations. Still other examples are optimization of process heat distribution in process plants, engineering aspects of crack propagation in energy related structures (e.g., components of nuclear reactors and synfuel plants) at high temperatures, reduction of fuel consumptiom in internal combustion engines without sacrificing performance, and a theoretical basis for improvements and cost reduction of solar power collectors.

The technical approaches to the solution of these problems include experimental and theoretical studies of friction-induced vibrations and wear, development of analytic and computational methods for modeling of turbulent heat transfer, extension of optimal control theory to include time dependent external constraints, advances in thermoeconomics (i.e., study of systems design under both economic and energy supply constraints), experimental and theoretical studies of macroscopic aspects of elasto-plastic deformations and creep at high temperature, reliable initiation of combustion in lean fuel-air mixtures, and the development of the theory of non-imaging optics.

Among the significant recent achievements is the development of a new theoretical basis for determining critical stresses at which surface damage in shaft bearings becomes important. A bearing surface can be damaged when the stress is large enough for the surface asperities (microscopic sharp points) to break through the lubricant oil film. Scientists supported by this activity have developed for the first time a method for estimating the force needed by a sharp object to penetrate through the tension of a liquid surface. This method will enable the computation of the critical stresses, and lead to the design of higher efficiency, more durable bearings.

Another important advance is an easily implemented practical algorithm for the design of resilient process heat distribution - i.e., systems which automatically adjust themselves so as to operate near optimum when individual subsystems fall short of rated performance. An expected result of this type of research is a reduction of redundancy of components in process plants. This will lead to reduction in capital costs as well as more efficient use of energy resources.

Representative projects started in FY 1981 include instrumentation for measuring viscosity and thermal conductivity of corrosive fluids at high temperature and high pressure, modeling of vibration and noise in heat exchangers, fast holographic methods for investigating transient two-phase flow, experimental research on crack propagation induced by surface flaws, and research on advanced ultrasonic transducers for non-destructive evaluation.

The Engineering Research activity addresses engineering areas essential for the progress of many energy technologies. Emphasis and high priority are accorded research topics filling gaps in urgently needed fundamental data and understanding essential for long-range advances in energy processes and systems. This is an important aspect of engineering research for DOE, complementing the shorter range focus required in the DOE technology programs. Attention is focused on interdisciplinary engineering research tasks which will be supported for three to eight years. Work is carried out in DOE laboratories, universities and the private sector. Another important role played by this activity is the graduate training of young engineers in the energy field. There is unanimous agreement that the supply of appropriately trained engineers will be a very serious problem.

The requested increase in FY 1982 will be used mainly to start new engineering programs aimed at enhancing energy production. This will strengthen and balance the fledgling engineering research activity which hitherto has stressed research initiatives in support of conservation measures. Specifically two important areas have been identified for future emphasis.

1. Development of adequate data bases is now perceived as a serious impediment to the future growth and evolution of the emerging synfuels industry, and economic exploitation of geothermal resources. It has been pointed out that this type of data has extremely high economic leverage. For instance, synthetic fuel installation will cost billions each, and poor data could decrease their efficiency by many percentage points.

2. Development of new instrumentation and measurement methodologies is essential for effective implementation of modern automation and process control systems and for advancing certain energy related aspects of robotics. In addition to recently completed workshops surveying instrumentation needs and priorities, engineering research is preparing a study of its long range role in this field as compared with that of the private sector.

Typically, an engineering research project starts yielding useful data and conclusions after three or four years. Thus in order for the results expected here to have a significant beneficial impact on the national energy problems within this decade and early in the next one, this research must be built up to a full productive capacity as soon as possible. The requested increase in effort in FY 1982 will allow the crucial problems to be addressed at an early date, with a good chance of getting timely solutions. A lesser increase will almost certainly delay the acquisition of the data and understanding, vital for future progress, with potentially grave and costly consequences.

Applied Mathematical Sciences

The Applied Mathematical Sciences activity serves as the DOE focal point for monitoring and advancing the state-of-the-art in mathematics, statistics, and computer science. The objective of this activity is to fill the many department-wide needs in those fields. Several DOE mission programs develop and refine specific techniques from the mathematic sciences applicable to their immediate needs. In contrast, Applied Mathematical Sciences concentrates on more broadly based, continuing needs throughout the DOE community. Emphasis is placed on research basic to the analysis, development, and use of large-scale computational models; the management and analysis of large, complex collections of information; and the effective use of present and prospective DOE computing resources.

The FY 1982 request for operating funds for Applied Mathematical Sciences is $14,500,000, a $3,100,000 increase over the amount appropriated in FY 1981. Corresponding to the above areas of emphasis, the Applied Mathematical Sciences research program has recently been organized into four subactivities: Analytical and Numerical Methods, Information Analysis Techniques, Advanced Computer Concepts and Special Projects.

Research on Analytical and Numerical Methods addresses questions basic to improved predictions of the feasibility, reliability, safety, and efficiency of energy systems. Many results are also applicable to the simulation of environmental or health effects and to modeling energy supply-demand. Analytical and Numerical Methods comprises three categories of research activities reflecting the prinicipal thrust of the program in previous years: applied analysis, computational mathematics, and numerical methods for partial differential equations.

The nature of this research is well illustrated by the following significant achievements. In the search for combustors in which fuels are burned cleanly and efficiently, mathematicians at Northwestern University set up a theoretical model for a particular type of gas burner. Their studies have led to predictions of flame speeds and temperatures as a function of gas inflow. These predictions were later confirmed by independent experiments at Sandia National Laboratory's combustion diagnostics facility. This collaborative effort is expected to have a significant impact on the design of environmentally sound combustors for efficient utilization of fossil fuels.

"Ellipsoid" algorithms for solving linear programming problems were introduced by Russian mathematicians in late 1979, and immediately attracted great interest. Such problems arise often, for example in optimal resource allocation. Current methods for their solution are computationally laborious, and claims were made that the "ellipsoid" algorithms would be computationally more efficient. A detailed numerical investigation of ellipsoid algorithms revealed serious practical difficulties and there remains little reason to believe that ellipsoid-based methods can compete with the previously developed simplex method.

In a quite different area, a major breakthrough in the analysis of binary alloy solidification has been accomplished at ORNL. Binary alloys are alloys composed of two metals; e.g., tungsten-iron, magnesium-aluminum, etc. In practice, castings of such alloys must be of uniform composition, but during solidification, depending on a variety of external parameters, the two metals may become segregated resulting in defective castings. This advance will make possible the effective computer simulation of the processes occurring in binary alloy solidification for industrial and energy related metallurgical applications, and will thereby improve the quality of the product.

In FY 1982, $7,200,000, an increase of $1,200,000, is requested for Analytical and Numerical Methods. This increase will be used primarily to strengthen the efforts in applied analysis and numerical methods for partial differential equations - both essential to advancing the solution of many vitally important problems in engineering research.

The research on Information Analysis Techniques seeks innovative approaches to the manipulation and analysis of large, complex collections of scientific, engineering, environmental, energy, demographic and economic data. It thus addresses questions basic to determining future national energy needs as well as the analysis of energy systems and their impacts. A new component of the Applied Mathematical Sciences research activity, it is initially organized into three categories: statistical methods, data management, and display and analysis systems.

Statistical methods addresses issues fundamental to analyzing both the input and the output of data intensive studies. Emphasis is on exploratory data analysis, experimental design, and sensitivity analysis applicable to large, complex data collections and multi-parameter models. Data management encompasses computer science research underlying the organization and retrieval of large, complex data collections. The interface with interactive display and analysis of numeric data is emphasized; as well as the interface with computational models.

