

DEPARTMENT OF ENERGY  
FISCAL YEAR 1981 CONGRESSIONAL BUDGET REQUEST  
ENERGY SUPPLY RESEARCH AND DEVELOPMENT  
VOLUME 3  
BASIC RESEARCH  
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Department of Energy  
FY 1981 CONGRESSIONAL BUDGET REQUEST

PROGRAM OVERVIEW

Supporting Research

The need to develop new and improved energy sources and to use energy more efficiently is increasingly recognized. Economists, industrialists and executives within the government are now realizing that basic research is essential for the kind of technological innovations which have helped establish the position of the United States in the world's economy. Funding of basic research is an investment in the future. Failure to recognize this 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 need for energy-related basic research is of critical importance.

The following four programs make up the Supporting Research category of the Department of Energy: (1) Basic Energy Sciences (BES); (2) Technical Assessment Projects (TAP); (3) University Research Support (URS); and (4) Technical Program and Policy Analysis (TPPA). All four of these programs are under the Director of Energy Research. These programs are dedicated to maintaining a strong national energy program that will provide a base of pertinent knowledge for future scientists, engineers and mathematicians in the development and improvement of energy alternatives to meet the Nation's critical energy needs.

Basic Energy Sciences is the major Department of Energy program which supports and administers basic research in the physical and biological sciences, engineering and mathematics in order to provide fundamental information leading to improvements in existing technologies and to discover new concepts, materials, processes and techniques important for the production and efficient use of energy. BES assembles, encourages and supports a body of the Nation's most competent researchers in physics, chemistry, biology, the materials and nuclear sciences, engineering, geosciences and mathematics, in order to expand the base of scientific knowledge pertinent to energy and energy-related topics. In addition, the program will continue to support construction and operation of pioneering and/or unique facilities for use by scientists throughout the Nation. Traditionally, these facilities have been used primarily by their in-house research staff and by university users throughout the United States. However, increasing interest is being shown by private concerns which cannot afford the capital investment required to build these facilities (e.g., the Combustion Research Facility at Sandia-Livermore and the National Synchrotron Light Source at Brookhaven National Laboratory).

The primary output of basic research is new fundamental knowledge which is expected to influence the long-term energy capability of the Nation. Direct commercialization of results from basic research occurs fairly often; however, more often the benefits accrue as the accumulated knowledge and understanding of detailed processes and properties become an integral part of the body of data on which applied technologies rest.

The following recent accomplishments represent the spectrum of major advances coming out of the BES program: Ion-implanted and laser annealed solar cells of silicon have resulted in higher efficiency photovoltaic materials. Amorphous silicon and other amorphous alloys have been prepared with new sputtering techniques, thus showing the possibility of using less expensive starting materials for solar applications. The use of a fluid energy mill to grind coal has made it possible to produce homogeneous fragments of heterogeneous coal. Subsequent separation of the macerals (organic substances) from each other by a special centrifugation technique is resulting in separation of coal into its homogeneous components for analysis. This is a major step toward detailed understanding of the many varieties of coal which is important

for optimal and clean use of this vital energy resource. Applications to coal liquefaction and gasification should arise from this development. Numerous other accomplishments have been made in a wide variety of areas such as superconductivity, artificial photosynthesis, the fermentation of wastes to alcohol, nuclear data measurements, and the geological structure of the earth. In addition, a new source of tunable x-rays has been discovered which is likely to become a powerful tool in materials research. Some of these accomplishments are discussed in greater detail below in the narrative justification.

The provision of separated isotopes to the research community, done within the Nuclear Science portion of the BES program, is the only direct revenue-producing activity within the program. Revenues from this activity in FY 1981 are estimated to be about \$1,500,000.

The Technical Assessment Projects program provides the capability for independent rigorous assessment of the base of research that underlies a variety of energy technologies. The assessment of the Solar Power Satellite (SPS) concept, to be completed in 1980, falls within this budget category. In FY 1981 the SPS program will continue assessment efforts in areas of critical concern identified in the initial assessment and will conduct planning for a possible future exploratory development program. In addition this program 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 with 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. These efforts are intended to provide the Director of Energy Research with the information required to fulfill his role of providing advice and recommendations to the Secretary on Department-wide research and development issues and strategy.

The University Research Support program consists of three interrelated activities directed at supporting university-based energy research, which is specialized in nature and focuses on long-range, cross-programmatic subjects. This program operates between the disciplinary-oriented basic research projects supported by the Basic Energy Sciences program and the applied research, engineering and development-oriented responsibilities of the individual outlay programs. A related goal of this program is to stimulate and expedite the technology transfer process through the support, on a selective basis, of cooperative research efforts between universities, industry and DOE national laboratories. The three activities in URS are the University Institutional Agreements Program (which includes the Minority Institutions Research Program), the University Reactor Fuel Assistance Program, and the University/Laboratory Cooperative Program. The University Institutional Agreements Program provides support on a competitive basis for campus-wide programs of exploratory or "proof of concept" energy research and for the enhancement of energy research and education capabilities at smaller, traditionally minority institutions. The University Reactor Fuel Assistance Program provides support to a small number of university nuclear research reactors for the actual fabrication cost of nuclear fuel. In addition support will be provided for the establishment of a lower enriched uranium fuel fabrication line for these reactors in compliance with Department of State requirements regarding nonproliferation. The University Laboratory Cooperative Program provides for the maintenance of energy-related education and training activities involving university faculty and students.

Technical Program and Policy Analysis provides funds for the personnel resources required by the Director of Energy Research to carry out his responsibilities under the Department of Energy Organization Act (P.L. 95-91) or as mandated by the Secretary, in areas beyond the scope of the assigned Energy Research programs. The program provides funds only for the salaries and related personnel expenses for the personnel who carry out the studies, analyses, monitoring and coordinating activities required to support the Director, and does not include any funds for outside contracts. Included among the responsibilities assigned in P.L. 95-91 are monitoring the Department's research and development programs in order to advise the Secretary with regard to any undesirable gaps or duplications; advising the Secretary with respect to the well-being and management of the multiprogram laboratories; and supervising or supporting research activities carried out by any of the Assistant Secretaries.

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

	FY 1979 Appropriation	FY 1980 Appropriation	FY 1981 Base	FY 1981 Request
Basic energy sciences				
Nuclear science				
Operating expenses .....	28,150	30,700	30,700	33,400
Capital equipment .....	1,300	1,300	1,300	1,400
Subtotal .....	29,450	32,000	32,000	34,800
Materials sciences				
Operating expenses .....	71,520	79,000	79,000	92,000
Capital equipment .....	5,900	6,300	6,300	7,600
Construction .....	16,670	11,650	11,650	300
Subtotal .....	94,090	96,950	96,950	99,900
Chemical sciences				
Operating expenses .....	48,000	55,100	55,100	63,300
Capital equipment .....	3,400	3,700	3,700	4,740
Construction .....	3,400	6,300	6,300	6,500
Subtotal .....	54,800	65,100	65,100	74,540
Engineering, mathematical and geosciences				
Operating expenses .....	15,700	20,100	20,100	28,600
Capital equipment .....	800	1,250	1,250	2,060
Subtotal .....	16,500	21,350	21,350	30,660
Advanced energy projects				
Operating expenses .....	3,800	5,000	5,000	8,000
Capital equipment .....	200	200	200	300
Subtotal .....	4,000	5,200	5,200	8,300
Biological energy research				
Operating expenses .....	4,000	6,000	6,000	8,800
Capital equipment .....	0	300	300	400
Subtotal .....	4,000	6,300	6,300	9,200
Program direction				
Operating expenses .....	1,896	2,156 <sup>a/</sup>	2,289	2,444
Subtotal .....	1,896	2,156	2,289	2,444
Total				
Operating expenses .....	173,066	198,056	198,189	236,544
Capital equipment .....	11,600	13,050	13,050	16,500
Construction .....	20,070	17,950	17,950	6,800
Basic energy sciences..	204,736	229,056	229,189	259,844

a/ Reflects comparability adjustment of \$40,000 for the transfer of one position from the former Assistant Secretary for Energy Technology.

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

Summary of Changes

FY 1980 Appropriation enacted .....	\$229,056
Built-in increases and decreases:	
Pay cost supplemental .....	+ 133
FY 1981 Base .....	\$229,189
Program Increases and Decreases	
<u>Basic Energy Sciences</u>	
Maintain current level and provide for selected expansions in basic research programs in:	
Materials sciences .....	+\$14,300
Chemical sciences .....	+ 9,240
Engineering .....	+ 2,200
Applied mathematical sciences .....	+ 3,100
Geosciences .....	+ 4,010
Biological energy research .....	+ 2,900
Maintain current level of research in nuclear sciences .....	+ 2,800
Expand support of advanced energy projects .....	+ 3,100
Continue general purpose projects for Ames Laboratory and Notre Dame Radiation Laboratory .....	+ 50
Personnel-related increases for the above programs .....	+ 155
Begin an accelerator improvement project at ORNL .....	+ 200
Complete construction of three research facilities .....	-11,400
FY 1981 Budget Request .....	\$259,844

Basic Energy Sciences

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

In FY 1981, the Basic Energy Sciences request is for \$259,844,000, an increase of \$30,655,000 over FY 1980. Of this request, \$234,100,000 is for operating expenses; \$16,500,000 is for capital equipment; \$6,800,000 is for construction; and \$2,444,000 is for program direction. Since the establishment of BES's predecessor agency, the Energy Research and Development Administration, the ratio of the Basic Energy Sciences budget to the budget of the energy technology programs it supports has declined markedly. It is important to reverse this trend if the long-term needs of the energy technology

programs are to be satisfied. The FY 1981 request is a step in that direction. Highlights of the FY 1981 request include continuing a strong base research program needed to meet long-term energy needs; increasing basic research on the chemistry of coal (particularly relating to liquefaction), combustion, high temperature materials, corrosion, catalysis, novel approaches to the use of solar energy and nuclear waste isolation; and expanding the base programs in engineering, geosciences, advanced energy projects and biological energy research to meet the increasing demand for basic and exploratory research in these areas. The request also provides for the funding necessary to complete the Chemical and Materials Sciences Laboratory at Lawrence Berkeley Laboratory (LBL) in California. These and other areas of emphasis in FY 1981 can be discussed in terms of the six major programs under basic energy sciences. These are: 1) nuclear science; 2) materials sciences; 3) chemical sciences; 4) engineering, mathematical and geosciences; 5) advanced energy projects; and 6) biological energy research.

### Nuclear Science

The Nuclear Science subprogram is comprised of two separate but related functions, the first of which supports research relevant to fission and fusion nuclear energy and a second which provides a national service in support of a wide range of research activities. The first function (low energy nuclear science) supports both basic and applied experimental research that uses particle accelerators, research reactors, and special nuclear materials. Low energy nuclear science, by definition, consists of experimental accelerator research using beams less massive than the nucleus of helium and whose maximum energy is insufficient to produce pi mesons (a subnuclear particle which is believed to be the fundamental carrier of the nuclear force). Nuclear research at higher energies or with higher mass beams is supported in the DOE Nuclear Physics program discussed in the Basic Sciences part of the budget. Low energy nuclear science also supports experiments at the Brookhaven High Flux Beam Reactor. It includes support for the measurement of nuclear data important to the development of fission and fusion energy technologies and nuclear waste management and for the systematic compilation and critical evaluation of this data. In addition, low energy nuclear science supports experimental research in the study of the chemical and physical properties of the heavy elements (those elements with atomic numbers greater than 83), principally the actinide elements.

The second function in the Nuclear Sciences program is isotope preparation. This activity provides support to Oak Ridge National Laboratory (ORNL) in Tennessee for the Calutron facility to separate stable isotopes, for the High Flux Isotope Reactor (HFIR) to produce heavy actinide elements, and for the Transuranium Processing Plant (TRU) to chemically process heavy elements produced by HFIR.

The FY 1981 request of \$34,800,000 (\$33,400,000 for operating expenses and \$1,400,000 for capital equipment) is necessary to maintain Nuclear Sciences at the FY 1980 program level.

### Operating Expenses

#### Nuclear Sciences Summary of Operating Expenses

	Budget Authority	
	<u>FY 1980</u>	<u>FY 1981</u>
Low energy nuclear science		
Nuclear research	\$12,030	\$13,260
Nuclear data measurements	4,930	5,210
Nuclear data compilation and evaluation	2,375	2,585
Heavy element chemistry	<u>3,380</u>	<u>3,720</u>
Subtotal, low energy nuclear science	22,715	24,775
Isotope preparation		
Electromagnetic isotope separation	1,300	1,405
Special isotope preparation	<u>6,685</u>	<u>7,220</u>
Subtotal, isotope preparation	7,985	8,625
Total, nuclear science	\$30,700	\$33,400

### Low Energy Nuclear Science

The operating expenses request for FY 1981 for low energy nuclear science is \$24,775,000, an increase of \$2,060,000 above the FY 1980 level. The work supported under this heading is carried out in four main areas: nuclear research; nuclear data measurements; nuclear data compilation and evaluation; and heavy element chemistry.

The FY 1981 request for low energy basic nuclear research is \$13,260,000, an increase of \$1,230,000 over the FY 1980 level. This request would support experimental research in basic low energy nuclear physics. These very fundamental studies, particularly involving neutrons, also provide information which is relevant to long-term development of fission and fusion energy systems.

The nuclear research component of low energy nuclear science is a highly developed area of science. Both the fascination of the strange subworld of the atomic nucleus and the confirmed promise of practical applications of the knowledge gained from research in this field have led to a large investment in facilities and manpower. This investment and the current maintenance support is still highly productive. Our long-term goal is a quantitative understanding of the structure of nuclei and the mechanisms by which nuclei interact with light ions. Low energy studies now generally require more precision, higher resolution, and often such refinements as the needed ability to control the orientations of the spins of the reacting nuclei. Fortunately, the development of electronics, detectors, ion sources and other instruments has continued to improve the quality of the measurements.

Protons and deuterons (a very simple nucleus consisting of one proton and one neutron bound together) have a property called intrinsic angular momentum or spin. This is best visualized by thinking of protons and deuterons as spinning balls. By orienting the protons' and deuterons' spin along or at right angles to the direction of the accelerated beam, scientists measure ways in which nuclear interactions depend upon spin. The device which orients the protons' and deuterons' spin is a polarized ion source. At the University of Wisconsin, a new type of polarized ion source has been developed and a prototype tested. When fully operational, the novel design of this polarized ion source is expected to provide oriented proton and deuteron beams five to ten times more intense than are now available. In FY 1980 and FY 1981, University of Wisconsin scientists will use this new capability to investigate the fundamental nuclear interaction between protons and neutrons.

A new facility that has just undergone initial tests is the TRISTAN II on-line isotope separator at the High Flux Beam Reactor (HFBR) at the Brookhaven National Laboratory. TRISTAN II sorts the fragments resulting from nuclear fission into groups. This is done by a system of magnets. By such sorting, scientists can identify individual fission fragments and study their nuclear properties. Interesting new programs (e.g., nuclear structure studies of neutron-rich nuclides and delayed neutron emission studies important to nuclear power development) are being developed by BNL and by a number of university user groups (Clark University, Iowa State University, University of Maryland, and the University of Oklahoma). New contracts with other university groups are expected to be approved during the current year. Experiments to study the mass-separated fission fragments by laser techniques will also be supported.

The cyclograaff accelerator at Duke University (the major facility at the Triangle Universities Nuclear Laboratory that 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, as demonstrated by recent publications. Three other accelerators are jointly supported by Nuclear Science and Nuclear Physics, since they are extensively used for both light- and heavy-ion research studies. These are the tandem Van de Graaffs at Yale University and the University of Washington and the 88-inch cyclotron at the Lawrence Berkeley Laboratory. Support for research groups of proven excellence will continue at these facilities.

The budget request for nuclear data measurements is \$5,210,000, an increase of \$280,000 over the FY 1980 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 phenomena. The funding request is divided almost equally between measurements needed for the fission and for the fusion programs.

The activities devoted to satisfying the highest priority nuclear data needs of the fusion program are coordinated by a working group that includes representatives from three national laboratories (ORNL, LASL, and LLL) and from two universities (Duke University and Ohio University). The largest of these activities is that conducted at the Oak Ridge Electron Linear Accelerator (ORELA), where, for example, recent measurements show that the neutron capture cross sections for niobium, under consideration for use in fusion power reactors, are ten times larger than those found for vanadium (another candidate). The LLL group makes use of the world's most intense source of 14-MeV fusion neutrons to accomplish difficult measurements of the charged-particle production from suggested fusion reactor construction materials. This information is especially needed for estimating the radiation damage effects resulting from neutron bombardment of the material. The university groups and LASL use tandem Van de Graaff accelerators to provide pulsed neutron sources for measurements of elastic and inelastic scattering from nuclides that are contained in materials being considered in the design of fusion power reactors. LASL is beginning precise absolute measurements at the lowest possible energies of reactions involving deuterium and tritium that are of great interest in fusion research, and also in the diagnostics of the performance of the Tokamak Fusion Test Reactor being built at Princeton.

The work supporting the fission program includes measurements at ORNL of the average number of neutrons released during the spontaneous fission of californium-252, the standard by which all other fissionable materials are measured. At ANL, measurements will be continued on the yields of fast-neutron-induced fission products using nearly mono-energetic neutrons over an energy range of 0.1 to 8 MeV on the important fissile and fertile nuclides. This data will permit accurate modeling of the fission product yield spectrum for any fission reactor neutron spectrum.

At LLL the development of a fast chemistry system continues and measurements are being made of nuclear properties of short-lived fission products needed for reactor-fuel decay-heat predictions. At ORNL, the program of measurement of actinide cross sections is continuing 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 and the State University of New York at Albany. Measurements of differential inelastic neutron scattering cross sections of thorium and uranium have been initiated at the University of Lowell in Massachusetts. Other programs contributing to nuclear data needs are located at the University of Michigan, 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 \$2,585,000, an increase of \$210,000 over the FY 1980 amount. These funds would 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 major portion 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 a major 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 the responsibility for the coordination of the United States' effort in the compilation and evaluation of nuclear structure and decay data, as well as for selected charged-particle reaction data of interest for applied purposes. It coordinates this effort via a recently established National Data Network (NDN), which includes data centers at BNL, INEL, LBL, ORNL, the National Bureau of Standards (NBS), and the University of Pennsylvania. All but the NBS effort is funded by Nuclear 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 the desired 4-year update cycle 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 1981 budget request for heavy element chemistry is \$3,720,000, an increase of \$340,000 over the amount appropriated in FY 1980. These funds are needed to maintain at the same level as in FY 1980 support for a wide range of research activities involving the fundamental chemical and physical properties of the actinide elements. These elements comprise more than 13% of the known elements and constitute a group in which the trends of fundamental chemical properties and behavior change and about which comparatively little information is known. An understanding of the behavior of the transuranium elements (part of the actinide series) in glasses and other waste forms and in environmental media is of pivotal importance to the solution of many nuclear waste management problems; however, the fundamental chemical knowledge of these elements pertinent to these forms and media is largely unknown. The research supported in this activity seeks to develop this knowledge. The actinide elements are all radioactive; therefore, most of this research is carried out at the national laboratories where the proper handling facilities are available. Some studies of uranium and thorium and of the other actinides at the tracer level are pursued at universities, but university-based scientists also pursue research at the laboratories in a user mode.

At Argonne National Laboratory a major area of interest is the nature of actinide species in aqueous solutions. Information on the reactions of the actinides and their complex behavior in environmental media is being developed. Part of this project has been pursued in collaboration with chemists at Florida State University. Scientists at ANL are also initiating a study of the fundamental properties of actinides in glasses to determine the nature and strength of the actinide-oxygen-silicon interaction. Information from this study will be important to an understanding of the properties and behavior of this proposed nuclear waste form.

At LBL, in one of the many projects being pursued, scientists are endeavoring to design benign chemical agents that will specifically bind and biologically isolate plutonium so that it can be discharged from the body. Good progress has been made, and tests show that certain of the agents remove plutonium as effectively as the drugs that are presently used in treating plutonium poisoning, and at one-tenth the dose. The new agents also have lower toxicity and fewer side effects than the presently used drugs. Further work and testing is needed to improve these agents to the point where they can be modified and used for another promising application: the removal of actinides from nuclear wastes.

At ORNL research is pursued in two general areas: the determination of data for a fundamental understanding of actinide reactions and properties, and the application of basic research techniques to the solution of the applied problem of understanding the behavior of actinides in nuclear waste management systems. New insights have been obtained from this research. One insight of particular fundamental and theoretical interest is the increasing stability of the low oxidation states in the higher actinides (einsteinium, fermium, mendelevium, and nobelium). Studies have been initiated on the interaction of actinides with geological media and definitive information has been obtained on a variety of minerals including several clays. Strong adsorption in these media has been demonstrated and further investigations are underway to explain the nature of the interaction to assist in the design of possible overpack materials around waste canisters. Collaborative studies with a program funded under the Division of Materials Sciences are being pursued in which new actinide-containing waste forms are tested in the Transuranium Research Laboratory for their chemical stability and ground-water leach rate.

At LASL two projects are funded for the study of the lesser known chemical properties of the technologically important actinides, protactinium and uranium, and for the investigation of the high temperature thermodynamics of the actinide metals and their compounds. Scientists at LASL are determining the vapor pressures and heats of vaporization and sublimation of the rare actinide metals berkelium, californium, and einsteinium on the milligram and microgram scale in collaboration with scientists at ORNL. These measurements are fundamental to a thorough understanding of the thermodynamic stability and chemical behavior of the actinide elements and compounds.

Actinide research at the universities is conducted in a number of areas, largely in a user mode at the national laboratories because of radioactivity handling problems. Of particular importance are the studies based at the University of Tennessee in the chemical, physical, spectroscopic, and magnetic properties of the very rare higher actinides: curium, berkelium, californium, and einsteinium. These studies represent a frontier in chemistry and provide valuable insights for our broad knowledge and understanding of chemical properties and principles. Funding is especially important at the universities because of the concomitant training of young investigators needed in this area of increasing importance.

#### Isotope Preparation

The second activity under Nuclear Science provides support for the production, separation, purification, and allocation of samples of stable isotopes and actinide research materials for scientific research and for medical and industrial applications. The FY 1981 budget request for isotope preparations is \$8,625,000, an increase of \$640,000 over the amount appropriated in FY 1980. These funds are needed to maintain the level of operations at ORNL for three isotope production and separation facilities: the Electromagnetic Isotope Separation Facility (Calutrons); the High Flux Isotope Reactor (HFIR), and the Transuranium Processing Plant (TRU). The Calutrons separate stable isotopes, enriching them from their natural abundance to levels in excess of 99% in some cases. HFIR irradiates targets to produce the high atomic number, high mass actinides berkelium, californium, einsteinium, and fermium; and TRU chemically processes these targets to separate and purify samples of these elements so they can be made available to the research community. The TRU facility also works closely with the scientists providing special services and for the preparation of special samples and targets not available in the routine operation. HFIR also provides irradiation services for non-routine isotope production, as well as ongoing user research programs on an "irradiation-unit recharge" basis. This is available to industry when similar services are not available commercially. This reactor has an isotope production, neutron irradiation and neutron beam research capability unique in the Western world.

This total production effort represents the sole source of this broad range of research materials in the Western world. The samples are made available to the national and international research community by loan or by sale on a full-cost-recovery basis. Samples of stable isotopes from the research materials collection or loan pool are made available to investigators for non-destructive research in support of fission and/or fusion nuclear energy technology. For those research projects where the isotopic materials are consumed and for medical and industrial applications, samples are sold on a full-cost-recovery basis. 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 made available at foreign institutions to which the United States' investigator has been invited as a "hands-on" collaborator.

#### Capital Equipment

The FY 1981 capital equipment request for Nuclear Science is \$1,400,000, an increase of \$100,000 over the amount appropriated in FY 1980. Of this \$1,400,000 total, \$875,000 is needed for nuclear research, nuclear data measurements, and nuclear data compilation and evaluation; \$525,000 is needed for heavy element chemistry and isotope preparation. These funds are needed to maintain the research effort at the forefront of the field and to ensure the high quality of research results. Advances in fission and fusion nuclear energy technology require supporting data of higher precision and accuracy. These requirements must be met by ever more careful measurements with sophisticated equipment of advanced design. Advances in our ability to understand

the fundamental properties and reactions of nuclei are closely coupled to our ability to equip research accelerators and reactors and to instrument experiments for the detection of nuclear emissions. Progress in the field of actinide chemistry, especially as it relates to the development of nuclear waste management technology, requires new equipment to determine the nature of the actinide species at extremely low levels of concentration. Isotope production operations have a continuing need for new and upgraded equipment.

Equipment requirements in FY 1981 include data acquisition and analysis systems; electronics to instrument a nuclear time-of-flight detection system; a thin wall target chamber; laser systems for the characterization of gas-phase actinide species; an automated x-ray diffractometer; a xenon and helium gaseous scintillator detector system; klystron power tubes; a fast printer/plotter for data output; a differential scanning calorimeter; a mass spectrometer; high speed/high vacuum pumping systems; fission chamber assemblies; actinide processing equipment racks; and product purification equipment.

### Materials Sciences

This subprogram seeks to understand materials properties and phenomena which affect all energy systems. The primary purpose is to provide the necessary base of materials knowledge required to advance the Nation's energy production, conversion, transmission and conservation programs. Emphasis is placed on areas where problems are known to exist or are anticipated and on areas of fundamental importance across all energy systems. 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. For example, major materials problems/opportunities lie in the path of successful energy development with solar photovoltaics (cost, reliability, storage), synfuels production (corrosion, erosion, catalyst deterioration) and nuclear waste isolation (glass/ceramic host materials, canister). In Materials Sciences, emphasis is placed where significant improvements in performance must depend on the selection of materials based on improved understanding of the underlying mechanisms that control their properties. The program 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. Research in Materials Sciences is conducted primarily by personnel trained in the disciplines of metallurgy, ceramics, engineering, solid state physics and materials chemistry. Some of the research is aimed at a single energy technology (e.g., photo-voltaic materials for direct conversion of solar energy), whereas other research is applicable to many technologies (e.g., the embrittlement of structural materials due to the presence of hydrogen).

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 program takes place primarily through the DOE Energy Materials Coordinating Committee (EMaCC), but also through Materials Sciences Research Assistance Task Forces and less formal contacts among staff members. 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 1979 the Council reviewed research needs and opportunities in the areas of high temperature ceramics and theory of surfaces; corrosion and novel materials were examined in FY 1980. Interagency communication and coordination are handled primarily through the Committee on Materials (COMAT), an interagency committee 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. The FY 1981 request of \$99,900,000 for Materials Sciences includes \$92,000,000 for operating expenses, \$7,600,000 for capital equipment and \$300,000 for construction.

## Operating Expenses

The FY 1981 request for operating expenses for Materials Sciences is \$92,000,000, an increase of \$13,000,000 over the FY 1980 level. This level is necessary to continue the Department's basic research program in materials which underpins all the energy technology programs. It will permit commitments to be met arising from new equipment and facilities under development or recently completed. Considering the increased costs associated with the Intense Pulsed Neutron Source (IPNS-I) at ANL, the National Synchrotron Light Source (NSLS) at BNL, and electron microscopy facilities at LBL, ORNL and ANL, selected new initiatives will be undertaken while phasing out some ongoing projects. Increasing emphasis will be placed on research at universities and to a lesser extent industry. Some reductions will take place in research involving amorphous beryllium alloys, superconductivity, high temperature borides, and radiation damage. Increased emphasis will be devoted to materials research related to solar energy, nuclear waste isolation, and fossil energy. Funding for selected user groups will provide exploitation of the unique new facilities funded by this program such as the electron microscopes, the NSLS, and the neutron sources.

The funding needs for the Materials Sciences subprogram can be discussed under three major topics: metallurgy and ceramics, solid state physics and materials chemistry. The following table shows the funding required for these three topics.

### Materials Sciences Summary of Operating Expenses

	Budget Authority	
	Estimate FY 1980	Estimate FY 1981
Metallurgy and ceramics	\$34,900	\$40,750
Solid state physics	33,210	38,600
Materials chemistry	<u>10,890</u>	<u>12,650</u>
Total, materials sciences	\$79,000	\$92,000

### Metallurgy and Ceramics

The primary purpose of research under the metallurgy and ceramics category is to establish a better understanding of the relationship between materials properties and structure, the methods by which materials are formed and how structures are prepared (processing). Ultimately, this understanding among properties, structure and processing will result in improving present materials and creating new materials to meet the important needs of all energy systems. The FY 1981 request of \$40,750,000 will support activity in metallurgy and ceramics at approximately the same level as in FY 1980. The request will permit the program to meet commitments at the three high voltage electron microscopes at ORNL, ANL and LBL, support activities related to the IPNS-I at ANL and support university user groups at these facilities. Buildup of research to utilize the atomic resolution microscope at LBL and the NSLS at BNL will continue. These new facilities will permit unprecedented research. As discussed below, selected new programs will be started, primarily at universities.

Significant added emphasis in this budget will occur in the areas of materials research related to fossil energy, especially synfuels, solar energy and nuclear waste isolation. Research in corrosion, erosion, high temperature mechanical behavior, amorphous materials and films for solar energy, leaching and synthesis of possible nuclear waste host materials, and canister materials for nuclear wastes will be strengthened or initiated. Work on conservation-related activities such as insulating materials, engine materials, and battery materials will also be emphasized.