An example of a project involving all the categories of Information Analysis Techniques is provided by computer scientists and statisticians at two national laboratories and three universities (LBL, PNL, Princeton, Stanford, and George Washington). The primary areas of interest are exploratory data analysis of very large data sets using state-of-the-art techniques involving color graphics, computer networks, and innovative archival mass storage devices such as optical disks.

In FY 1982, $2,700,000, an increase of $630,000, is requested for Information Analysis Techniques. This will provide for new work along the lines of the work just cited, and on display techniques for multi-dimensional analysis in fluid dynamics which will provide an essential set of tools for energy systems analysis.

Research in Advanced Computer Concepts is a subactivity which is based upon three premises: 1) the computer industry will continue to improve cost-performance ratios for hardware, 2) hardware systems will increasingly be tailored to specific classes of applications, and 3) the cost of software development and maintenance will dominate all other computing costs. Based upon these premises, three categories of Advanced Computer Concepts are distinguished: software engineering, distributed systems and high performance systems.

The nature of work in this subactivity is illustrated by the following examples. Several years ago the Applied Mathematical Sciences program sponsored an investigation of computer networks as a technique for resource sharing among DOE laboratories. The principal finding was that the main barrier to resource sharing had little to do with networks per se. The problem was the necessity of learning many new operating systems, command languages, and different styles of user interfaces once network access had been accomplished. To attack this problem, the advanced systems group at LBL began developing a Virtual Operating System which would provide a uniform user environment on any computer system. Over a period of two years, the usefulness of this project has been widely recognized, as illustrated by the formation of a Software Tools Users Group that now claims over 1000 members. In the process of investigating the principles of virtual operating systems, the LBL group produced a practical and useful set of software tools that has been implemented on over 25 different computer systems. Both industry and other government agencies have been eager to assimilate the practical aspects of this research, and the results have been widely published. Current work is aimed at developing interprocess communication elements which will allow computer networks involving different kinds of computers to behave as a single, integrated computational resource.

At the level of electronic components, the art of computer building is advancing rapidly. Single, fingernail sized electronic "chips" are already as powerful as yesterday's minicomputers, and by the end of this decade very small computers, each as powerful as some of today's largest, should become available. This technological progress is bound to trigger major changes in the way computer systems are designed and used. A particularly exciting possibility is to combine thousands or tens of thousands of these powerful one-chip computers into "ultracomputers" capable of computing hundreds of times faster than is now feasible. This would allow computational study of many important chemical, meteorological, physical, and biological models which presently lie out of reach. Projects to study supercomputer designs and programming strategies are being supported at the Courant Institute of Mathematical Sciences of New York University, M.I.T., and LLNL among others.

In FY 1982, $4,000,000, an increase of $1,020,000, is requested for research in Advanced Computer Concepts. This increase will permit innovative work in high performance systems including prototypes of parallel processor arrays, together with associated algorithm development.

In FY 1982, $600,000, an increase of $250,000, is requested for Special Projects to support conference and working groups to evaluate program directions; liaison activities to stimulate interactions between Applied Mathematical Sciences researchers and DOE computer users; and operating costs for Research Computing Facilities established over the last several years at DOE laboratories. Examples of these activities include a High Speed

Computer Workshop sponsored by LLNL and LANSL which includes representatives from all the major mainframe manufacturers and scientists from the DOE community, the Berkeley Workshop on Distributed Data Measurement and Computer Networks, the Software Clinics experiment at ANL, LANSL, and NYU, and several visiting scientist programs which serve to bring distinguished visitors from the universities to the national laboratories.

Each part of the Applied Mathematical Sciences activity has been designed with the help and advice of leading mathematical and computer scientists from universities and DOE laboratories to assure the broadest and greatest impact on the nation's energy R&D enterprise. Many of them are expert in industry's needs in the cognizant areas. Close liaison is maintained with other Federal agencies in the selection of areas of emphasis and of individual research tasks. This is high leverage research. In favorable cases, the results may be of great benefit simultaneously to a number of different energy technologies. The requested increase will be an exceptionally sound investment.

Geosciences

The objective of the Geosciences activity is to develop a quantitative and predictive understanding of geological, geophysical and geochemical structures and processes in the solid earth and in solar-terrestrial relationships. This understanding is to assure an effective knowledge base for energy resource recognition, evaluation and utilization in an environmentally acceptable manner.

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

The FY 1982 request for operating expenses for Geosciences is $12,800,000, an increase of $3,500,000 above the FY 1981 level. Within the FY 1982 request, $7,000,000 is for continuing the existing base program in geology, geophysics and geochemistry. The base program is the major Geosciences subactivity, and consists of approximately 60 individual research efforts directed toward a specific energy technology, national security, conservation of the environment, or the safety objectives of the Department of Energy. Individual research efforts may contribute to all four of these objectives. Thus, the base program is designed to develop a broad, basic understanding of geoscience materials and processes necessary for the attainment of long-term Department of Energy goals.

One important area in the base program is the development of field geophysical interpretation techniques to delineate the physical nature and associated geologic activity of targets of energy resources. In FY 1980, a fluid-filled crack model has been developed to interpret seismic wave generation, transmission, scattering and attenuation in geothermal areas. The model is based on studies of the hot dry rock system at Fenton Hill, New Mexico, and on the magma body in Kilauea Iki, Hawaii. Through the model, the volcanic tremor data at Kilauea Iki were related to the rate of magma transport during an eruption. The fluid-filled crack model will be useful for interpreting volcanic tremors observed recently at Mount St. Helens. In other work typical of this area of research, a sound velocity log run in a one kilometer deep borehole in granite showed that waveform distortion could predict fractured regions, which are important in different ways to the geothermal and nuclear waste isolation technologies.

A large emphasis is given in the base program to the study of physical and chemical properties of rocks and magma. Much attention has been given to the nature and mechanics of the formation and sealing of small microfractures in rocks because of their important role in controlling physical properties such as permeability. Recent work has clarified how permeability depends on both crack size and smoothness. Additionally, in FY 1980, it has been shown that microcracks are important pathways for uranium migration and concentration; this study will help guide uranium exploration. In other research, measurements of the density of silicate liquids over a range of compositions have shown that silicate liquids mix ideally with respect to volume. When the volume measurements are considered with previous heat capacity measurements, the simple solution model which results can predict equilibrium temperatures, immiscibility and a wide range of other thermodynamic properties of magma.

The remaining $5,800,000 in operating expenses is for five additional subactivities which will impact numerous current and future energy processes and systems. One of these efforts, Geochemical Migration in the Earth's Crust, was started in FY 1979. Two others, the Continental Scientific Drilling Program and Rock Mechanics, were started in FY 1980. The FY 1982 request provides for strengthening the work in these three areas and for starting work in two other highly important areas: Organic Geochemistry, an area of fundamental importance in understanding the formation and diagenesis of coal, petroleum and other fossil fuels, and Regional Geological Studies to interpret crustal structure and tectonics in terms of energy-related uses.

The studies of the migration of chemical species in the earth's crust apply to radioactive waste isolation and rock-fluid interactions relating to in-situ mining and geothermal energy. In FY 1982, $1,000,000 is required for this effort in Geochemical Migration. Work completed in FY 1980 on the actinide elements in groundwater has elucidated the sequence of oxidation states and their relative stabilities. The more highly charged actinides are found to be more insoluble and have a higher affinity for adsorption than the less highly charged actinide ions. A geologic study of rare earth element migration, where a granite has intruded carbonates interbedded with silts, serves as an analog for long-term actinide element migration. Results show that migration of the trace elements has taken place over distances of several kilometers. The trace element concentration gradients from the granite pluton contact are greater in the silt than in the carbonate zone. By throwing light on the migration of radioactive species, these results have significant importance to designing methods for isolating radioactive wastes.

In FY 1982, $3,200,000 is required for the DOE portion of the National Continental Scientific Drilling Program (CSDP). The CSDP is a cooperative interagency program of experimentation and drilling at selected sites for the development of information on the underlying structure, dynamics and chemical processes of the North American Continent. The resulting knowledge will be important in predicting deposits of energy resources, in establishing a scientific base of information relevant to nuclear waste isolation, and in the assessment of hazards associated with the siting of major energy-related facilities.

In FY 1982, $2,200,000 is required for studies on magma-hydrothermal systems, an area in which the DOE geoscience program has a special interest. During the past year four DOE laboratories jointly completed a comparative site assessment for deep drill holes into such systems. The study focused on the five most promising geothermal sites under which complicated magma-hydrothermal systems may exist. In the future, drill holes will be needed as "research facilities" to ascertain physical and chemical properties of rocks under those in-situ conditions which pertain to energy resources or waste isolation.

The remaining $1,000,000 will be used in situations where other energy-related geologic information can uniquely be obtained from drilling, downhole experimentation, logging and sampling. One way to minimize the high cost of drilling is to use or deepen holes drilled by the DOE technology programs, by other government agencies, or by industry and thereby to maximize the scientific returns from these holes at minimal additional costs. Work completed so far includes documentation for the first time of the full range of DOE drilling activities; this information base will help open up opportunities for studies in regions of special interest in DOE. Shallow holes may be required in scientifically-critical locations where no holes exist and surface geophysical information is ambiguous. Experimentation with shallow holes and holes of opportunity can contribute useful or definitive data to our knowledge of basement rock, heat flow, in situ stress and regions of complicated structure such as the folded Appalachians.

In FY 1982, $800,000 is required for energy-related studies in Rock Mechanics. These efforts are needed in order to (1) define in-situ conditions of the earth's subsurface; (2) determine the constitutive behavior of rock under different subsurface conditions; (3) generate predictive numerical models based on a sound knowledge of rock physics; and (4) obtain field data to validate such predictive models. Such long-range efforts will provide a better basis for the design and operation of all types of subsurface facilities from oil and gas storage caverns to radioactive waste disposal repositories and lead to the development of better siting and design criteria for earthquake protection. Specifically, mechanical property tests of crystalline rocks for the range of temperature and pressure likely to be encountered in geothermal recovery and in excavation and maintenance of underground waste projects show that crystalline rocks will be drillable by conventional techniques, because of brittle behavior right up to temperatures of partial melting.

Another recent result is the production of multiple hydraulic fractures at intermediate loading rates. This knowledge can be applied to produce greater stimulation of a geothermal rock mass or an oil or gas reservoir than if either static or explosive loading were used. Seismic velocity has been measured in the negative effective pressure region where internal fluid pressures exceed confining pressure. The velocity change is relatively large over a small pressure range. These results are important to situations of induced fluid injection such as in secondary recovery in oil fields or in hot dry rock geothermal reservoirs.

Also, in FY 1982, $400,000 will be required for a new program in Organic Geochemistry. The rapid development of sophisticated instrumentation for identifying and quantifying organic compounds on molecular, elemental and isotopic levels can be applied to problems dealing with the origin, spatial and temporal distributions and fates of carbonaceous materials. The origin of modern organic geochemistry may be traced to studies involving the nature of petroleum. The discipline is largely concerned with natural gases, petroleum and coal. In a current project electron microprobe work already has been accepted as a valid method for direct organic sulfur analysis in coal. A workshop was held in December 1980 to define the geoscience problems associated with the efficient discovery and utilization of carbonaceous fuels and to design strategies for solving these problems.

A new initiative in Regional Geologic Studies will require $400,000 in FY 1982. The evolution, dynamics, stratigraphy, petrology, and structure of major tectonic provinces need to be studied in an integrated, concerted fashion. The emphasis will be to increase basic geologic knowledge for application to those energy resource or waste disposal problems occurring within each tectonic province. Currently, a consortium of five universities is proposing to study the Alaskan Peninsula as a model magmatic arc. Arc systems are characterized by volcanic chains and parallel trenches which mark where lithospheric plates descend into the asthenosphere creating some of the world's most explosive volcanoes and largest earthquakes. Exploration for hydrocarbons and geothermal energy in arc systems will probably increase substantially in the near future. An improved understanding of basic geologic processes operating in arcs should be of considerable value to developing an effective technology for prospecting in these complex rock formations. Future regional studies may focus on the Appalachian Mountains (where a major overthrust has recently been discovered), the Basin and Range Province, the Midcontinent Basement, and the Colorado Plateau.

Capital Equipment

The FY 1982 request for capital equipment for Engineering, Mathematical and Geosciences is $2,550,000, an increase of $790,000 above the FY 1981 level.

Engineering Research projects will require $400,000 in equipment funds in FY 1982 for effective implementation of the new thermophysical/thermochemical data bases program, research on instrumentation for non-destructive evaluation, experimental studies of vibrational noise due to turbulent heat transfer, investigation of reduction of friction, as well as to meet high priority needs arising from ongoing research, such as measurement methodology for hostile environments and studies of crack propagation in engineering structures.

In addition, $950,000 is requested for capital equipment in Applied Mathematical Sciences. The most compelling needs are at the Research Computing Facilities (RCF's) being developed at several DOE national laboratories and universities. Each RCF consists of one or more minicomputers to serve a key part of the research program. The RCF's are linked by existing computer networks to facilitate access by researchers without a local RCF, stimulate interactions among various supported research groups, and provide a resource for research on distributed systems. The RCF's also serve as gateways to large-scale scientific computers and other DOE computing resources. The Research Computing Facilities will provide the resources needed to explore innovations in use of new computer technology, while also pointing the way to new technological frontiers. The applied mathematical sciences computer research community needs to use the computer itself as the object of experimentation. This experimentation is clearly incompatible with the stability of the computing environment required to serve the computing needs of other disciplines.

For Geosciences, $1,200,000 is required for capital equipment in FY 1982. These funds are needed to provide equipment of vital importance to the DOE's Geosciences research program. Examples of geoscience equipment needs at several national laboratories are as follows. At LASL an X-ray diffractometer, scanning electron microscope, Raman spectrometer, mechanical creep testing machine, ion microprobe and transmission electron microscope are needed for petrographic analysis and rock mechanics. At Sandia-A, a downhole seismic system, plasma source spectrometer, scanning electron microscope and digital seismic signal processing system are needed for magma energy related research. At LLNL, ultrasonic velocity equipment is needed for rock mechanics, seismometers are needed for seismology, and computer interfaces are needed for underground imaging. In addition to providing capital equipment to the DOE laboratories, $200,000 will be reserved for academic institutions in FY 1982. Obsolescence of capital equipment has been an increasingly serious problem for universities in the past several years. New generations of analytical and computing capabilities can spur on a broad range of energy-related geoscience research from geochemistry to seismology. For example, energy dispersive x-ray systems now permit chemical analysis down to 100 Angstrom resolution, through which the spatial distribution of uranium and thorium along grain boundaries in rock can be determined. Such instruments would constitute an important increase in capability for understanding uranium ore genesis or for studies of nuclear waste isolation.

Advanced Energy Projects

The objective of Advanced Energy Projects 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, either because of their unconventional nature or for any other reason, do not easily fit into the existing Department of Energy program structure. Most of the projects supported fall into a category known as "high risk, high potential pay-off." In FY 1982, $9,000,000 is requested for operating expenses, an increase of $2,650,000 over FY 1981; the request for capital equipment funds is $400,000, representing a $100,000 increase.