Progress during the past year in this category has been significant, as described in more detail below. By building on this progress and using the new techniques now becoming available (e.g., analytical electron microscopy, laser diagnostics, synchrotron radiation), it is expected that not only will we be able to predict materials behavior as a function of time, stress and a variety of environments but also create new metal and ceramic structures to meet the severe engineering requirements for emerging energy

systems. Research in metallurgy and ceramics is separated into five subcategories: structure of materials, mechanical properties, physical properties, radiation effects and engineering materials.

Research in the structure of materials is undertaken to enhance our ability to control the properties of metallic and ceramic solids by changing their structure. The scope of this research includes atomic, electronic, and defect structures of metals and ceramics as well as the microchemistry of complex alloys and multiphase ceramics. The key to the development of new and improved materials for more efficient energy conversion systems lies in understanding the role of materials processing, as well as the effects of technological in-service exposure conditions on the resultant structure. Structure of materials research includes examination under very high magnification by using advanced techniques such as electron microscopy (high voltage; analytical; atomic resolution; and scanning transmission); x-ray photoelectron spectroscopy; and extended x-ray fine absorption analysis.

An example of a recent accomplishment concerns the use of analytical electron microscopy at ORNL to study the effectiveness of certain processing methods in preparing "synthetic" rocks which might provide stable hosts for radioactive waste storage. During the laboratory processing of one sample (Synroc-A), an undesirable formation of a thin glass film separating the crystalline phases was detected. This film is undesirable because of its poor leaching resistance. The resultant structural information on these phases is being used to improve the processing methods.

Progress on the development of silicon nitride, a ceramic material of potential use in high temperature automobile and truck turbine engines, has been substantially enhanced by the use of new microscopic techniques to study the process used to fabricate test parts. The process used (sintering) produces finished, fabricated parts through solidifying powdered starting materials at high temperatures. The process is enhanced through the use of a variety of special additives, called sintering agents. These agents, however, can weaken the final part and can significantly affect its properties unless carefully controlled. New microscopic techniques permit studying the location and quantities of these agents, thus enabling the development of sintering methods to produce higher quality, high temperature silicon nitride parts.

New research areas for FY 1981 include university efforts in three different kinds of electron microscopy: analytical, atomic resolution, and high voltage. Initial university research on both the NSLS and the IPNS-I will be applied to forefront problems concerning the structure of metals and ceramics. The FY 1981 request of \$9,900,000 for structure of materials is required to sustain work started in FY 1980 research in such areas as: behavior of refractory materials in hostile environments; sintering studies of complex ceramic materials to achieve control over their resulting structure and properties; electrically conducting ceramics for magnetohydrodynamics (MHD); and high temperature battery materials. Other areas of work which will continue to be supported include atomic structure studies of hydrides for energy storage applications and electronic structure studies of superconductors with high transition temperatures.

Research in the mechanical properties subcategory seeks to understand materials behavior under stress, i.e., the elastic and plastic deformation and fracture of metals and ceramics. Major accomplishments during the past year include evaluating design crack growth parameters and assessing defect interactions related to alloy embrittlement and phase transformations.

Recent university research has shown significant progress in the study of ceramic and metal fracture at high temperatures. This research is important in order to provide better design criteria for high temperature energy system components such as large steam turbines or advanced gas turbines. Conditions were identified under which the primary crack would grow based on its interactions with other smaller cracks and cavities in silicon nitride structures. This knowledge will provide guidance on acceptable flaw and phase distributions in high temperature structural ceramics.

Certain materials fracture catastrophically near or below room temperature. Recent studies have shown promise of understanding and preventing this phenomena. In steels, sulfur and oxygen segregation to grain boundaries is known to lower fracture resistance. Although much has been reported about segregation, the preference of impurities to segregate to boundaries of different orientations was established for the first time at Pacific Northwest Laboratory for the case of sulfur and oxygen in iron. This detailed information is a prerequisite for designing alloys with increased resistance to embrittlement. Similarly, information is being obtained on stress corrosion cracking of stainless steels in the presence of water at Brookhaven National Laboratory. Scientists there have developed a new method for studying extremely small areas of surface films on these steels. The process of film formation can be related to the susceptibility of cracking and thus can provide early warning of a problem.

The budget request of \$8,200,000 for mechanical properties is required to strengthen the current level of effort at the national laboratories while allowing growth of university research. Greater emphasis will continue to be placed on: structural ceramics using high resolution microscopy to identify the effect of grain boundary phases on deformation and fracture mechanisms; influence of environment and impurities on alloys, including hydrogen embrittlement and attack as well as sulfide cracking of steels; interaction among various elements in alloys; and in-situ observations of fracture in high voltage electron microscopes. Alloy design research will be held at its current level and will focus on transformations, processing, grain boundary structure, and surface modification. Efforts on ferrous alloys will increase while those on refractory metals will decrease.

Physical properties research is concerned with increasing the understanding of thermal, optical, transport, and electrical properties of materials, including the effect of processing treatments. Areas of recent or future expanded emphasis encompass corrosion mechanism of metals and environmental degradation of ceramics; solar photovoltaics; transport in radioactive waste forms; sintering to achieve fully densified carbides, oxides, and nitrides; and fast ion conduction for battery and other energy storage applications.

Accomplishments in 1979 included a new process developed at Ames Laboratory for preparing multifilamentary superconducting wire at significantly reduced cost. Superconducting wire is used in magnets for MHD, fusion energy research and high energy physics and has potential for use in power transmission and generation equipment. The next phase is to scale up the process for commercial production.

A good example of basic and applied research in cooperation is now underway at the Varian Associates Solid State Laboratory. Several DOE solar projects are co-located with a Materials Sciences supported program. The thrust of these several DOE contracts is to develop multigap solar cells with an efficiency of >30 percent in concentrated sunlight. The usual single gap silicon cells have efficiencies in the range of 15 percent. The materials sciences program at Varian has demonstrated a total solar cell efficiency of 28.5 percent for a cell of aluminum-gallium arsenide in combination with a cell of silicon, i.e., for a two band gap solar cell.

New initiatives for FY 1981 will be in the areas of protective coatings, environmental degradation and corrosion behavior, the utilization of the Combustion Research Facility at Sandia-Livermore for studying the interaction of combustion products with surfaces, and increased support of university contract research. The FY 1981 budget request of \$10,370,000 for physical properties research will permit expansion of current work in the following areas: mass transport in ceramics for MHD applications and in nuclear wastes; environmental degradation and ion transport in solid electrolytes for high temperature battery applications; investigations of solar absorptivity of fluids for increased solar conversion efficiency; and studies of ion implantation for metallurgical applications.

Experimental and theoretical research in the radiation effects subcategory explores materials behavior when exposed to radiation. Primary emphasis is directed toward the stability of metals, ceramics and glasses when exposed to radioactive waste, fission or fusion reactor environments. A smaller effort is on the use of energetic ions (electrically charged nuclei) to alter the structure and properties of materials used for non-nuclear energy systems. Basic research results continue to be incorporated into reactor technology programs. For example, the design of components for an advanced reactor test facility is based on performance of low swelling steels first developed by this research program.

One area that requires further emphasis is the development of methods which simulate in a short time the long time in-reactor radiation effects on materials. For this, theory is particularly important in order for designers to have confidence that neutron damage can be simulated using electrons or ions. At Oak Ridge National Laboratory, detailed modeling of material damage during heavy ion bombardment demonstrated material swelling at a much shallower depth than calculated from the beam parameters only. Electron microscopy studies have shown this to be correct and now, with this information, heavy ion-bombarded material can be evaluated at the depth of maximum damage, thus improving the validity of this simulation technique.

In the area of mechanisms of phase stability and void swelling under irradiation, new theoretical and experimental results were obtained at ANL. The theory predicts that specific radiation-induced defects will be attracted to solute atoms of different sizes. These phenomena of radiation-induced segregation and precipitation have been experimentally observed in both dilute and concentrated alloys. This type of research provides the underpinning needed for the development of more radiation resistant structural alloys.

New research will exploit the high voltage electron microscope/tandem accelerator at ANL, which will become operational in FY 1980. Also planned are increased efforts on the effects of low level radiation (simulating nuclear waste) on complex glasses and ceramics; on microstructural changes in alloys under dual ion irradiation and irradiation creep; and on the transfer of research techniques of surface modification and defect characterization in materials related to solar and fossil energy applications. The programs measuring and modeling fundamental damage parameters will continue at their current levels, whereas those on neutron irradiation of structural alloys and superconductors will be decreased. \$7,200,000 for radiation effects is required to strengthen the level of effort.

Research in engineering materials is aimed at increasing our understanding of more complex phenomena and materials which generally are closer to "real" world conditions and problems. The focus is still basic research, although it is expected that model systems will be chosen and parameters controlled so that generalizations and extrapolations can be made. An FY 1981 budget of \$5,080,000 is needed for this important area to strengthen ongoing programs in erosion-corrosion concerning mechanics of fluid flow and development of analytical models to define particle trajectories and erosion mechanisms (important for coal conversion systems), modeling of the solidification process during welding (of value in the fabrication of pressure vessels for fossil or nuclear plants), and the use of dynamic photoelasticity for the characterization of ultrasonic wave interactions with surface cracks (to assist in detecting the onset of materials failure). Continued buildup of new programs initiated in FY 1980 on non-destructive evaluation, ceramic processing, erosion/corrosion, ceramics-metal interface effects, and in-situ gas-solid reaction studies using high voltage electron microscopy will be permitted in this request. In FY 1981, work on high temperature semiconductors, nondestructive evaluation, coatings, erosion, processing, and multiaxial mechanical behavior of structural ceramics and metals will also be emphasized.



An example of an accomplishment under this category is the recent discovery of an alternative way of analyzing the detailed shape of an acoustic emission wave. A moving crack emits an acoustic wave which can be used nondestructively to detect and monitor cracks in structures. The new discovery showed that an elastic wave (e.g., from a crack) in a medium carries a wave momentum which is distinct from the particle momentum (e.g., background noise) of the medium. Thus crack growth can perhaps be monitored using appropriately designed acoustic wave receivers under service conditions (noise) not possible now.

Among the most severe problems in coal conversion systems are corrosion, erosion and interactive combinations of the two. Prevention of excessive corrosion depends on the formation of a protective scale (usually chromium oxide or aluminum oxide) on the material. In order for this to be effective, the oxide must form rapidly, it must be resistant to penetration by harmful elements, and it must adhere well to the material. A recent investigation of erosion resistance of stainless steel oxide scales has shown that their resistance depends on the atmosphere in which the scales are formed. Detrimental behavior was observed under certain conditions where the oxide flaked off completely, exposing a clean metal surface. These results suggest two goals for the development of erosion-corrosion resistant alloys: improvement in the oxide-metal interfacial strength to alleviate the flaking problem, and strengthening of the scales to reduce their erosion rates.

#### Solid State Physics

The FY 1981 request for solid state physics is \$38,600,000. Solid state physics research is directed towards fundamental research on solids, liquids, and gases in which the interactions of electrons, atoms, and crystal imperfections are investigated with the most advanced kinds of instrumentation. Understanding how these factors influence solid behavior under conditions of temperature, pressure, magnetic field, radiation, and unusual environment is important to all energy technologies. The research includes coupled experimental and theoretical work, especially focused on promising new materials for sequestering nuclear wastes, crystalline and amorphous solar materials, and unusual hydrogen storage materials. Increased efforts will also be given to startup of the National Synchrotron Light Source at BNL and continued use of the Intense Pulsed Neutron Source at ANL.

A number of important accomplishments occurred during the past year including the following: 1) It was found that new leach-resistant synthetic nuclear waste solids were resistant to saline and molten salt leaching to the highest degree yet reported, and offer considerable promise in efforts to solve the high level nuclear waste problem. 2) Novel experiments with liquids as thermodynamic media were performed with conceptually new heat engines, that may ultimately prove important for the utilization of low grade heat. 3) Hydrogen storage in solid materials is one potential method for storing energy during off-peak hours. Research with niobium and tantalum covered with a few layers of palladium resulted in the ability to store hydrogen at a greatly increased rate compared to a single layer coverage. This discovery may assist efforts in the potential large scale storage of hydrogen for energy systems. 4) Totally new materials have been prepared using the ion implantation-laser annealing technique, including supersaturated solid solutions, which are inherently unstable, and often cannot be prepared by any other means. In principle, the ion implantation, laser annealing method not only has advanced solar cell technology applications, but holds considerable promise for producing totally new materials which may impact on many other energy technologies that are materials limited.

The major areas of investigation under the solid state physics category include neutron scattering, experimental research, theoretical research, particle-solid interactions, and engineering physics.

Neutron scattering research uses neutrons as unique probes for the study of condensed matter. Information about certain properties of materials, such as hydrogen in solids, and micromagnetic phenomena, cannot be obtained by other means. Additionally, this method is utilized to study polymer properties, hydride storage structures, and the

mechanisms of void formation in nuclear reactor materials. Neutron scattering research is conducted at high intensity research reactors at various DOE laboratories and in the future will also be done at IPNS-I, now under construction at ANL. The reactors have incurred escalating costs of nuclear fuel and electrical power beyond those of the consumer price index rate of inflation. These added costs plus the buildup of research at the new pulsed systems and the expansion of user mode operation, are placing increased budgetary pressures on this area of research. To partially offset this effect, the shutdown of the CP-5 reactor at ANL in FY 1980 and the Bulk Shielding Reactor (BSR) at ORNL in early FY 1981 is planned. In order to sustain a minimum viable program in neutron scattering research in FY 1981, \$9,270,000 is required.

Experimental research covers all facets of solid state physics experiments on metal solids and liquids, alloys, semiconductors, insulators, and compounds. The synthesis and testing of new non-leachable nuclear waste materials will be accelerated. Ion-implantation and laser annealing, already proven important to solar materials fabrication, will be extended to superconductors, protective weld coatings and supersaturated compounds. In-situ electron microscope studies of fracture will be extended to high temperature materials such as carbides and borides, which have potential use in hot, highly stressed parts such as in turbines. The preparation and characterization of modified amorphous silicon for solar applications will be continued at an increased level. Research at the NSLS will be strengthened through support of participating research teams made up of university, laboratory, and industrial personnel on a broad spectrum of surface-catalytic, trace impurity, and electronic-state studies important to many energy systems. These early efforts will be confined to beam line, instrument, and computer checkouts while the NSLS is under construction. In FY 1981, \$600,000 is specifically earmarked for NSLS-related research and development and early operational costs for the vacuum ultraviolet ring. New lasers, high quality mirrors, and optical coatings research will be pursued with advanced preparation and spectroscopic techniques. With regard to the latter, those polymer and other surface coatings for solar materials will be investigated under simulated long-term terrestrial conditions, with advanced microscopic measurements of degradation. To support this experimental research effort in FY 1981, \$18,970,000 is required.