The Advanced Energy Projects program was first instituted in FY 1978 to provide a vehicle for supporting work on new ideas in danger of falling into programmatic cracks. It accepts unsolicited proposals from researchers at universities, industry and government laboratories. There are no limitations as to the technical approaches proposed: among the projects presently supported, some are directly related to specific technologies such as coal (example: ultrasonic grinding of coal), nuclear (example: uranium retrieval from seawater), solar (example: new, thus far unexplored, means of concentrating solar radiation), and, some are so novel, far-reaching and potentially relevant to various technologies that they do not fit any of the common categories (example: x-ray lasers, new schemes for accelerating particles big enough to be seen by the naked eye). The one restriction imposed upon projects supported is that their duration be limited in time, usually not to exceed three years; the program does not fund continuous, evolutionary research. Following a period of support by Advanced Energy Projects, a project is expected either to be picked up for further funding by a specialized program (within or without the government) or else be dropped.

In the short time since its inception the Advanced Energy Projects subprogram became a Department-wide focal point for research in such areas as:

- new methods for direct heat-to-electricity conversion;
- new designs for efficient heat engines;
- new methods of accelerating charged particles--with a potential for eventually replacing costly accelerators; and
- new approaches to solar energy concentration.

At the time of this writing, the first set of projects initiated under the auspices of Advanced Energy Projects has not yet been completed. Still, a number of accomplishments can already be listed. Those developed within the last fiscal year include:

- A new method for solar cell fabrication, called Arc Plasma Spraying. This technique, developed by scientists at a small company, offers the promise of a significant cost reduction in mass scale fabrication of solar cells.

- A new concept in heat energy utilization, known as the Energy Exchanger, has been identified by the DOE Office of Coal Utilization as a likely candidate for application in pressurized fluidized bed systems where it would significantly improve overall system efficiency. The Energy Exchanger was conceived by scientists working for a small business company; exploratory research under a three-year sponsorship of the Advanced Energy Projects program resulted in a successful development and testing of a bench-scale model.

- A new method of electrolytic production of pure silicon, analogous to that commonly used in the production of aluminum. This method, developed by scientists at Stanford University, offers a potential for drastically cutting the cost of pure silicon, and thereby of silicon-based solar cells.

One of the projects completed earlier, and reported in last year's budget submission, involved a new method for extracting oil from tar sands using radiofrequency heating; that project continues as a multi-million dollar field-testing program, under continued Federal and private funding.

To summarize: Three years after its inception the Advanced Energy Projects program has fully realized its stated objectives, having developed into a technically ambitious, scientifically advanced and programmatically vigorous activity.

Operating Expenses

The goal of Advanced Energy Projects is to initiate support of about twenty new concepts during each year. The choice of the number twenty takes into account both past experience and the pressure of highly rated proposals which must be declined for lack of funds. In FY 1978, the program's first year of operation, twenty-one projects were selected for support. In FY 1979 and FY 1980, available funding permitted, respectively, only thirteen and fourteen projects to be started. The annual funding level per project in FY 1980 varied between about $60,000 and $250,000.

The FY 1982 request of $9,000,000 in operating funds is justified as follows: new energy-related technical concepts are being born continuously; it is impossible to predict exactly what new ideas will be proposed in FY 1982 but one can state with certainty that many will emerge. It is imperative that the best be explored. The amount requested would permit the initiation in FY 1982 of about sixteen new projects for exploratory research--in addition to continuing the support of projects initiated in FY 1980 and FY 1981.

Capital Equipment

The FY 1982 request for capital equipment funds is $400,000. Some of the research efforts supported by Advanced Energy Projects require advanced instrumentation and other ancillary equipment. This request addresses these important equipment needs. Without the required equipment, it would be impossible to explore fully certain of the projects selected for support under Advanced Energy Projects.

Biological Energy Research

The principal objective of the Biological Energy Research (BER) subprogram is to generate the fundamental biological data base for the Department's efforts towards increasing biomass production for energy use, using biological transformations of biomass to fuels and chemicals (bioconversion) and using biological systems for resource recovery (bioprocessing). The subprogram has two activities, Botanical Sciences and Microbiological Sciences. The research is aimed at developing a broad, intensive understanding of the biological factors involved with plant biomass productivity, conversion of biomass and other organic materials by microorganisms into fuel and chemicals, and use of biological systems for sparing energy resources (conservation).

While the DOE Biomass Energy Systems program stresses near- to mid-term research and development needs, the BER program is oriented towards longer term and fundamental research. BER is the only basic biological program in the Federal Government specifically aimed at using biological systems for energy applications. While there are a number of problem areas common with U.S. Department of Agriculture (USDA) programs, the major difference is that DOE has primary interest in biomass production for fuels and chemicals. The species of plants used are usually different and the growing areas will be somewhat different from those of interest to USDA, with DOE focussing particularly on the use of marginal lands and aquatic areas.

Some recent accomplishments reflect the nature of this young program which was established in FY 1979.

- Recently, it has been discovered that small polysaccharides (chains of sugars) act as regulators of plant growth and plant defense against attack by disease organisms. Plant disease-causing fungi and bacteria produce specific small polysaccharides that act as hormones (messengers) causing the plant to produce new antibiotics, protective enzymes, and new growth to resist pathogen attack. In addition, injury or trauma to plant cells causes release of specific enzymes that, in turn, release short polysaccharides from the plant's own cell wall. These cause specific changes in the plant depending on the type of "hormone" released. The data supports a novel hypothesis: the specificity of plant growth and response to disease relies upon a set of polysaccharide hormone-messengers. This new knowledge will add significantly to our ability to design plants that are intended specifically for improved biomass production.

- The molecular basis for cooperativity between different microorganisms in binary fermentations is under study. Bioconversion of cellulosic biomass to ethanol has been difficult because of low levels of ethanol produced by strains of microorganisms that degrade cellulose easily. Experiments have been performed on simultaneous fermentations by two bacterial strains both tolerant to high temperatures, one that breaks down the cellulose to smaller units and the second that produces high yields of ethanol. The second organism was found to enhance cellulose breakdown enzymes. Using such binary systems of bacteria, high-temperature conversions of cellulosic biomass to liquid fuels such as ethanol have been achieved. These experiments provide the basic science support for fitting microbial systems to modern fermentation technology for cellulosic biomass conversion.

- Recent work has provided better insight into how plants synthesize cellulose, the most abundant organic chemical in nature and the principal component of biomass. The system under study uses cotton as a model in which cellulose biosynthesis is followed in fiber development. While the exact mechanism by which plants make cellulose is still not clear, recent research indicates that the synthesis proceeds from a precursor, uridine diphospho glucose (UDP-glucose) and requires an intact cell membrane with a gradient of positively charged ions. This membrane charge may provide energy for a yet unknown step in the process of cellulose production.

- Study of the molecular basis of genetic phenomena in corn is leading to a better understanding of controlling elements that determine and modulate gene activity. These controlling elements are discrete pieces of DNA called insertion sequences that allow changes in both gene position and expression in bacteria and animal cells. Using developing corn kernels that make specific storage protein and the enzyme, sucrose synthetase, as model systems, recent research has shown how specific genetic loci in plants may be turned on and off and moved about within chromosomes by the controlling elements. The work is significant in providing us with information about existing "gene-vehicles" in corn that can be manipulated by plant-molecular geneticists in the future for plant improvement in many new directions such as biomass yield.

The FY 1982 budget request for the Biological Energy Research subprogram is $10,000,000 of which $9,500,000 is for operating expenses and $500,000 is for capital equipment. The BER subprogram was initiated in FY 1979 with the objective of filling an important gap in the Federal research establishment, namely to provide an effort towards filling fundamental, long-term research needs relating to the use of biological materials in energy systems. During FY 1980 and FY 1981 the program has experienced moderate and careful growth in scope and depth. This fact has been quite beneficial in beginning to provide the type of fundamental program in the plant and microbial sciences essential for examining the various options to utilize biological systems in energy matters. The FY 1982 request continues this pattern of careful growth requisite to making innovative use of biosystems.