Theoretical research is closely coupled to the experimental investigations discussed above and makes extensive use of the large-scale computers within the DOE complex. Problems especially amenable to this type of investigation include those dynamic processes such as rapid crack propagation in materials, atomic collision cascades in nuclear and fusion damage studies, metal-electrolyte interface phenomena in batteries, and the interaction of laser light with materials. Where complex effects are important, as in many energy systems, it is clear that a strong theoretical effort is vital. To support these theoretical research efforts, \$4,170,000 is required for FY 1981.

Under particle-solid interactions, the damaging effects of electrons, ions, atoms, and fission fragments with varying energies in solids are followed with experiments at controlled temperatures and environments. Experiments conducted at 4° Kelvin in nuclear reactors are essential for evaluating superconducting magnets for fusion reactor systems. The understanding of the synergistic effects of different particle-radiations is necessary for the analysis of damage in fission and fusion systems, whether on surfaces or in bulk materials. Although this is a relatively small area of research, it continues to be important. \$1,990,000 is requested for FY 1981.

Engineering physics research is an expanding area. Closed-cycle refrigeration and higher temperature superconducting devices will be field tested in known oil and gas areas to investigate the applicability and sensitivity of these electronic devices in detecting and mapping deep deposits from the surface of the earth. The synthesis of new high level waste forms will be followed with leaching and spectroscopic studies to determine the long-life stability of these compounds. Material processing by new techniques of ion-beam mixing and laser rastering (fast scanning) of coatings will be emphasized in the search for improved protective coatings for specialized uses in energy systems. The new use of specific liquids as thermodynamic media will be explored for potential improvements in low grade heat utilization, and in prime mover systems. Computer-controlled microscopic machining and grinding will be extended from metals and alloys to ceramic materials with flat and controlled curved surfaces for potential solar and laser applications. In FY 1981, \$4,200,000 is required for engineering physics research.

## Materials Chemistry

The FY 1981 request for materials chemistry is \$12,650,000. Materials chemistry research is directed towards understanding the chemical properties of materials of different composition and structure and in various environments. This research also serves to identify how the laws of chemistry can be used to determine chemical properties and phenomena in materials. Chemical phenomena together with a variety of physical experimental techniques are utilized to examine chemical corrosion and compatibility and the chemical stability of materials in hostile fossil and geothermal environments. Investigations with tritium recovery, liquid lithium transport, and fused salt thermodynamics have led to important advances relating to fusion research. Electrochemical research is conducted on materials which are important to storage batteries, fuel cells, and potential hydrogen generating systems. Particle studies utilizing oxygen and sulfur isotope techniques have been adapted to atmospheric pollutant control concepts. Studies of impurity coverage on catalyst surfaces are undertaken with the view of controlling poisoning effects in these systems.

A few of the important accomplishments in materials chemistry during the past year include the following: 1) A new process was developed to reduce sulphur dioxide pollution and recover re-usable additives. 2) An improved performance lithium aluminum alloy electrode for use in high temperature batteries was developed by modifying the older electrode with magnesium. 3) Research on the interaction of nuclear fuel with its cladding was aimed at eliminating hazardous corrosion effects with the potential of fuel cladding failure. By determining the temperature range of the deleterious reaction for the formation of cesium chromate, elimination of this adverse process was made possible by studies of thermodynamic stability.

The major areas within materials chemistry include chemical structure, engineering chemistry and high temperature and surface chemistry.

Research in chemical structure is related to the atomic structure of materials and corresponding chemical activity. The tools for investigating these properties include steady-state and pulsed neutrons, x-rays and electrons. These probes are utilized to study metal clusters as catalysts, methanation catalysts, detergents for enhanced oil recovery, amorphous derivatives from coal, and nucleation and bubble growth at gas-electrolyte-electrode interfaces. Chemically modified zeolites, materials of considerable importance to petroleum refining catalyzation, will be investigated using intense pulsed neutrons to locate light atoms which may be important in catalyzing reactions. The relationship between chemical structure and unusually high electrical conductivity in inorganic and organic materials will be studied in carefully synthesized specimens with both x-ray and neutron techniques. These materials may be useful as new electrical conducting materials as well as in advanced battery systems. Other diffraction studies on liquid hydrocarbons will be directed towards determining the status of rotational isomers which may be important to processes occurring in internal combustion cycles. In FY 1981, \$3,250,000 is required for this effort.

Engineering chemistry includes those activities related to chemical processes of mass transport, materials separation systems, thermodynamic behavior, scaling and corrosion mechanisms in geothermal environments, and advanced nuclear fuel characterization. The FY 1981 request includes \$4,840,000 for these studies. Emphasis will be given to conversion of atmospheric pollutants such as sulfur dioxide into safe solid materials in a regenerative form. The thermodynamics of advanced nuclear fuels and their interactions with fuel cladding surfaces will be investigated to determine cladding integrity. New physical techniques including laser spectroscopy will be utilized in studying how to efficiently remove deleterious fine particles from coal conversion liquids. This research is important to several fossil fuel conversion techniques. Variable processing conditions will be used to examine the stability of polyethylene materials for electrical insulation. Breakdown of insulation in major power systems is a significant factor in power outages. This research is aimed at finding stable polymers which may alleviate this problem. Research on advanced batteries will include the preparation of new cathodic materials, the use of calorimetry and the prevention of electrolytic degradation. Studies will be initiated on the

recovery of potassium seed material from complex ceramic mixtures for recycling in coal-fired MHD systems. Recovery of aluminum and iron constituents from coal fly ash using recently advanced techniques of material separation will also be pursued.

High temperature and surface chemistry includes those activities of catalytic and surface electrochemical reactions, the thermodynamic mechanisms in high temperature batteries, theoretical and experimental verification of the stability of solids and mixed salts laser fluorescence spectroscopy of metal cluster catalysts and condensation processes in coal combustion systems. Experiments will be conducted on the deleterious effects of chemical composition changes in molten salt mixtures. These changes result from the polarization effects which are common in high current battery systems.

Vibrational effects in polymers will be related to their structure using new methods of spectroscopy. These studies are important in understanding the properties of polymers used in several energy technologies, including solar, and also to electrical transmission systems. Surface studies include those of well-characterized surfaces of a variety of catalytic materials including transition metals and alloys by means of low energy electron diffraction methods. Additional efforts will be given to understanding the chemical effects of microinclusions in welded alloys. These studies are important in understanding failure phenomena in materials that are joined by welding processes. To support these research efforts, \$4,560 000 is required in FY 1981.

#### Capital Equipment

The FY 1981 capital equipment request of \$7 600,000 for Materials Sciences is essential to keep the program at the forefront of research in materials. The program is moving into new research areas with the development of facilities such as the Intense Pulsed Neutron Source, the National Synchrotron Light Source, and the LBL high voltage and atomic resolution electron microscopes. These new activities require spectrometers, smaller microscopes, and related electronic equipment in order to efficiently utilize the facilities and conduct effective research programs. Energy-related research generally requires higher temperatures, extremely careful control of the atmosphere and highly accurate analysis of observations, all which point to expensive equipment. New projects which will need significant outlays of capital equipment include: solar-related research, studies of the effect of combustion on surfaces, nuclear waste isolation materials preparation and high temperature corrosion research related to synfuels.

Equipment funds are needed to acquire surface modification and analysis apparatus for studying the role of surface composition on materials behavior. High resolution electron microscopes are needed to study the relationship of properties to structure in materials at resolution distances of several atoms. Ion implantation equipment is needed to extend the voltage range of existing ion implantation facilities in order to study both radiation effects and chemical doping on a micro-scale. High temperature furnaces and crystal-growing apparatus are required to study the properties of ceramics and to prepare single crystals of metals and ceramics for basic research. New initiatives in nondestructive evaluation and welding need electronic equipment for analysis. Superconducting magnets are needed to study the electronic and magnetic structure of alloys at low temperatures. Optical and x-ray spectrometers are needed to outfit experiment stations at the NSLS.

In addition to the above examples of equipment needs for new or growing programs, there is a need to provide funds for replacement equipment. High priority will be given to replacement of small conventional items such as furnaces, vacuum pumps, x-ray tubes, etc., which are required to avoid unscheduled outages caused by malfunctioning antiquated equipment.

### Construction

The \$300 000 requested for construction is for General Plant Projects for Ames Laboratory (\$275,000) and the Notre Dame Radiation Laboratory (\$25,000). These funds will permit minor additions and modifications to these facilities which will assist in maintaining them as safe and productive laboratories for conducting research and development.

### Chemical Sciences

The research activities supported by Chemical Sciences advance the basic knowledge and understanding of energy-related chemical and physical phenomena, specifically the behavior of liquids, gases, plasmas (extremely hot mixtures of ions and electrons) and the individual particles which make them up: molecules, atoms, ions, electrons. This research also includes studies of some solids (e.g. coal, catalysts and chlorophyll).

The types of phenomena and processes studied by these basic researchers emphasize those which are likely to become important in the long (and sometimes near) term to energy technologists. Thus the areas under study are chosen with a range of time scales in view. Some areas, like research on the chemical effects of catalysts, may lead to discoveries which can be picked up quickly by industrial process designers to achieve previously impossible efficiencies of fossil fuel conversion to more usable forms, for example, liquefaction of coal. Other areas, like the research on water-splitting photo-chemistry to produce hydrogen, the cleanest of all fuels, are producing results which are longer range in impact and which may reach a state of attractiveness to solar energy technologists in the mid-term (ten years or so). Still others, like research on radiation emitted by ions (electrically charged atoms) moving very fast through crystal foils, are producing new information with a high likelihood of usefulness in future energy applications because the phenomena observed are manifestations of energy; it is too early, however, to specify the likely uses.

A large share of the Chemical Sciences activities is carried out in DOE laboratories because of their unique equipment and their enhanced opportunities for these basic researchers to interact with research and development teams in related energy technology areas. Most of the remainder of the activities are carried out at universities, and a small part takes place in industrial laboratories. Where useful, laboratory scientists supported by Chemical Sciences are working closely with important industrial laboratories such as those of the automotive industry. Plans for the funding pattern are shown below.

<u>Research Sites</u>	<u>Operating Expenses</u>	
	<u>FY 1980</u>	<u>FY 1981</u>
DOE Laboratories	\$ 38,400	\$ 43,100
Universities	15,200	18,400
Other	1,500	1,800
Total	\$ 55,100	\$ 63,300

In addition to the laboratory-based interactions between the basic researchers supported by Chemical Sciences and the technology teams, headquarters-based coordination is also stressed. Up-to-date word on needs for understanding, problems encountered, opportunities presented by new discoveries, comparing of findings and coordinating of activities are handled by the Combustion Research Coordinating Panel, the Hydrogen Coordinating Committee, Solar Photochemistry Research Conferences, Coal Chemistry Research Meetings and Catalysis Workshops. In addition, Chemical Sciences staff serve in advisory capacities for energy technology activities, visit and review the activities at the multiprogram laboratories and maintain frequent contact with energy technology staffs.

Of the FY 1981 request for \$74,400,000 for Chemical Sciences, \$63,300,000 is for operating expenses, \$4,740,000 is for capital equipment and \$6,500,000 is for construction. Each is discussed in turn below.

Operating Expenses

The Chemical Sciences request for \$63,300,000 in operating expenses is \$8,200,000 above the level of FY 1980. This increase is necessary to begin effective use of the new Combustion Research Facility and to strengthen the research efforts in the highest priority energy-related areas, heretofore inadequately covered. These include research in solar-related photochemistry, the chemical physics of photosynthesis, organic chemistry and other fundamental properties of coal, and clarifying the still poorly understood chemical effects of catalysts. In addition, research underlying separation of chemical species to facilitate safe storage of nuclear wastes is to be strengthened. Added emphasis in the chemical effects of lasers and in the fundamental physics of lasers is called for by the energy-related advances these devices have already enabled, even though they are still limited in the wavelengths (energies) they can produce.

The overall level of \$63,300,000 is necessary for the foregoing purposes and at the same time supports efforts, some ongoing and some replacements, in basic research which is expected to produce knowledge useful to other areas of energy technology. The ongoing research, in addition to the areas mentioned above, includes studies basic to energy conservation interests, such as hydrogen's behavior in forming hydrides which could serve as hydrogen storage media, and thermochemical formation of hydrogen from water. It includes fusion-related studies, emphasizing behavior of highly charged ions which can sap the energy of a fusion-intended plasma. It also includes research on the chemical effects of gases like nitrogen dioxide, which play important environmental roles. Equally important is the maintaining and selective strengthening, with internal trade-offs, of long-term research into chemical and physical phenomena on the submicroscopic scale, because the understanding of such phenomena is basic to their effective use in energy systems.

The operating request for Chemical Sciences is best discussed in two parts: Fundamental Interactions and Processes and Techniques. Of the two, Fundamental Interactions deals mainly with a longer range and more fundamental set of activities while Processes and Techniques mainly supports research with nearer term payoffs for energy systems. The estimated funding of these activities is shown in the following table.

Chemical Sciences  
Summary of Operating Expenses

	FY 1980 Estimated Budget <u>Authority</u>	FY 1981 Estimated Budget <u>Authority</u>
Fundamental Interactions	\$ 32,505	\$ 37,630
Processes and Techniques	<u>22,595</u>	<u>25,670</u>
Total Chemical Sciences	\$ 55,100	\$ 63,300

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 of types which are central to questions of successful conversion, storage and conservation of energy, including possible environmental effects. The specific research areas encompassed by these activities are: photochemical and radiation sciences, chemical physics and atomic physics.

The scope of the Fundamental Interactions research can be seen in some of its recent accomplishments. Some years ago we reported the concept of the artificial leaf, advanced by researchers at the Argonne National Laboratory. It consisted of a device incorporating chlorophyll in a plastic membrane between two solutions, one an oxidizing agent and the other a reducing agent. It (inefficiently) converted sunlight into electricity. Recently, based on growing understanding of photosynthetic processes, this same group has succeeded in preparing a substance made up of a type of synthetic molecule which behaves like chlorophyll but which is much more durable under laboratory working conditions. Together with scientists at the University of Illinois they have shown that the synthetic molecules undergo the same important photochemical processes as do chlorophyll molecules in natural photosynthetic systems. This puts them one step closer to the goal of preparing a synthetic system that will convert sunlight's energy to electricity or fuel with good efficiency and durability.

Researchers at Oak Ridge National Laboratory have adapted a technique (known as electron spin resonance spectroscopy) to the study of radicals (short-lived reactive molecules) in fluids at high temperatures and pressures such as those expected in coal liquefaction processes. They have already shown that, under these conditions, unpredicted reactions leading to undesirable polymeric products take place. This might open the way to explaining and then preventing formation of the troublesome asphaltens often seen in coal liquefaction. This advance also shows promise as a tool in investigating the mechanism of soot formation during combustion, which is an important environmental concern, especially with diesel engines.