Operating Expenses

The FY 1982 request for $9,500,000 in operating funds for Biological Energy Research represents an increase of $2,250,000 over the FY 1981 level. Although some of this increase is necessary to cover cost-of-living for current research efforts, most of the increase is designed for university laboratories in support of expanded botanical and microbiological research.

Of the total operating expenses requested, approximately $5,500,000 is planned for research concerning how plants convert solar energy into biomass and what the limitations to these conversions are (Botanical Sciences). The following describes the principal research areas in the botanical sciences identified for expansion in FY 1982. The mechanisms by which plants adapt to sub-optimal growing conditions are expected to receive increased attention. These studies are crucial if marginal lands are ever expected to be used effectively. The goals will be to better understand the functions of plants under stress in biochemical and physiological terms and in particular, to understand the key role of roots in regulating plant growth, as well as to understand root-soil microorganism interactions. The manner in which genetic information is expressed in higher plants at the physiological and biochemical levels will be investigated. These studies are closely related to other research involving the transfer of genetic information in plant systems. Such investigations are essential in bringing the promising tools of genetic manipulation closer to realization for the improvement of plants as biomass crops. The way in which plants partition the solar energy they trap will be studied. This will include attempts at understanding the regulatory mechanisms in plants which determine which chemical compounds are produced and where in the plant. Such information is exceedingly important for devising strategies for chemical and genetic control of the products that may be produced by future biomass crops.

The remaining $4,000,000 in the request for operating expenses is planned for research on the conversion of biomass to energy rich organic chemicals by microbial activity (Microbiological Sciences). A stronger basic foundation of knowledge concerning microbial fermentations is essential to the eventual application of fungi and bacteria to a variety of modern production systems for fuel and chemical feedstock production from biomass. The "microbiology" portion of Biological Energy Research will focus on the following areas. Under investigation will be many diverse fungi and bacteria that have special capabilities such as rapid digestion of cellulose, fermentation at high temperatures, high tolerance to solvents, and binding of cells to solid supports. The understanding of the molecular nature of such special capabilities will permit a rational approach to designing processes and bioreactors using specialized fungi and bacteria to carry out specific tasks for the conversion of biomass to fuels and chemicals. Directly related to successful biomass conversion is the rapid degradation of biopolymers. The bulk of the renewable biomass resources consists of the biopolymers, cellulose, hemicellulose and lignin. Thus, detailed basic biochemical research is planned on the numerous biocatalysts produced by microbes that degrade and digest these molecules. This is essential for future manipulation of these properties for development of new processes. In addition, some studies will be directed toward combinations of microbes that work either in parallel or in series to loosen and digest complex biopolymers and provide substrates for gaseous or liquid fuels produced by other microbes.

Undergirding all of these investigations is a new effort to begin an in-depth study of the genetics of bacteria which can only grow in the absence of oxygen (obligate anaerobes). These various organisms are vital to fuel and chemical production from biomass and yet, surprisingly, almost nothing is known of their genetics. This portion of the program will pioneer genetic research of anaerobic microorganisms, and at the same time exploit modern recombinant DNA and genetic engineering technology. The aim will be to use the power of modern genetics to reveal the mechanisms of microbial breakdown of biopolymers and the regulation and pathways of metabolism by major groups of important fermenting organisms which heretofore have been little understood.

Capital Equipment

Funds in the amount of $500,000 are requested for capital equipment in order to provide the analytical tools and other instruments for carrying out the research of the BER program. Items such as fermentors, high pressure liquid chromatography-mass spectrometer combinations, spectrophotometers, centrifuges, and radioisotope counting equipment are essential to maintaining a research program which is contemporary and vigorous. Without these instruments, some of the studies could not be performed at all.

Inertial Plasma Physics Research

The overall objective of the Inertial Plasma Physics Research subprogram is to explore the physics associated with the interaction of high power laser beams with matter. This includes the study of the conditions appropriate in condensed matter for significant energy release, fundamental properties of highly condensed matter and their relationship to astrophysical processes, (i.e. laboratory astrophysics), laser photochemistry, x-ray biophysics and the investigation of energy transfer in dense biological systems, materials development for radiation applications and many others. The University of Rochester operates the National Laser Users Facility (NLUF) which is centered around three laser systems: (1) the 24 beam symmetrical illumination OMEGA system (12 terrawatts, 4 kilojoules) which uses neodymium glass laser at 1.05 micrometer wavelength, (2) the Glass Development Laser, and (3) the Diagnostic Evaluation Laser. Also included are large scale computation facilities. These systems are available to scientists both within and outside the University of Rochester to conduct research in the above areas. In FY 1981 the University performed high energy density plasma physics research in the following areas: interaction physics, beam characterization, ultraviolet materials and direct illumination studies. Major accomplishments during FY 1981 include: (1) completion of the 24 beam OMEGA laser system ahead of time, under budget, with system performance exceeding contractual objectives, (2) demonstration of high conversion efficiency (>80%) of 1.054 micrometer high power laser radiation to third harmonic (0.3513 micrometer) thereby opening up the possibility of utilization of these facilities for high power short wavelength interaction studies (in principle this allows higher efficiency implosions to be carried out with significantly lower input energy), (3) demonstration of strong coupling (>80%) of third harmonic (0.3513 micrometer) radiation with solid targets in agreement with the higher absorption efficiency predicted theoretically, (4) demonstration of the highest brightness x-ray laboratory source to date, using 0.3513 micrometer radiation and metallic targets producing x-rays in the 1-10 KeV range, which makes possible nanosecond time resolved material structure and biophysics studies, and (5) development of subpicosecond laser radiation sources and the demonstration of the use of these in fundamental time resolved photobiology energy conversion studies.

Operating Expenses

In addition to its value for understanding basic processes in matter, this research will also lead to a better understanding of phenomena occurring in inertial fusion targets when illuminated by laser drivers; hence the work resulting from this program is highly relevant to the effort in the area of inertial confinement fusion. A second attractive feature of the program is that, being located at a university campus, it provides a unique vehicle for training students in the increasingly important field of high power laser technology and high energy density physics. A third feature of the program is the significant industry, New York State and University participation in operations amounting to $42,400,000 out of a total program cost of $76,700,000 or 55% of the total over five years through FY 1981.

In FY 1982, $7,400,000 for operating funds are requested. This breaks down as follows: $5,330,000 for in-house research, $1,000,000 for users research and $1,070,000 for NLUF management and operations.

The in-house research has as its goal the implementation of implosion experiments on a 6 to 12-beam symmetrical irradiation facility. Research will be conducted in two major areas. (1) single/two beam - short wavelength studies - continuation of work begun during FY 1981 on interaction physics at 0.3513 micrometer including experiments and theoretical support and studies on ultraviolet optical materials ($2,400,000) and (2) direct illumination - uniformity - the objective of this work is to design and conduct appropriate experiments which will provide data relevant for assessing the uniformity of energy deposition and transport attainable for directly illuminated targets ($2,930,000).

User Research: $1,000,000 is requested for support of research to be performed at the NLUF by scientists from outside the University of Rochester.

NLUF Management and Operations: $1,070,000 is requested for management of the NLUF ($200,000), as well as for operating the facility under the users program ($870,000).

Capital Equipment

The requested amount of $1,600,000 will allow the acquisition of equipment required for the NLUF and available for use by all NLUF users at no charge. These items include the 24 beam OMEGA target chamber ($197,000), diagnostic equipment for user experiments including electronic x-ray cameras and oscilloscopes ($649,000) and spare parts for the laser system to maintain its operability during FY 1982 ($754,000).

Program Direction

Basic Energy Sciences is a broadly diversified program requiring staff with expertise covering many subfields in the areas of chemistry, physics, engineering, metallurgy, geosciences, biology, mathematics and computer science, as well as in administration, procurement and financial management. Some of the non-technical support is shared with the Office of High Energy and Nuclear Physics and the Office of Energy Research, although funding for all of their efforts comes from this specific request. Basic Energy Sciences staff are responsible for development, direction and management of complex technical programs, each involving one or more of the scientific areas mentioned above. 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.

The FY 1982 request for Program Direction for the Basic Energy Sciences program is $2,900,000, an increase of $332,000 above the current base. The request is necessary to provide for the salaries, benefits, travel and related expenses associated with the 63 staff years of effort required to administer the program. This is an increase in staff of eight above FY 1981. The principal factors justifying the need for additional staff are:

- During the last several years, there has been a marked expansion of the areas of research covered and an accompanying change in emphasis of the Basic Energy Sciences program coincident with the additional mission requirements of ERDA and DOE beyond those of the AEC.

- The recently intensified emphasis on integrating research results with needed support for the applied technologies has required considerably more staff attention to interact with other DOE program offices to coordinate basic research with the applied program development projects, to participate in the identification of Departmental technology base needs, and to contribute to the comprehensive planning needed to achieve an interrelated program.

- There has been a marked increase in the past year of the need for staff specialists to plan and monitor the construction and operation of complex and unique scientific facilities.

- The basic science programs have recorded a near doubling since FY 1977 of the number of unsolicited research proposals that they must evaluate and consider for funding. This essentually uncontrollable infusion of scientific ideas is crucial to the programs and each must be evaluated and considered for funding, a major requirement on staff time.

Department of Energy
FY 1982 CONGRESSIONAL BUDGET REQUEST

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

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

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

3. Date A-E work initiated: 1st Qtr. FY 1982

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3a. Date physical construction starts: 3rd Qtr. FY 1983

4. Date construction ends: 3rd Qtr. FY 1985

5. Previous cost estimate: None
Date:

6. Current cost estimate: $17,000
Date: 1/81

7. Financial Schedule:

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1982	$17,000	$ 3,500	$ 3,500	$2,400
1983	0	9,500	9,500	7,600
1984	0	4,000	4,000	6,000
1985	0	0	0	1,000

8. Brief Physical Description of Project:

The proposed project will consist of a new multi-story building to be approximately 50,000 sq.ft. Particular attention will be paid to make the design energy efficient and to take advantage of the latest active and passive solar heating techniques. The building will house research laboratories, offices, and service areas, and the project will also include special equipment for high temperature materials research in the areas of mechanical behavior, environmental interactions, physical property measurements, structural characterization, materials synthesis and preparation, and high temperature chemistry.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

8. Brief Physical Description of Project (cont'd):

Principles of energy conservation will be emphasized in every aspect of the design of the High Temperature Materials Laboratory (HTML). The environmental control systems will be designed for the best utilization of energy through the use of heat recovery systems, the installation of the minimum necessary number of fume hoods, and the use of systems operations management techniques. Roof mounted solar collectors will be installed to collect heat for domestic hot water requirements, for process hot water to preheat outside air directed to laboratories with hoods, and for other applications where economically feasible.

Laboratories will be provided for the research groupings to be housed in the building (Mechanical Behavior, Environmental Interactions, Physical Properties, Structural Characterization, Materials Synthesis and Preparation, and High Temperature Chemistry). The laboratories will include a large mechanical behavior laboratory on the second floor, several standard size laboratories, and smaller laboratories for individual research activities. Office space will be provided to accommodate requirements for both single and multiple occupancy. Service and support areas will include mechanical and electrical shops, a loading dock and a penthouse for the ventilation system. A combination freight and passenger elevator will be located near the dock entrance to facilitate deliveries to the upper floor and the equipment penthouse, and as an aid to handicapped persons. Improvements to the land will include a new paved access road and service driveways, parking areas for government vehicles, walks, and landscaping. Utilities will be extended from existing distribution systems. Planned long-term experiments, which may run continuously for a decade or longer, will be protected against power failure by emergency power from diesel motor-generator sets. Drainage from the facility will flow to the existing plant collection and treatment systems.

9. Purpose, Justification of Need for, and Scope of Project:

The purpose of the HTML is to provide appropriate space and equipment to conduct research designed to provide an understanding and useful application of the relationships between a material's properties at elevated temperatures and its structure, composition, and environment. It is intended that the materials to be studied will be directly related to the needs, both short- and long-term, of the DOE energy systems development. The HTML will also provide the concentration of expertise to provide solutions for complex short-range elevated temperature materials problems in fossil and advanced energy systems. The size of the proposed HTML and the special equipment needs were arrived at through a careful consideration of the variety of research programs needed to accomplish these aims and an understanding, based on our experience, of the critical size of the individual research groups.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee	2. Project No. 82-E-322

9. Purpose, Justification of Need for, and Scope of Project (cont'd):

Need for High Temperature Materials Research

Materials limitations dominate virtually all of our advanced concepts for energy production and use. These limitations are most commonly associated with mechanical or chemical stability at elevated temperatures in more adverse environments. For example, component failures due to erosion and corrosion processes are the chief causes of shutdowns in synthetic fuel pilot plants. Corrosive attack of the cathodes in high temperature batteries based on the Na-S cell limits the performance of such batteries, which might otherwise be used for electric vehicle propulsion and in electric energy storage systems. An understanding of elevated-temperature-materials behavior would affect the United States energy program in the following areas:

1. Higher operating temperatures of energy-producing systems, as governed by the Carnot cycle, would increase the efficiency of the conversion of heat energy.

2. The reliability of structural components in service at elevated temperatures would be improved.

3. The high temperature materials problems that limit the feasibility of some advanced systems would be solved.

4. The conservation of fuel and scarce materials would be achieved.

5. Broad exploratory research holds the potential for the discovery of new properties of known materials and for the development of new classes of materials. New physical phenomena may be discovered that might allow entirely new energy systems to be invented. Such long-term research holds the possibility of contributing to the energy needs of the United States in a revolutionary way.

Need for a High Temperature Materials Laboratory

Neither private industry nor another government agency is likely to fund the basic research needed to support energy systems materials needs. A comprehensive, DOE-supported laboratory is the most efficient medium- to long-range approach to the deficiencies that now exist. A DOE-dedicated laboratory, with its specialized equipment and personnel, would serve as an important national resource. Those factors favoring a HTML are listed below:

1. A HTML with its staff of professionals from several disciplines would be capable of addressing broad multi-faceted or multi-disciplinary questions concerning high temperature materials research.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

9. Purpose, Justification of Need for, and Scope of Project (cont'd):

2. A HTML would serve as a DOE resource, housing equipment and expertise in the specialized area of high temperature materials synthesis.

3. A HTML would improve the resolution and detection of high temperature materials phenomena through the development of uniform procedures for preparing, analyzing, and testing materials.

4. A HTML would permit difficult property measurements at high temperatures.

5. A HTML would be able to respond in a coordinated fashion to a problem in the use of materials at elevated temperatures requiring immediate attention and understanding.

6. A HTML would be able to attack the problem of predicting long-term (10 to 30 years) service behavior from short-term tests.

7. A HTML would provide a center for broad exploratory research on matter at high temperatures (>2000°C), a regime that is relatively unexplored.

8. A HTML, encompassing both fundamental and applied research, would expedite the transfer of fundamental information and results to technology.