A new method has been devised at Argonne National Laboratory for studying the structure of extremely reactive electrically charged molecules (called ions). These ions do not have lives long enough to permit determination of their structures by conventional means. The method, an outgrowth of research on the physics of atoms, involves passing the ions very rapidly through a thin carbon foil. The electrons binding the constituent atoms of the ion are removed in this process and the ion, now subject to strong electrostatic repulsion among its parts, literally explodes when it leaves the foil. From the locations of the collected fragments and measurement of their energies, the geometrical structure of the original ion can be accurately deduced. This technique has revolutionized the study of such species and opened up many new research directions. These ionic species influence many energetic processes encountered in energy conversion and conservation such as combustion, MHD and fusion. In addition, they are responsible for and participate in many of the important atmospheric chemical reactions involving pollutants. Knowledge of the structures of these ions is important in the study of their chemistry and in diagnostics of flame phenomena and fusion plasma behavior.

The FY 1981 request for Fundamental Interactions is \$37,630,000, an increase of \$5,125,000 over the FY 1980 level.

Of this total, \$7,700,000 will be devoted to research in solar-related photochemistry, an increase of \$1,500,000 over FY 1980. The most promising work in artificial photosynthesis, homogeneous and heterogeneous photochemistry, photoelectrochemistry and molecular energy storage will be extended 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 using solar energy. This has great potential for energy conservation. Under the umbrella of the United States-Japan Agreement on Cooperation in Research and Development in Energy and Related Fields, an Implementing Arrangement is being negotiated for jointly-funded research in photoconversion and photosynthesis research. Some of the FY 1981 funds will be used to provide support for photo-chemistry research under this Arrangement.

It is planned that combustion research will increase by \$2,400,000 to \$6,900,000. Of this increase, \$2,000,000 will be added for activities at Sandia Laboratories-Livermore, bringing them to the level necessary for operation and use of the combustion Research Facility for its first full year. In-house researchers and outside users from universities, national laboratories and industry will use the

advanced lasers and other diagnostic equipment on scientific problems related to fundamental combustion kinetics, to engine research and to coal combustion. The remaining increase will be used at other laboratories and universities, to tackle other important new combustion problems, the principal one being a requirement for understanding of the mechanisms of soot formation in diesel fuel burning. Knowledge of these mechanisms is necessary if steps are to be taken to reduce these polluting emissions.

The fossil-related research in Fundamental Interactions consists largely of theoretical and spectroscopic studies of catalytic phenomena. The fusion-related atomic physics effort is devoted to studies of highly charged heavy ions and their energy-degrading role in fusion plasmas. An increase of \$200,000 is requested in each of these two areas, bringing each to a total of \$2,200,000. This will permit most ongoing programs to proceed, and will allow the initiation of some important new work while lesser priority research is terminated.

Smaller groups of important projects in non-solar photochemistry, radiation chemistry and chemical physics are devoted to problems in areas related to the environment, to fission energy and conservation. Some of the photochemical reactions under study have strong possibilities of explaining and pointing toward solutions of energy-related atmospheric pollution. In the related area of radiation chemistry, study of the effects of radiation from actinide elements on liquids used for chemical processing is ongoing. The actinide elements are among the important products found in spent nuclear fuel. Within the chemical physics activities is included the study of the chemical structures of hydrides, substances of high potential for conserving energy by storing hydrogen. The total funding requested for these particular groups of research activity is \$1,400,000, which represents essentially no change in the funding level from FY 1980.

The largest single category of research in Fundamental Interactions is the long-term fundamental research underlying not only progress in energy technologies but also in almost all of the other Chemical Science activities. This research in chemical and atomic physics, radiation chemistry and photochemistry explores the basic causes of chemical and physical interactions in order to systematize our knowledge of these fields and give us the predictive power needed to design new systems for energy conversion, storage and conservation. It consists of theoretical and experimental studies of reaction rates and mechanisms, interactions of light and other radiation with matter, the forces between small particles and similar phenomena on a submicroscopic scale. The emphasis here is on the phenomena rather than the specific energy system, since knowledge of the former is needed to design the latter intelligently.

The total request for long term energy research is for \$17,230,000, an increase of \$900,000. This will not permit continuation of all present research. By judicious phasing out of some research, however, it is planned to augment certain of the more critical research areas. One example is the program of fundamental laser chemistry and physics research. The unique characteristics of lasers have provided advances in understanding in areas such as photosynthesis and solar energy conversion, combustion, and fusion. There is a great need to broaden the wavelength region accessible with existing lasers for the demanding research programs in these areas. The new funds will specifically be devoted to explorations of the fundamental chemistry and physics of lasers. Another type of long-term research to be increased within the funds requested is support of chemistry activities planned for the National Synchrotron Light Source, which will provide very intense light over a wide range of wavelengths. Equipment must be assembled and tested and experiments designed well in advance of the operation of the facility.

#### 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, bearing on liquid fuels from fossil and biomass resources, nuclear waste processing and isolation, fusion, hydrogen, chemical engineering aspects of combustion and other energy processes. This research also provides the understanding which increases the probability of generating new ideas and creative solutions.

Several accomplishments of the past year illustrate that the basic understanding contributed by this activity can point to resolution of practical problems. The first accomplishment will achieve a significant improvement in processing of fuels through catalysis, including petroleum refining and the upgrading of coal-derived liquids. It has shown how basic understanding of molecule-surface interactions can lead to a new concept for regenerating sulfur-poisoned nickel catalysts, thereby reducing both capital investment for plant equipment and operating costs of technological processes. The concept, developed by a University of Delaware chemical engineer, is based on a new insight into the usual two-stage regeneration process using sophisticated physical techniques. The discovery is that in the usual process the oxidation phase of removing sulfur from the surface of the used (poisoned) catalyst occurs at a slower rate than the oxidation of the nickel surface itself. This oxidation formed a nickel oxide layer which trapped the sulfur atoms before they could be oxidized. Consequently, in the next step of regeneration, namely that of removing the oxygen from the surface with hydrogen, it was found that the sulfur, which was buried by the nickel oxide, remained on the surface and prevented the nickel from returning to its initial unpoisoned activity. Knowing this led to the idea that oxidation by exposure to exceptionally diluted oxygen concentrations (a few parts per million) would favor the kinetics of sulfur oxidation and lead to complete removal of the sulfur before it could be buried by the nickel oxide. After such treatment it was found that subsequent removal of the oxygen from the nickel oxide did indeed result in a totally reactivated catalyst. This concept is being patented.

Another accomplishment will have a significant impact on knowledge of coal constituents. The problem of separating coal samples into their individual macerals (organic substances bound together in particles) was attacked by an Argonne chemist. He found that the traditional grinding of coal heated the macerals so that they stuck together, making separation impossible. With great ingenuity he learned how to achieve the needed separations by adapting two techniques: a fluid energy mill and a density-gradient centrifuge. In the mill, demineralized coal particles are carried by an inert gas into the grinding zone, where collisions among them cause fragmentation into individual maceral particles. These are swept out of the grinding zone by spiraling gas action, and are then fed into a centrifuge containing a fluid having a large difference in density between layers. This sorts the particles into uniform fractions differing in density, and the sorted particles are then filtered from the fluid. This achievement should open the door to significant new chemical understanding of purer fractions of coals, providing needed insight into how different coals can be more efficiently converted to liquid fuels.

The FY 1981 request for Processes and Techniques operating funds is for \$25,670,000, an increase of \$3,075,000 over FY 1980. The increase is largely to be used for initiatives in fossil-related organic chemistry, separations, analytical chemistry and catalysis (\$1,350,000); combustion-related fluid dynamics and turbulence (\$430,000); and fission product separation chemistry related to nuclear waste isolation (\$420,000). The remaining \$875,000 increase is for research including solar-related chemistry of biomass conversion, separations chemistry of recovering metals from low grade resources such as fly ash, inorganic chemistry related to hydrogen production and storage concepts, and work on new analytical techniques. The Processes and Techniques request is divided into subactivities called chemical energy, separations research, analysis, and chemical engineering sciences.

In FY 1981 chemical energy research requires \$12,780,000, an increase of \$1,370,000 over FY 1980. 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 supported (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 technological solutions of immediate problems such as new techniques for regeneration of sulfur-poisoned catalysts, and can lay the foundation for future improved catalyst systems. This work includes fundamental organometallic chemistry which underlies the transformations of small molecules like carbon monoxide and hydrogen to produce bulk chemicals and synthetic fuels. Research in inorganic chemistry and thermochemistry addresses questions bearing on the devising and refining of 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 on 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 understanding for use by technologists in learning 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 research is \$6,730,000, an increase of \$795,000 over FY 1980. 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. The increase is primarily for research on the chemistry of complex molecular groupings, their stability and selectivity to enhance the separation of components of spent nuclear fuel in order 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 volumes 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 "cooling", 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 the 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.

In FY 1981, \$4,480,000, an increase of \$365,000 over FY 1980, is required to continue most of the ongoing research in the analysis subactivity. This research concentrates on the basic aspects of analytic techniques to increase precision, lower detection limits and decrease the costs of analysis. Modifying existing techniques and inventing new ones provides expanded analytical capabilities which are of significant benefit to many technologies. Trace analyses of molecular species, especially organic, are studied to provide more effective and more efficient capabilities for detection of species encountered 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.

The request for chemical engineering sciences is \$1,680,000, an increase of \$545,000 over FY 1980. The amount requested 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, a frequently encountered situation in energy processes. The resulting developments of more physically precise models provide to energy technologies relationships needed to replace those based more on empiricism. Most of the increase is for new turbulence research to improve the capability for modeling complex combustion

phenomena. Emphasis will be given to improving and/or developing the scientific basis for engineering generalizations, unifying theories and innovative processes.

#### Capital Equipment

The FY 1981 request for capital equipment for Chemical Sciences is \$4,740,000, an increase of \$1,040,000 above the FY 1980 level. This increase is vitally important for two major reasons: preparing for efficient use of two new facilities by in-house and outside users, and reducing the valuable scientific time wasted while repairs and modifications are made to outdated equipment. 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 catalysis 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. Of the total request for equipment, \$3,345,000 is intended to fulfill the above need for such newly developed, widely capable equipment.

Of the total request, \$955,000 is required for the Combustion Research Facility at Sandia Laboratories-Livermore which will begin operation during the first quarter of FY 1981. Here, the need for equipment is twofold. The Facility will be user-oriented; researchers from university, industrial and national laboratories will come to the Facility to do combustion research using its equipment. 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.

At Brookhaven National Laboratory, the National Synchrotron Light Source (NSLS) will begin operations near the middle of FY 1981. Approximately \$300,000 of the equipment funds requested is expected to be used at BNL for the preparation of chemistry experiments at the NSLS. This facility will be a powerful new source for research in the short ultraviolet and x-ray regions of the spectrum. These funds will help ensure completion of sufficient beam lines and associated equipment to establish a vigorous in-house and user-oriented chemistry research program.

In addition, \$140,000 will be provided to Ames Laboratory for general purpose equipment. This multipurpose equipment, which is essential to the proper day-to-day operations at the laboratories, cannot be identified specifically with any one Department of Energy program. Included are the needs of the laboratory service and support divisions, as well as equipment required to respond to health, safety, security and environmental considerations.

#### Construction

Of the \$6,500,000 request for construction funding for Chemical Sciences, \$6,300,000 is for completion of the Chemical and Materials Sciences Laboratory at LBL, construction of which is being initiated in FY 1980. Approximately 50,000 square feet of laboratory and office space will be provided as an addition to an existing laboratory building. The purposes of this project are two-fold: expanded research capabilities and improved efficiency and effectiveness of ongoing programs. The capabilities being expanded will serve not only Chemical Sciences but also Materials Sciences activities, including an atomic resolution microscope with the extraordinary power to resolve and image individual atoms. This microscope, with ancillary equipment, will permit better understanding of the behavior of materials such as catalysts, coatings and thin-film solar devices at the very fundamental atomic level. These are all central to the

needs of advancing energy technologies. 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. By bringing together presently scattered research collaborators and by easing overcrowding of their individual teams, the efficiency of LBL research will be improved, especially in the Materials and Molecular Research Division. The total estimated cost of constructing this facility is \$12,600,000, of which \$6,300,000 was appropriated in FY 1980. The remaining \$6,300,000, requested in FY 1981, will allow completion of architect-engineering services, procurement of the necessary equipment and completion of the construction activities.

The other \$200,000 in the construction request is for an accelerator improvement and modification project at Oak Ridge National Laboratory. Capabilities at the EN-tandem accelerator have evolved for purposes of research in nuclear physics, to the point that they now meet some needs for modern research in atomic (i.e., non-nuclear) physics. This is a field of very fundamental research which has significant and broad long-term importance in energy, with definite impact on fusion and combustion research and likely impacts on MHD and the protection of the environment. The purpose of the requested improvement is to enhance greatly the atomic physics capabilities of the EN-tandem. With the modification, this will be the first accelerator in a government-owned, contractor operated laboratory dedicated to carrying out atomic physics experiments. The funds will be used mainly to install a high resolution magnetic spectrograph which has been surplusd at Los Alamos Scientific Laboratory. The remainder will be used to acquire auxiliary equipment and to make necessary modification in detection and data acquisition systems. For a relatively small investment, the project will provide an important research capability at ORNL for conducting important new experiments in the atomic physics portion of the Chemical Sciences subprogram.

Engineering, Mathematics and Geosciences .....\$ 21,400 \$ 30,700

Skills in many disciplines are needed in attacking our nation's energy problems. This subprogram supports use of the talents of outstanding researchers in the disciplines of mechanical, structural and electrical engineering, mathematics, statistics, computer sciences, geology, geochemistry and geophysics. It focuses this talent on research tasks chosen for their long-term importance to meeting the nation's energy needs.

The FY 1981 request for Engineering, Mathematics and Geosciences is \$30,660,000, an increase of \$9,310,000 above the FY 1980 level. This activity started as DOE was formed with a very small base relative to the associated energy research needs. The requested increase reflects the importance of the results already being realized, the overwhelming flow of truly excellent ideas for further research, and the resulting high priority assigned by DOE to getting more researchers actively engaged in these areas of energy research.

Operating Expenses

The FY 1981 request for operating expenses for Engineering, Mathematics and Geosciences is \$28,600,000, compared to the FY 1980 level of \$20,100,000. The distribution of the FY 1981 request among the three main areas is shown in the following table:

Engineering, Mathematics and Geosciences  
Summary of Operating Expenses

	FY 1980 Estimated Budget <u>Authority</u>	FY 1981 Estimated Budget <u>Authority</u>
Engineering research .....	\$ 1,900	\$ 4,000
Applied mathematical sciences .....	10,200	13,000
Geosciences .....	<u>8,000</u>	<u>11,600</u>
Total, Engineering, Mathematics and Geosciences	\$ 20,100	\$ 28,600

## Engineering Research

In FY 1981, \$4,000,000 in operating funds is required for energy-related engineering research, an increase of \$2,100,000 over FY 1980. The choice of research topics has been and will continue to be guided by the need to solve within this decade some of the most urgent energy related engineering problems. The payoffs from well managed engineering research can be very high. Leaders at the recent workshop on Process and Systems Dynamics and Control estimate, for example, that exceptionally large savings can be realized for each dollar invested in properly selected engineering research tasks. Three other workshops were held to assist in identifying the most fruitful research areas. These workshops involved over 200 engineers including many heads of engineering departments in industry, universities and Federal laboratories. Typically, a 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 1981 will allow additional 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.

Research under this heading addresses engineering areas essential for the progress of many energy technologies. Emphasis and high priority are accorded to research topics filling gaps in fundamental data and understanding essential for long-range advances in energy processes and systems. This is an essential 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. Initial high priority basic engineering research areas have been identified as follows: tribology (the study of friction and lubrication), percolation (fluid flow through porous materials), heat transfer, process control (including sensors, actuators and microelectronics), structural engineering materials, engineering aspects of combustion and resource recovery. In FY 1980 some research projects were started in the following areas: surface-fluid interactions in support of research in tribology and percolation; studies of non-imaging optics for design of more efficient solar collectors; research on high temperature electronics for control systems in hostile environments (combustors, geothermal wells, etc.); methods for solid-solid and solid-liquid separation for resource recovery; modeling of elastoplastic deformation and crack propagation in engineering structures. The remainder of the FY 1980 funds were used to continue supporting projects started in FY 1979, including automatic on-line process analysis, automation of non-destructive testing of materials, the combustion of lean fuel-air mixtures and combustion studies, heat pipe and heat exchange research, system vibrations and wear.

These research efforts have the objectives of raising energy systems efficiencies, opening new technological opportunities, improving reliability and extending the useful life of energy systems. For example, a series of elements in a new type of process control strategy has been demonstrated at LLL using a highly automated, laboratory-scale pilot plant. The plant adapts itself to changes in the chemical composition of the inputs and changes in the desired mix of products using control algorithms designed to give increasingly sophisticated numerical models of the chemical process. These innovations may lead to early replacement of conventional pilot plants with "smart" ones (i.e., ones with sophisticated feedback control systems). In turn, that holds great promise for improvements over the next 5-10 years in coal liquefaction and other chemical processing.

The funds requested for FY 1981 will be used to continue ongoing projects where they remain fruitful and to start other high priority studies in tribology (ball bearings, journal bearings, and automobile tires); percolation (tertiary oil recovery, geothermal applications, and nuclear waste disposal); automation and process control (adaptive systems and energy conserving control strategies); heat transfer and heat exchangers (basic aspects of heat pipes and development of new materials, techniques and processes

for heat exchange components and systems in mobile and stationary plants); structural engineering materials research (plastic deformation, non-destructive evaluation and testing).

#### Applied Mathematical Sciences

Applied Mathematical Sciences serves as the DOE focal point for monitoring and advancing the state of the art in applied mathematics, statistics, and computer science. The work is concentrated on broadly shared continuing needs throughout the DOE community. Emphasis is placed on research basic to the analysis, development, and use of large-scale computational models of the type arising throughout DOE technology programs; the management and analysis of large, complex collections of information; and the effective use of DOE computing resources.

Two accomplishments of the past year indicate the substance of the effort in applied mathematical sciences. In the area of partial differential equations we have developed and implemented the first reliable method for solving equations of magnetohydrodynamics in three dimensions. These equations are fundamental to the description of magnetic fusion devices such as tokamaks, mirror machines and others. The availability of this new method is already impacting the future course of the magnetic fusion process.

Mathematicians and computer scientists at Argonne National Laboratory, working jointly with colleagues at the University of Maryland, the University of New Mexico, and the University of California at San Diego, recently completed a venture sponsored jointly with NSF. The objective was better understanding of the process of creating quality numerical software for energy applications using automated programming aids. The resulting collection of software for solving systems of linear equations, called LINPACK, was distributed to over 150 requestor sites during the first three months of availability. Over 1200 copies of the associated monograph have been purchased by computer users, numerical analysts, and educators during the same period.

The FY 1981 request for operating funds for Applied Mathematical Sciences is \$13,000,000, a \$2,800,000 increase over the amount appropriated in FY 1980. Corresponding to the main areas of emphasis, Applied Mathematical Sciences has recently been organized into four components: analytical and numerical methods, information analysis techniques, advanced computer concepts, and special projects.

\$6,000,000, an increase of \$925,000, is required for analytical and numerical methods. This research 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 the environmental or health effects of energy production and to modeling energy supply and demand. Analytical and numerical methods covers three categories of research reflecting the principal thrust of the program in previous years: applied analysis, computational mathematics, and numerical methods for partial differential equations. Applied analysis concentrates on techniques to develop and analyze mathematical models of scientific, engineering, and socio-economic phenomena. It also includes the analysis of the transition from a mathematical model to corresponding approximate computational models. Computational mathematics involves the design and analysis of algorithms for basic computational problems (e.g., linear algebra, optimization, approximation and interpolation, and differential equations). Emphasis is also placed on creating transportable, high-quality software suitable for a wide body of users instead of for a specific computer center. Numerical methods for partial differential equations deals with a class of equations which play a dominant role in the modeling of energy systems. Currently, this research emphasizes methods applicable to computational fluid dynamics; FY 1981 plans, however, include methods applicable to structural mechanics and heat transfer. The principal objective is to develop methodology and tools to solve currently intractable problems.

\$2,400,000, an increase of \$650,000, is required for information analysis techniques, in which innovative approaches are sought to the manipulation and analysis of large, complex collections of scientific, engineering, environmental, energy, and socio-economic data. It thus addresses questions basic to energy policy activities and analysis of energy systems. It covers three categories of research: statistical

methods, data management, and display and analysis systems. Statistical methods emphasizes exploratory data analysis, experimental design, and sensitivity analysis applicable to large, complex data collections and multi-parameter models. Data management research seeks better ways to organize and retrieve large, complex sets of data. Currently, the interface with interactive display and analysis of numeric data is emphasized; FY 1981 plans include the interface with computational models. Display and analysis systems studies methods for making graphics, data management, and analysis tools more unified and easier to use. Initial efforts focus on the display and analysis of data coded by geographical areas. Research in information analysis techniques is directly applicable to problems impeding the development of the Energy Information Administration's (EIA's) National Energy Information System and Energy Emergency Management Information System and the analysis of regional environmental impacts. The resulting synergistic effects of interactions with EIA, with the Department's environmental programs and with other Federal agencies (Department of Labor and the Department of Commerce's National Telecommunications and Information Agency and Office of Federal Statistical Policy) significantly contributes to the improved use of information for domestic policy decisions.

\$4,000,000, an increase of \$1,025,000, is required for research in advanced computer concepts, which covers the categories called software engineering, distributed systems, and high performance systems. Software engineering includes research on programming languages and automated programming aids, with emphasis on ultimate applicability to large-scale computational models and better understanding of the process of creating transportable, high-quality software implementations of algorithms for basic computational problems. Distributed systems includes research on both local and remote computer networks. Research on local networks emphasizes performance of links between worker computers (e.g., supercomputers), mass-storage systems, and interactive access. Research on remote networks addresses the problem of resource utilization in a heterogeneous environment (e.g., program development on a highly interactive system with automated programming aids for Fortran programming, program execution on a supercomputer, and analysis of results on an interactive graphics facility). High performance systems responds to the fact that computer hardware development has reached the fundamental limit imposed by the speed of light. Increased computing power will ultimately depend upon parallel execution of instructions. High performance systems, therefore, emphasizes two critical areas: the match between algorithmic structure of large-scale computational models and the possible architectural structure of future supercomputers; and the transportability of applications software between successive generations of supercomputers. Several activities in advanced computer concepts are pursued jointly with the NSF's Computer Science Research Program and the DOD Defense Advanced Research Project Agency's (DARPA's) Information Processing Techniques Research Program. For example, NSF is supporting investigations of fundamental changes in computer architectures and DARPA is supporting related implications of Very Large Scale Integration (VLSI) technology, while DOE supports their impact on the solution of partial differential equations describing energy systems on the supercomputers of the future.

\$600,000, an increase of \$200,000, is required for special projects to support conferences and working groups to evaluate program directions; liaison activities to stimulate interactions between researchers funded by this program and DOE computer users; and selected special projects outside the previously defined topic areas. A particularly significant liaison effort is the establishment of prototypical "software clinics" at ANL, LASL, and New York University. Numerical analysts and computer scientists will use computer networks to bring the best available expertise to bear on selected user problems. The resulting insights will undoubtedly influence the future directions of research in the applied mathematical sciences.

### Geosciences

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; hydrologic and marine sciences; 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 1981 request for operating expenses for Geosciences is \$11,600,000, an increase of \$3,600,000 above the FY 1980 level. Approximately \$6,900,000 of the request is for continuing the existing base programs in geology, geophysics, geochemistry. One focus of the base program involves detailed examination of the nature and mechanics of the formation of small microfractures in rocks. These studies have shown that cracks are a dynamic feature in rocks, and that the nature of filling the cracks and surface roughness are important parameters in controlling physical properties, such as acoustic velocity, internal friction and permeability. These results are important in evaluating fluid flow in hydrothermal (geothermal) systems and estimating limits for the escape of radioactive nuclides from breached disposal sites.

In another area typical of the base program, high temperature studies on the thermodynamic properties of brines have lead to powerful theoretical models that allow us to predict the properties of complex mixtures of salts over a broad range of temperature, composition and solute concentrations. Such models have numerous applications for understanding and predicting the behavior of natural geothermal systems.

The remaining \$4,700,000 in operating expenses is for five areas of special emphasis which will impact numerous current and future energy processes and systems, but which will have particular significance for the geologic disposal of radioactive wastes. One of these efforts, called geochemical migration, was started in FY 1979. Two others, the continental scientific drilling program and rock mechanics were started in FY 1980. The FY 1981 request provides for strengthening the work in these three areas, and for starting work in two other highly important areas: ocean margin drilling and mineral hosts for element isolation.

The studies of the migration of chemical species in the earth's crust are a joint venture in cooperation with the NSF and the United States Geological Survey (USGS). This effort involves the study of radioactive waste isolation, the concentration of hydrocarbon resources (oil and gas), and rock-fluid interactions relating to in-situ mining and geothermal energy. In FY 1981, \$1,000,000 is required for this effort in geochemical migration. Work completed so far has defined the range of plutonium species that will occur in natural solutions, has shown that the decreasing adsorptive capacities of clay for the cesium ion at higher temperatures means that this ion may move substantially faster through a clay backfill than previously expected, and has suggested that hematite (iron oxide) may be an effective barrier to the migration of iodate ions. By throwing light on the migration of radioactive species, all three of these results have significant importance to designing methods for isolating radioactive wastes.

\$1,600,000 is required in FY 1981 for studies on magma-hydrothermal systems--the DOE portion of the National Continental Scientific Drilling Program (CSDP)--including experimental "piggybacking" on drill-holes emplaced by the DOE technology programs to maximize the scientific returns from these holes at minimum cost. The CSDP is an interagency program of experimentation and drilling at selected sites for the development of information on the continent's underlying structure and dynamics. The resulting knowledge will be important in predicting deposits of energy resources, in establishing a scientific base of information relevant to nuclear waste disposition, and in the assessment of hazards associated with the siting of major energy-related facilities. 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.



\$700,000 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. Recent results include a model that quantifies the timing, shape and rate at which explosive pulses may be used to generate and control and nature of fractures in rock. This type of work will help develop processes for the release of natural gas trapped in formations of low porosity.

Also in FY 1981, \$400,000 will be required for the investigation of mineral hosts for element isolation. In this new area, the ability of different minerals to maintain their integrity under wide ranges of temperatures and pressure will be compared. The most enduring will then be studied for their abilities to contain radioactive wastes without serious breakdown caused by radiation and heat from the contained wastes. In preliminary studies, for example, synthesis of  $UO_2$  (uraninite) and  $ThO_2$  (thorianite) have yielded large crystals suitable for study of the effects of radiation damage on crystals and will lead to an evaluation of these minerals as potential hosts for radioactive waste materials.

\$1,000,000 is required to initiate a new program of research that bears on the evaluation of the petroleum potential of the outer continental margin. The major thrusts will be in fields of organic geochemistry, the development of new geophysical studies and techniques to examine the continental and oceanic plate margins, and the development of equipment for automated core logging and analysis. The studies will be coordinated closely with the planned next phase of the Deep Sea Drilling Project, Ocean Margin Drilling currently being organized by NSF.

#### Capital Equipment

The FY 1981 request for capital equipment for Engineering, Mathematical and Geosciences is \$2,060,000, an increase of \$810,000 above the FY 1980 level.

Engineering Research projects will require \$200,000 in equipment funds in FY 1981 for effective start of studies on reducing friction, percolation, heat transfer and process control, as well as to meet the highest priority needs arising from ongoing research, such as those in the area of separations for resource recovery.

\$900,000 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 will consist of one or more minicomputers to serve a key part of the research program. The RCF's will be 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 will 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. The establishment of RCF's is consistent with the recommendations of a select panel of academic and industrial representatives reported in "Rejuvenating Experimental Computer Sciences: A Report to the National Science Foundation and Others." The plans are being coordinated closely with NSF and DARPA.

For Geosciences, \$960,000 is required for capital equipment in FY 1981. These funds are needed to provide equipment of vital importance to the base research program in geosciences as well as for the five areas of special emphases. Major equipment needs at LLL include an ion beam scanner, a telemetered digital seismic system, automated density-measuring equipment and prototype geophysical tools for

underground imaging. At LBL a high temperature vapor pressure measuring system is required, a graphics terminal and a drop calorimeter for measurement of heats of fusion of minerals. At ANL, a high temperature, high pressure calorimeter is needed, plus a thermometer-microprocessor system. The request will also provide an anoxic chamber, an oxygen analyzer, a high pressure pump and computer interfacing equipment for Battelle-Pacific Northwest Laboratories.

#### 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. In FY 1981, operating funds of \$8,000,000 and capital equipment funds of \$300,000 are requested.

#### 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 is clearly a judgmental call. It takes into account past experience, the pressure of highly rated proposals which had to be declined for lack of funds, as well as availability of Federal staff to operate and monitor this activity. Each project selected is supported for a limited time only, typically not to exceed three years. After such a period, the concept is expected to either prove itself to a point where a source of further support can be identified, or else be dropped. Projects are considered on the basis of proposals submitted by researchers from universities, industry and national laboratories. Proposals from all sources are treated on an equal basis: all are subjected to a detailed technical peer review by individually selected panels of experts.