Criteria for a High Temperature Materials Laboratory

To meet the above specification, a HTML must meet the following criteria:

1. It must have a strong basic materials science program in the areas of high temperature materials, and it must have strong links with the academic community.

2. It must have companion programs that extend from basic and applied research to engineering development related to the DOE mission.

3. It must work closely with industry to provide facilities and results that will further United States technology.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

9. Purpose, Justification of Need For, and Scope of Project (cont'd):

On the basis of applying these criteria to existing United States laboratories (industrial, nonprofit, and federal government) and university research centers, it was concluded that no facility now exists that has the required characteristics of the HTML.

The Oak Ridge Site

ORNL is a suitable site for the establishment of a HTML because it has: (1) a strong materials science program to form the nucleus of the basic research effort on high temperature materials, (2) many important projects in applied research and engineering for DOE-high-temperature-materials needs, (3) a long history of expertise in the area of high temperature materials technology, and (4) the extensive support facilities of a large multi-disciplinary energy-mission laboratory.

Research Programs for HTML

The research on high temperature materials will be organized into four broad groupings. Areas of expertise encompassed by the staffs of these groups are as follows:

1. Mechanical Behavior will include studies of creep, fatigue, fracture, and mechanical modeling.

2. Physical Properties will concentrate on thermal, electrical, optical, elastic, and magnetic properties, and thermometry.

3. The Structural Characterization Group will contain facilities for high temperature x-ray and electron diffraction, electron and optical microscopy, and surface characterization methods. The chief research areas will be phase stability and the kinetics of phase transformations.

4. The Materials Synthesis and Preparation Group will provide specimens for the other groups in the HTML, will provide samples for external researchers, and will conduct research on synthesis techniques (i.e., directionally solidified eutectics).

Estimates of Annual Costs of Operations

The estimates of the annual costs of operations (FY 1982 dollars) for the research activities described in previous sections are based upon 85 people physically housed in the facility. The estimated annual costs of materials, supplies, and services is $2,300,000. The estimated costs of the utilities is $1,000,000. The estimated annual costs of personnel including fringe benefits and overhead is $6,000,000.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

10. Details of cost estimate*

	Item Cost	Total Cost
a. Engineering, design and inspection at 20% of construction costs, item b.....		$ 2,100
b. Construction costs		10,200
1. Land improvements	$ 600	
2. Building construction (approximately 50,000 sq.ft. at $123 per sq.ft) ..	6,200	
3. Special facilities (laboratory hoods and exhaust system, special temperature and humidity controls, and special equipment for research)	2,600	
4. Utilities (electrical power, water and communications)	800	
c. Standard equipment, office and laboratory furniture, and movable equipment		1,700
Subtotal		14,000
d. Contingency at approximately 20% of above costs		3,000
Total Project Cost		$ 17,000

*This cost estimate is based on partial conceptual design.

11. Method of Performance

Design and inspection will be on the basis of a negotiated architect-engineer contract. To the extent feasible, construction and procurement will be accomplshed by fixed-price contracts and subcontracts awarded on the basis of competitive bidding.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

12. Pending Schedule of Project Funding and Other Related Funding Requirements

	Prior Years	FY 1982	FY 1983	FY 1984	FY 1985	Total
a. Total project funding						
1. Total facility costs	$ 0	$ 2,400	$ 7,600	$ 6,000	$ 1,000	$17,000
Total facility costs	$ 0	$ 2,400	$ 7,600	$ 6,000	$ 1,000	$17,000
2. Other project funding						
a. Direct R&D necessary to complete construction	$ 580	$ 0	$ 0	$ 0	$ 0	$ 580
Total other project funding	$ 580	$ 0	$ 0	$ 0	$ 0	$ 580
Total project funding	$ 580	$ 2,400	$ 7,600	$ 6,000	$ 1,000	$17,580*

*This total includes $580,000 for conceptual design prior to FY 1982.

12. Pending Schedule of Project Funding and Other Related Funding Requirements (cont'd)

b. Total related funding requirement (estimates life of project: 50 years)

1. Facility operating costs	$ 1,000
2. Programmatic operating directly related to the facility	8,300
3. Capital equipment not related to construction but related to the programmatic effort in the facility	1,000
Total Other Related Annual Funding Requirements	$10,300*

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

a. Total project funding

1. Total Facility Costs

See items 8, 9 and 10.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: High temperature materials laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 82-E-322

13. Narrative Explanation of Total Project Funding and Other Related Funding Requirements (cont'd)

2. Other Project Funding

R&D necessary to complete construction

Approximately $580,000 was spent on conceptual design prior to FY 1982.

*These costs are expressed in FY 1982 dollars.

b. Total related funding requirement

1. Facility Operating Costs

These estimated costs are for utilities for the building and program activities, maintenance of the building and its systems, and janitorial services.

2. Programmatic Operating Expenses Directly Related to the Facility

Programmatic operating expenses, directly related to the activities described in Item 9, cover consumable materials and supplies' costs, personnel costs including fringe benefits, and miscellaneous costs.

3. Capital Equipment Not Related to Construction but Related to the Programmatic Effort in the Facility

Capital equipment for programmatic activities is described in Item 9.

Department of Energy
FY 1982 CONGRESSIONAL BUDGET REQUEST

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

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

Office of Basic Energy Sciences (OBES)

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No. 82-E-321

3. Date A-E work initiated: 1st Qtr. FY 1982

5. Previous cost estimate: None
Date:

3a. Date physical construction starts: 2nd Qtr. FY 1982

6. Current cost estimate: $ 700
Date: 1/81

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

7. Financial Schedule:

Fiscal Year	Authorization	Appropriations	Obligations	Costs
1982	$ 700	$ 700	$ 700	$ 400
1983	0	0	0	300

8. Brief Physical Description of Project:

This subproject provides for additions, modifications, and improvements to major research accelerators, research reactors and ancillary experimental facilities. The requested funds are necessary to maintain and improve reliability and efficiency of operations and to provide new experimental capabilities as required for execution of the planned research program. Listed below are the laboratories and a description of each project:

Argonne National Laboratory $ 400

A system will be installed in the Intense Pulsed Neutron Source to bend and focus the accelerating proton beam.

Office of Basic Energy Sciences (OBES)

1. Title and location of project: Accelerator improvements and modifications, various locations

2. Project No. 82-E-321

8. Brief Physical Description of Project (cont'd):

Brookhaven National Laboratory $ 300

A reactor beam collimator and a small hot cell will be installed for the High Flux Beam Reactor (HFBR). A multipole high field wiggler will be inserted in a straight section of the National Synchrotron Light Source (NSLS) X-ray ring.

9. Purpose, Justification of Need for, and Scope of Project:

Argonne National Laboratory

Straight section length is very limited in the rapid cycling synchrotron of the IPNS due to the original machine and magnet design. Additional length for kicker and system magnets allows them to operate at a lower magnetic field strength which will make operation more reliable and reduce operating costs for the kicker magnet power supplies which comprise a substantial part of our operating costs. The additional magnetic fields available along with the planned diagnostic improvements will also provide for a cleaner operation which will reduce background radiation levels in the synchrotron tunnel. Increases in reliability and decreases in operating cost will enhance the neutron per dollar ratio, making the program more cost effective.

Brookhaven National Laboratory

A new tapered hole, reactor beam collimator will be fabricated and installed in the reactor shield to provide a suitable shape beam and maximal flux suitable for the TRISTAN Isotope Separator source at the HFBR. Samples irradiated in HFBR verticle thimbles are difficult to handle on the Operations Level because of induced radioactivity and tritium contamination. A small hot cell will be installed on the Operations Level with suitable off-gas, remote handling, and decontamination systems.