In FY 1978, the program's first year of operation, twenty-one projects were selected for support. In FY 1979, available funding permitted only thirteen projects to be started. The subject matter of those projects covered, for example, new heat engines, new and "exotic" photovoltaic materials, new concepts in solar energy collection, research aimed at developing x-ray lasers and new methods of accelerating charged particles. Although the program is only two years old, several significant accomplishments can already be mentioned. Among those is a laboratory-scale verification and preliminary economic evaluation of a new method for extracting oil from tar sands using RF heating; based on the results obtained in an eighteen-month study supported by Advanced Energy Projects, this concept is now field-tested under a multimillion dollar program combining Federal and private funds. Another achievement is the discovery of "channeling radiation" -- extremely narrow beams of x-rays emitted by electrons passing through specially aligned crystals. Potential energy-related applications are in the materials research area. Other possible applications include x-ray lithography and medical diagnostics.

The following tables illustrate the distribution of FY 1979 operating expenses among various sectors and among different technologies.

#### Distribution of FY 1979 Operating Expenses by Sector

	<u>\$</u>	<u>% of total</u>
Universities	\$1,797	47%
Industry	1,450	38%
DOE Labs	447	12%
Federal Labs	106	3%
Total	<u>\$3,800</u>	<u>100%</u>

Distribution of FY 1979 Operating Expenses by Technology

	<u>\$</u>	<u>% of total</u>
Solar	\$2,044	54%
Conservation	600	16%
Fossil	162	4%
Multitechnology	549	14%
Advanced Concepts	445	12%
Total	<u>\$3,800</u>	<u>100%</u>

The above distributions resulted from the selection of the best of the many unsolicited proposals received. The annual funding level per project in FY 1979 varied between about \$60,000 and \$218,000 with an average of about \$165,000.

The FY 1981 request of \$8,000,000 in operating funds is justified as follows: New energy related concepts are being born continuously. The amount requested would permit the achievement in FY 1981 of the goal of initiating about twenty new projects for support of exploratory research (in addition to continuing the support of projects initiated in FY 1979 and FY 1980).

Capital Equipment

The FY 1981 request for capital equipment funds is \$300,000. 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 provide the biological foundation of information for the Department's efforts for biomass production of fuels and chemicals, biological transformations of organic materials (bioconversion) for conservation and using biological systems (bioprocessing) for resource recovery. The program has two facets, botanical investigations and microbiological studies. 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 using microorganisms into fuel and chemicals, and with ideas for using 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 in energy matters. While there are a number of problem areas common with U.S. Department of Agriculture (USDA) programs, the difference is that USDA is concerned with food, fiber and forage while DOE has interest in fuels and chemicals. The species of plants used are usually different and the growing areas will be somewhat different with DOE focussing particularly on the use of marginal lands and aquatic areas.

Even though the BER program was just recently established in FY 1979, a number of accomplishments are representative of the character of the developing program.

- o Investigations on recently isolated bacteria and algae from natural sources including oil bearing sediments, coal areas, ponds near oil wells and others have shown that some of these organisms can synthesize quantities of hydrocarbons which resemble petroleum. The patterns of these hydrocarbons suggest that significant geological maturing might not have been necessary for petroleum formation. These findings also suggest that the bioconversion of various forms of biomass into petroleum-like products is a possibility in the coming years.

- o A possible biochemical indicator of drought resistance in plants has been identified. Such a biochemical indicator would be very useful in screening plant varieties with a high probability of drought tolerance for biomass production on marginal lands where water availability is a problem.
- o A bacterium capable of producing ethyl alcohol from sugars with good efficiency under strictly anaerobic (lacking free oxygen) conditions and at high temperatures has been found. Such a system, if it can be developed successfully in conjunction with cellulose degrading organisms might provide a means of using a continuous stream rather than a batch process for fermentation of residues to alcohol. This could lead to more efficient alcohol fuel production systems.
- o In biology, recognition between organisms is accomplished at the molecular level. In the last three decades, there have been two classes of information-carrying molecules, nucleic acids (like RNA and DNA) and proteins, which have received the most attention. A third class of molecule, the polysaccharides (polymers of sugars), is also responsible for biological recognition processes. In particular, the polysaccharides appear to have key roles in plant host-pathogen relations as well as where organisms form mutually beneficial relationships (symbiosis) as in nitrogen fixation. A significant advance leading to a better understanding of recognition processes involving polysaccharides has been made with the development of an analytical method yielding structural details of these molecules. This very basic information has the potential for suggesting strategies of improved plant protection or of symbiotic relationships leading to energy conservation.
- o The existence of a natural flowering-inhibitor hormone in plants has been demonstrated for the first time. Prevention of flowering is an important element in the production of biomass since flowering diverts the plant from continued vegetative growth and reduces biomass yields. This discovery suggests strategies for inhibition of flowering by chemical control, thereby enhancing total biomass production.

The FY 1981 request for Biological Energy Research is \$9,200,000 of which \$8,800,000 is for operating expenses and \$400,000 is for capital equipment. Initiated in FY 1979, the BER program aims at an area of energy sciences which until recently has been virtually ignored as far as long-term research; the program is beginning to fill that gap with careful, phased growth in building an effort with the scope and quality consistent with providing the requisite background to examine many options for utilizing biological systems in energy matters.

#### Operating Expenses

The FY 1981 request of \$8,800,000 in operating funds for Biological Energy Research represents an increase of \$2,800,000 over the FY 1980 level. Some of the increase will occur in the program at the Michigan State University/DOE Plant Research Laboratory, one of the strongest plant science laboratories in the Nation, while the remainder of the increases will be for investigations in a number of other universities and laboratories around the country.

Of the requested amount, about \$5,400,000 is planned for research for gaining a better understanding of how plants function in producing biomass. The main areas of investigation to be emphasized for growth in FY 1981 include:

Studies on the chemical diversity of selected plant species known to contain hydrocarbons of energy interest, and the regulation of biochemical pathways of synthesis of hydrocarbons including genetic control of the key reactions. This information is essential in order to conceive of the development of hydrocarbon plant growing as a source of fuel and chemicals.

The mechanisms by which plants adapt to non-optimal growth conditions. This includes investigations seeking chemical or physical indicators of adaptation which might then be used in any projected genetic improvement program. Studies on the key role of root function in regulating plant growth will also be emphasized. Included in the studies on roots will be work on how soil microorganisms interact

with the root in making available to the plant, water and soil nutrients which otherwise might be limited. The importance of these relationships have until recently only been suspected.

An understanding of the physiological genetics of plants using model systems will be stressed. This is of considerable significance if the promising tools of genetic manipulation are to be used most effectively in the future.

Investigations on the biological aspects of photosynthesis are to be enhanced as part of the U.S.-Japan Cooperative Program on Photoconversion and Photosynthesis.

The other major leg of the BER program accounting for \$3,400,000 of the FY 1981 request involves microbiological research. The major increases would focus on several areas:

Rapid development of a much better foundation of information concerning anaerobic microorganisms. Many fermentations which are in use today or are projected utilize anaerobic organisms. These organisms have many diverse capabilities which have not been exploited because too little is known about them. An example of their potential importance is as follows: Most of the synthetic fuels processes involve sizable emissions of gases including carbon monoxide, hydrogen and methane. Some anaerobic micro-organisms have the capability of utilizing some of these gases to synthesize larger molecules such as butyric acid, a starting material used in industry for making other more complex chemicals. With adequate information about the biochemistry, physiology and genetics of the anaerobes, it should become possible to design a strategy to get rid of unwanted and toxic waste gases and at the same time derive a bonus of a useful material.

Defining the ways in which microbial systems synthesize hydrocarbons (see the above discussion of achievements). Related to this work are other investigations aimed at understanding biochemical pathways for degrading materials such as cellulose and lignin. These latter materials would serve as the resource to use for conversion into hydrocarbons; that is, the concept is to have sequential or simultaneous microbial cultures which perform a series of events such as: cellulose --> sugars --> acetate --> hydrocarbons. Each of these individual simplified steps is known but the overall system is not yet demonstrable.

The basic microbiology relating to the use of microorganisms in enhanced oil recovery from depleted wells. Evidence is now available to demonstrate that injections of certain microbes and nutrient media to sustain them can result in subsequent oil recovery. The basis for this is unclear. The organisms which are effective need to be identified along with their biochemical characteristics which confer oil recovery capability in order to use the microbial systems more effectively.

With respect to the certain future of increased use of microorganisms for conversion processes, it is essential that the research base be developed promptly. Under consideration is the concept of support of broad based projects in one or more universities with developing departments of microbiology. This would encourage research while also developing the needed personnel to carry out the studies in the future.

#### Capital Equipment

The request for \$400,000 in capital equipment funds is required to provide rapid, efficient analytical tools for measuring hydrocarbons and other classes of biochemicals in organisms, utilizing techniques of high-pressure liquid chromatography, gas chromatography-mass spectrometry combinations, radioactive labeling analysis, and other analytical methods. In addition, a variety of separation techniques using centrifuges, column techniques, and others are needed to support our biological research effort. Without such techniques and equipment, the progress of this program would be seriously impaired and certain studies would be impossible to carry out.

### Program Direction

Basic Energy Sciences is a broadly diversified program requiring staff with expertise in scientific areas such as chemistry, physics, engineering, metallurgy, geosciences, biology, mathematics and computer science, as well as in administrative, procurement and financial management. Basic Energy Sciences staff are responsible for program development, direction and management of complex technical programs in these scientific areas. Their activities include assessing scientific needs and priorities of the program, developing long-range program plans, technical review of proposals from laboratories and universities, and monitoring the progress of ongoing university contracts, laboratory programs and construction projects.

The FY 1981 request for Program Direction for the Basic Energy Sciences program is \$2,444,000, an increase of \$155,000 above the current base. The request is necessary to provide for the salaries, benefits, travel and related expenses associated with the 57 staff years of effort required to administer the program. The request provides an increase of three staff years in FY 1981, which is necessary to provide for additional workload resulting from the growth and increased diversity in the research programs supported under Basic Energy Sciences in FY 1981.

The present staff is carrying an extremely heavy workload. For example, the Basic Energy Sciences program expects to receive approximately 1275 new and renewal proposals and will process approximately 600 procurement requests during FY 1980. These numbers are expected to grow in FY 1981 as the program continues to expand. The corresponding numbers in FY 1977 were 750 proposals and 400 procurement requests. The staff consisted of 50 employees in FY 1977 and there has been an increase of only 3 since that time. It is becoming virtually impossible for the staff to properly review and process all of these proposals without additional staffing assistance. Technical expertise and assistance are needed in the areas of applied mathematics, the organic chemistry of coal, catalytic chemistry and microbiology. In order to effectively carry out the objectives of Basic Energy Sciences, it is essential that additional staff be hired as soon as possible.

Supporting Research  
 Energy Supply Research and Development - Operating Expenses  
 (Tabular dollars in thousands. Narrative material in whole dollars)

	FY 1979 Appropriation	FY 1980 Appropriation	FY 1981 Base	FY 1981 Request
<b>Technical assessment projects</b>				
Assessment projects				
Operating expenses .....	2,200	2,500	2,500	3,200
Subtotal .....	2,200	2,500	2,500	3,200
Satellite power systems				
Operating expenses .....	4,600	5,000	5,000	5,500
Capital equipment .....	0	500	500	0
Subtotal .....	4,600	5,500	5,500	5,500
Advanced technology projects				
Operating expenses .....	3,500	5,000	5,000	12,000
Subtotal .....	3,500	5,000	5,000	12,000
Program direction				
Operating expenses .....	375	466	496	540
Subtotal .....	375	466	496	540
<b>Total</b>				
Operating expenses .....	10,675	12,966	12,996	21,240
Capital equipment .....	0	500	500	0
Technical assessment projects .....	10,675	13,466	13,496	21,240

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

Summary of Changes

FY 1980 Appropriation enacted .....	\$ 13,466
Built-in increases and decreases:	
Pay cost supplemental .....	+ 30
FY 1981 Base .....	\$ 13,496
<b>Program Increases and Decreases</b>	
<u>Technical Assessment Projects</u>	
Initiate new assessments as required to provide more comprehensive analysis of DOE's R&D programs .....	+ 700
Expand support of advanced technology projects .....	+ 7,000
Personnel-related increases for the above programs .....	+ 44
FY 1981 Budget Request .....	\$ 21,240

Technical Assessment Projects

Technical Assessment Projects provides the Department with independent, objective analyses and assessments of research and technical needs and opportunities, including conceptual development and evaluation of the Satellite Power System. In addition, this program supports advanced technology projects designed to develop engineering and economic data on innovative, potentially high payoff ideas which do not fit readily into existing Department of Energy programs. These assessments and projects are carried out under the auspices of the Director of Energy Research in order to fulfill his mandated responsi-

bility to advise the Secretary on the Department's R&D programs. In FY 1981, \$21,240,000 is required for Technical Assessment Projects, an increase of \$7,774,000 over the amount appropriated for FY 1980.

This program is discussed below in terms of the following three subprograms: (1) assessment projects; (2) satellite power systems; and (3) advanced technology projects.

#### Assessment Projects

This program is aimed at providing DOE with the capability for independent, objective analysis of the Department's technical needs and opportunities. Its objectives include providing for rigorous assessment of existing or proposed technological initiatives, and examining the base of research that underlies a broad range of energy technologies, such as heat transfer and materials. It also provides support to the Director of Energy Research, in fulfilling his responsibility to independently advise the Secretary on the Department's research and development activities, in order to help make its program more effective, and to avoid costly mistakes. The Assessment Projects subprogram is carried out through studies, workshops, panels, and other mechanisms which allow the Department to make use of the best scientific and technical talent. Projects are identified through staff analysis, contact with other DOE program staffs, contact with outside experts, and through the various R&D program planning functions of the Department.

Assessments initiated in FY 1979 included, among others, a determination of the long-range research needs in coal liquefaction (developed by the Fossil Energy Working Group) and an evaluation of the technical readiness of ocean thermal energy conversion technology. A review of the R&D balance within the Department's technology base activities was also carried out. Technology base activities include basic and applied research as well as exploratory development programs. Special investigations of technical issues such as tritium penetration and LNG safety were also conducted.

In FY 1980, assessments are planned in such areas as the technical potential of biomass options, the long-range research needs in oil shale, alternatives to silicon for photovoltaics, and the status of R&D needs associated with indirect coal liquefaction processes.

The FY 1981 budget request of \$3,200,000, an increase of \$700,000 over the amount appropriated for Assessment Projects in FY 1980, will be used to continue assessments initiated in FY 1980, as well as to initiate a number of new ones. Emphasis will be placed on the expansion of the technology base activities to minimize potential failures or cost overruns in the Department's high-cost pilot and demonstration activities. Incorrect assessments of technical risks or inadequate R&D support have led to problems with these large facilities after they are well under construction.

#### Satellite Power Systems

The Satellite Power System (SPS) is one option being considered by DOE as a post-year 2000 energy source. The SPS concept is designed to capture solar energy with satellites in a geostationary orbit (a point in space about 22,000 miles above the Earth, which maintains a fixed position relative to Earth) and converting it, in space, to electrical energy by means of solar cells. In turn, this energy would be converted to radio frequency (RF) energy and sent to Earth in a focused beam aimed at a ground receiving antenna (rectenna) where it would be reconverted to electricity for distribution in a utility grid.