A multiple high flux field wiggler will be inserted in a straight section of the NSLS x-ray ring. It will greatly enhance the machine performance for short wavelength users. A three pole, 6 Telsa wiggler magnet is being considered. The magnet is of a cold iron core with either NbTi or Nb_3Sn coils. The bore tube is capable of withstanding a baking temperature of 150^oC and pressure differential of 20 psi. The dewar consists of an inner helium vessel, radiation heat shield and vacuum tank. The wiggler will be connected in a closed loop cycle to a refrigerator which will be used to cool the magnet from 88^oK to 4.35^oK. A liquid nitrogen recooling loop will be incorporated into both the magnet and inner vessel to reduce the requirement for refrigeration capacity. A fall flow purifier will be installed to increase the reliability of the wiggler performance. A helium gas recovery system and a 500 liter storage dewar will also be provided at the NSLS.

CONSTRUCTION PROJECT DATA SHEETS

Office of Basic Energy Sciences (OBES)

1. Title and location of project: Accelerator improvements and modifications, various locations	2. Project No. 82-E-321

10. Details of Cost Estimate*

	Total Cost
a. Engineering, design, inspection and component assembly and fabrication	$ 700
Total Project Cost	$ 700

*See breakdown of $700,000 in Item 8.

11. Method of Performance

Design will be by contractor staff. To the extent feasible, construction and procurement will be accomplished by fixed-price subcontracts awarded on the basis of competitive bidding.

Department of Energy
FY 1982 CONGRESSIONAL BUDGET REQUEST

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

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

Office of Basic Energy Sciences (OBES)

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

2. Project No. 82-E-320

3. Date A-E work initiated: 1st Qtr. FY 1982

5. Previous cost estimate: None
Date:

6. Current cost estimate: $ 300
Date: 1/81

3a. Date physical construction starts: 2nd Qtr. FY 1982

4. Date construction ends: 4th Qtr. FY 1983

7. Financial Schedule:

Fiscal Year	Obligations	Costs			
		FY 1980	FY 1981	FY 1982	FY 1983
Prior Year Projects	xxx	$ 254	$ 0	$ 0	$ 0
FY 1980 Projects	$ 250	28	222	0	0
FY 1981 Projects	300	0	200	100	0
FY 1982 Projects	300	0	0	200	100

8. Brief Physical Description of Project:

This project is required to provide for minor new construction, other capital alterations and additions, and for buildings and utility systems. Where applicable, the request also includes the cost of installed capital equipment integral to a subproject. Funding of this type is essential for maintaining the productivity and usefulness of DOE-owned facilities. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may be expected to result in additions, deletions, and changes in the currently planned subprojects. In general, the estimated funding for each location is preliminary in nature, and is intended primarily to indicate the relative magnitude of the requirements. No significnt R&D program is anticipated as a prerequisite for design and construction of the subprojects under consideration.

CONSTRUCTION PROJECT DATA SHEETS

Office of Basic Energy Sciences (OBES)

1. Title and location of project: General plant projects, various locations   2. Project No. 82-E-320

8. Brief Physical Description of Project (cont'd):

The currently estimated distribution of FY 1982 funds by office is as follows:

Ames Laboratory	$ 275
Notre Dame Radiation Laboratory	25
Total project cost	$ 300

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 varous locations:

Ames Laboratory $ 275

Requirements include: expansion of the laboratory energy management control system ($105,700); renovations for handicapped personnel ($23,800); a piping collection system, pumps, and controls for the return of steam condensate to the central steam system ($26,500); a closed loop cooling system for research equipment and spot cooling needs in the Metallurgy Building ($69,900); humidity generator upgrade for Spedding Hall and Development Building ($26,500); and miscellaneous small projects ($22,600).

Notre Dame Radiation Laboratory $ 25

Requirements include: building modifications to properly house staff members to optimize laboratory research space; and additional shielding within existing store room area for radiation protection purposes.

10. Details of Cost Estimate

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

11. Method of Performance

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

Department of Energy
FY 1982 CONGRESSIONAL BUDGET REQUEST

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

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

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

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

5. Previous cost estimate: $12,600
Date: 1/80

3a. Date physical construction starts: 2nd Qtr. FY 1981

6. Current cost estimate: $13 400
Less amount for PE&D 0
Net cost estimate: $13,400
Date: 1/81

4. Date construction ends: 4th Qtr. FY 1983

7. Financial schedule

375

Fiscal Year	Authorization	Appropriation	Obligations	Costs
1980	$ 4,300	$ 4,300	$ 4,300	$ 45
1981	3,000	3,000	3,000	2,255
1982	6,100	6,100	~~6,100~~ 0	~~6,900~~ 2,000
1983	0	0	0	~~4,200~~ 3,000

8. Brief physical description of project
This project will provide a laboratory-office addition to Building 62 of approximately 49,000 gross square feet for chemical and materials sciences research. As presently conceived, it will be a three-story concrete and steel framed building with partial basement. A separate silo will house a 1000 kV Atomic Resolution Microscope (ARM)1/ a computer control system, and a bridge crane. Other major equipment will include a 200 kV High Resolution Electron Microscope (HREM) with scanning transmission capability, a beam scattering chamber, an environmental chamber, an auger microprobe with a field transmission source, and x-ray and electron spectroscopy systems. The building will be equipped with an elevator and

1/Electron microscope technology has advanced to the point where it is possible to purchase a 1000 kV microscope for the same price as the originally conceived 500 kV instrument. The 1000 kV machine will permit higher resolution.

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

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

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, 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 on corrosion, embrittlement and solid state transformations;

C. The identification 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.

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)

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 1000 kV machine. These facilities will also require laboratory space, instrumentation and staff for specimen 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 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 catalysts, 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 operating 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 a fraction of the total Materials and Molecular Research Division 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.

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)

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 adsorbate-bonded surfaces, and 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.

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 other 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 being conducted in different locations and under overcrowded conditions will allow the more efficient use of shared facilities and provide for improved interdisciplinary interactions in the conduct of collaborative efforts.

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*

a. Engineering, design and inspection at about 18% of construction costs, item b		$ 1,150[1/]
b. Construction costs		6,150
1. Improvements to land	$ 255[2/]	
2. Building (49,000 sq. ft. gross at about $115/sq. ft)....	5,620[3/]	
3. Utilities	275[2/]	
c. Standard equipment		$ 5,050
1. ARM & associated equipment	$3,520[3/]	
2. Chemical sciences equipment	1,000[4/]	
3. Bridge crane, laboratory furniture and fume hoods	530[5/]	
d. Contingencies @ approximately 14% of items a & b. above		1,050
Total project costs		$13,400

*Based upon a completed Title I design, partial Title II and repackaging and rescheduling work.

1/Increase due to:
- a) New resource plan requires packaging work in a manner different from that originally planned
- b) New, stretched out schedule
- c) Escalation

2/Reestimate based on Title I design

3/Based on bids

4/Increase based on escalation

5/Increase based on escalation rate for fume hoods and furniture (17%) and Title I 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

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. Pending 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	$ 45	$ 2,255	$ 6,900	$ 4,200	$13,400
Total facility costs	$ 0	$ 45	$ 2,255	$ 6,900	$ 4,200	$13,400

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

1. Facility operating costs	$ 150
2. Programmatic operating expenses directly related to the facility	5,000
Total other related annual funding requirements	$ 5,150

*In FY 1982 Dollar Terms

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

B. Total related funding requirements
1. Facility operating costs: includes estimated cost for janitorial service and utilities such as light, heat, water, telephone.
2. Programmatic operating expenses related to this facility. The program activities to be conducted in the facility are described in Section 9 above.