Presently the SPS program is working on the completion of the Concept Development and Evaluation Program (CDEP). This three year study, which was undertaken in conjunction with NASA, was intended to provide an initial assessment of the SPS concept and to provide a basis for making more informed decisions about SPS work. The CDEP has already identified a number of serious concerns about which it may be necessary to develop additional information, beyond the scope of the initial three year program, before any firm recommendation to proceed with an SPS Ground Based Exploratory Development (GBED) program could be supported.



The funds requested in FY 1981 will be used to study further the microwave bio-effects, the microwave communications effects, the non-microwave bio-effects, and the atmospheric effects of SPS. In addition, further systems definition will be undertaken, along with the development of an implementation plan for the GBED program if the decision is made to move forward with such a program. These areas are discussed in further detail below.

#### Microwave Bio-effects

The national concern for the effects of microwaves has significantly increased with the Presidential initiative to review the 1966 microwave occupational guidelines. The SPS requirements and activities are being coordinated with, and take advantage of, the current multiagency work in this area. Additional funding is required to tailor this work to the SPS frequency and power density levels, to provide new molecular biophysical theories on nonthermal microwave effects, and to design experiments to test the theories. Implementation planning will be completed, but no experiments will be initiated unless a GBED program is recommended and adopted by the administration and the Congress. Study results will be directly usable by the overall Federal microwave health and safety program being coordinated by the Environmental Protection Agency.

#### Microwave - Communications Effects

The SPS assessment work so far completed has shown that other effects of the microwave beams upon RF communications are of serious concern and will require additional experimental and analytical work to provide the necessary understanding and to develop and evaluate mitigating strategies.

The work falls into two categories: the effects resulting from disruption of the natural ionosphere and from the direct interference of the SPS beam with RF systems (microwave links, television, navigations systems, etc.).

The ionospheric experiments conducted at Platteville, Colorado, and Arecibo, Puerto Rico, have resulted in a new theory. This theory could significantly reduce future experimental costs by reducing the need for major facility upgrades. Physically, the validated theory will indicate if higher microwave power densities are environmentally acceptable. If so, the SPS system costs could be significantly reduced as a result of the reduced land area and rectenna size requirements. FY 1981 funding is required to continue experiments and theory development at the Platteville and the Arecibo facilities.

The studies of the effects of direct interference of the SPS beam with RF systems have taken advantage of a large body of data already accumulated by cognizant agencies in the United States. The potential seriousness of the problem has been delineated and mitigating strategies have been evaluated. The supporting experiments and analyses to extend these results to equipment, forecast to be in existence in the year 2000, and to judge what mitigation may already have been included, will require continued experimental and analytical work in FY 1981.

#### Non-microwave Bio-effects

This area is concerned mainly with the environmental effects of space on the personnel required to assemble and operate the SPS. The population required is in the hundreds; the stay times in space will be measured in months. Maximum advantage is being taken of the NASA space operations experience; however, additional work will be required to review the results of estimated manned operating limits and to define the environment at geosynchronous orbit (GEO), a region in which manned experience is nil. Funding is also required to maintain continuity and for design implementation plans, if the SPS program is continued.

### Atmospheric Effects

The effects of the launch vehicles and of the vehicles for transferring personnel and equipment from low earth orbit (LEO) to geosynchronous orbit are of concern because of the large scale of activity. The launched vehicles will be about 10 times the size of the space shuttle and will be launched on daily schedules. The orbit transfer vehicles will operate routinely in a hitherto lightly explored region between LEO and GEO. A comprehensive study of the impact of these systems on the total atmospheric system (the troposphere, stratosphere, ionosphere, mesosphere, and magnetosphere) is under way. The experimental and analytical work of NASA, DOE, and other contractors delineates specific impact studies and experiments (including the shuttle environmental assessment, sounding rocket flights, and monitoring launches of launch vehicles) that require additional FY 1981 funding. These include the impact of the orbital transfer vehicles on the magnetosphere and ionosphere.

### Systems Definitions

Systems definition activities require additional funding to refine the FY 1980 assessments of emerging technologies. These emerging technologies include solid state microwave systems and advanced systems for RF generation (gyrocons, etc.) which could significantly reduce weight, improve reliability, and result in major cost and environmental advantages. A preliminary laser concept, utilizing the laser as a power transmission system, has implied orders of magnitude reduction in land requirements for receiving antennae; but the state of the science for SPS use, such as solar-pumped lasers, requires further analysis. Advanced reference systems and the critical supporting investigations will be defined to provide an implementation plan for a possible continuation of the SPS program.

### Plan for Possible Program Continuation

The results of the initial CDEP are planned to be completed by late 1980. The proposed FY 1981 program covers transition activities and implementation planning for a possible new start on a GBED program in FY 1982, should such a program be supportable by the continuing assessment activities and the subsequent decisions of the Administration and the Congress.

### Advanced Technology Projects

The objective of Advanced Technology Projects (ATP) is to develop engineering and economic data on innovative concepts which have potentially high payoffs but which do not readily fit into existing Department of Energy programs. This program also serves as a mechanism for accelerating the transition of ideas which have been shown to be feasible from an engineering standpoint to the appropriate project organization within the Department for further development. Such projects might not be funded originally by an energy technology program for several reasons. For example, the potential high-payoff of these projects is usually accompanied by high risk, which makes them relatively unattractive funding choices for mainline program organizations. In addition, projects of this type typically fall outside of the main mission of most R&D organizations, and are therefore frequently not able to compete because available funds are all required for the pursuit of major ongoing programs. Further, this program also provides a source of funding for meritorious proposals that cut across several energy technology programs. Projects selected for funding under Advanced Technology Projects are evaluated on the basis of their specific goals and are assessed on their potential impact on the energy problem concerned. They are also reviewed, prior to funding, by potential supporting program groups as to their predicted benefits.

The FY 1981 budget request for Advanced Technology Projects is \$12,000,000, an increase of \$7,000,000 over the amount appropriated in FY 1980. The FY 1981 request will be used to initiate a number of new projects, as well as to continue projects initiated in FY 1979 and FY 1980. The level requested is based on the funds required to support the second year of projects initiated in FY 1980 and third and final year of projects initiated in FY 1979. In addition, an estimate of the amount required for new projects was made based on an extrapolation from the number of proposals received to date, the number accepted for funding, and their dollar value. Approximately two-thirds of the request is required for the continuation of ongoing projects and one-third is to

permit initiation of new projects. Typically, the duration of these projects will be for no longer than three years, by which time the decision will be made whether to transfer the project to another Department of Energy organization for further funding and development, or to drop it. Several of the projects of particular interest to mission-oriented organizations have been jointly funded with those organizations.

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

Several major new initiatives were begun in FY 1979 and FY 1980 which are aimed at providing verification of technological feasibility, as well as the basic engineering data required in order to judge the potential impact of a new energy concept on the national energy situation. Specific projects funded, which are planned for continuation in FY 1981, include:

- development of electrolytic cell-fuel cell solar energy systems for residences;
- demonstrations of the engineering feasibility of advanced catalytic systems, including synthesis of gasoline, and cogeneration of high-BTU gas and electricity;
- advanced aerial geophysical exploration for geothermal resources;
- computational concepts for very large (perhaps ten times) reductions in computer time for two-phase flow problems, particularly important in reactor safety problems;
- in-situ evaluation of radiofrequency heating of tar sands;
- new combustion technology concepts;
- demonstration of a room-temperature high energy density lithium-vanadium battery;
- demonstration of a high lifetime hydrocarbon lubricant;
- demonstration of rapid, low-cost production of ethanol from sugars.

The \$12,000,000 requested for FY 1981 would result in several major benefits. First, significant cost savings in design and implementation of second generation energy technologies including combustion, exploration, gasification, and product fabrication would be achieved by making it possible to advance conservative time schedules and by providing engineering data for pre-commercial design development. Second, multi-disciplinary and inter-programmatic activities would be verified to provide new program directions for further exploitation in other Department of Energy program organizations. Third, where unexpected technology problems are found, they would be redirected to other program divisions for further work in response to end-user requirements.

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

#### Program Direction

The FY 1981 request for Program Direction for the Technical Assessment Projects program is \$540,000, an increase of \$44,000 above the current base. This increase will provide for one additional full-time permanent staff year, from 12 in FY 1980 to 13 in FY 1981. This position would be used to provide needed technical support in order to help carry out the expanded efforts under the Advanced Technology Projects subprogram.

Basic Research  
 Energy Supply Research and Development - Operating Expenses  
 (Tabular dollars in thousands. Narrative materials in whole dollars.)

	FY 1979 Appropriation	FY 1980 Appropriation	FY 1981 Base	FY 1981 Request
<u>University research support (ER)</u>				
University institutional agreements:				
Operating expenses.....	800 <sup>a/</sup>	2,300	2,300	7,700
Subtotal.....	800	2,300	2,300	7,700
University reactor fuel assistance:				
Operating expenses.....	2,000	1,700	1,700	2,500
Subtotal.....	2,000	1,700	1,700	2,500
University/laboratory cooperative program:				
Operating expenses.....	3,155	2,800	2,800	3,800
Subtotal.....	3,155	2,800	2,800	3,000
Program direction:				
Operating expenses.....	244 <sup>b/</sup>	267 <sup>b/</sup>	278	320
Subtotal.....	244	267	278	320
Total, university research support	6,199	7,067	7,078	14,320

<sup>a/</sup>Additional \$1,400,000 budgeted under other programs.

<sup>b/</sup>Reflects comparability adjustment for transfer of three positions from former Assistant Secretary for Institutional Relations to Energy Research in the amounts of \$95,000 and \$96,000 respectively.

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

Summary of Changes

FY 1980 Appropriation enacted .....	\$7,067
Built-in increases and decreases:	
Pay cost supplemental.....	11
FY 1981 Base.....	\$7,078
Program Increases and Decreases	
<u>University Research Support Program</u>	
Support five new university institutional research awards (three awards on a replacement basis for projects completed in prior years).....	\$+ 800
Support goal-oriented and/or multidisciplinary university energy research programs.....	\$+3,000
Add five new research projects in minority institutions research program.....	\$+ 600
Increase number of minority research apprenticeships to 500.....	\$+1,000
Establish low enriched fuel fabrication line, reinstate support for reactor sharing.....	\$+ 800
Increase operating levels at 12 contractor sites in University/Laboratory Cooperative Program.....	\$+1,000
Provide for salary, fringe benefit increases in program direction.....	\$+ 42
FY 1981 Budget Request.....	\$14,320

	<u>FY 1980</u> <u>Appropriation</u>	<u>FY 1981</u> <u>Base</u>	<u>FY 1981</u> <u>Request</u>
<u>University institutional agreements</u>	\$2,300	\$2,300	\$7,700

The university institutional agreements program provides support at universities and colleges for energy-related research focused on longer-term research problems which, in many cases, cut across the individual energy technologies under development by the Department.

Three program subactivities are included in this program. The first is directed at strengthening the energy research and management capabilities at a small number of major universities with significant and deep involvement in energy research and development. Research awards are made following review and acceptance of unsolicited research proposals prepared and submitted to the Office of Energy Research by the principal campus official concerned with scientific and technical research, for example, a vice president for research or a director of a campus-wide energy laboratory or institute. Awards are normally made for three years, subject to the annual review of program performance and the availability of funds. Significant flexibility is provided to the participating universities in this program to propose and carry out a mix of research and education-oriented projects. Normally, these awards include support for the following general activities: (1) small-scale or exploratory energy research projects supported for the purpose of testing promising new research ideas and concepts; (2) the development of university-wide energy education programs including new courses at the graduate level, workshops, and symposia; (3) information dissemination efforts including conferences and training sessions, and personnel exchanges directed at improving the flow of research findings to development groups in industry.

Special emphasis in these awards is placed on involving postdoctoral researchers and young faculty in applied energy research. Cost sharing is also provided by the participating universities from industrial and other private sources. Cooperative research projects with industrial research groups may also be included as part of an institution's overall plan as a means of enhancing and expediting the transfer of university research results to commercial application. This is the only Department of Energy program which provides opportunities to universities to contribute to the National Energy Program on a campus-wide and multidisciplinary level.

Seven universities currently are supported under this program: the University of Puerto Rico, the Massachusetts Institute of Technology, the California Institute of Technology, Stanford University, the Utah Consortium for Energy Research and Education (consisting of the University of Utah, Brigham Young University, and Utah State University), the University of Illinois at Urbana, and Purdue University. The University of Puerto Rico's support is part of the Department's commitment to the University to assist in the development and operation of a university-wide Center for Energy and Environment Research. Two new research awards are scheduled for FY 1980 to replace projects which were completed in FY 1979.

The second program subactivity in the university institutional agreements program is a new initiative proposed for FY 1981, directed at the gap in DOE support of energy R&D between the disciplinary-oriented research programs supported on a project-by-project basis through the Basic Energy Sciences Program and the engineering scale and demonstration-oriented programs in the technology development programs. This initiative is designed to fill that gap through the support of interdisciplinary teams focused on goal oriented basic research in areas critical to the technologies. Support would be provided for scientific and technical research and for socioeconomic and environmental research, as appropriate to the nature of the problem under study. Emphasis would be placed on novel concepts and on problems common to more than one technology requiring a multidisciplinary scientific attack. Incremental improvements of existing technical approaches, properly the responsibility of the technology programs, will not be supported. Examples of initial research areas for this program effort include advanced energy conversion systems, high temperature materials, electrochemistry, surface science and energy risk analysis. Further identification of high priority program areas will

be carried out in close coordination with the DOE technology programs. Close collaboration would also be maintained among the participating universities, the DOE National Laboratories and private industry.

This program effort would be initiated by DOE through the release of a broad competitive solicitation. Each university interested in developing proposals for this program will have to meet certain minimum eligibility requirements including evidence of superior established research and educational competence in energy-related fields, the potential pool of involved faculty and students, and strong institutional commitment to the program. Criteria used to evaluate and select the projects for support will include the scientific/technical merit of the proposed research (particularly in terms of new concepts or approaches) the demonstrated superior capabilities and experience of the faculty to be involved in the program, the existing research facilities and equipment available for the proposed program, multidisciplinary and/or goal-oriented research experience at the proposing university, and the likelihood of significant contributions that would either contribute directly to technology development programs or lead to development projects attractive to those programs. Evidence of institutional commitment such as dedicated faculty positions and, if appropriate, private sector interest such as cost-sharing would be evaluated within the context of specific proposals. The research program subsequently supported would build on existing research capabilities, while at the same time providing the program stability necessary to attract new people and ideas into energy R&D. If proposals are of sufficiently high quality, additional awards under this new effort would be made in subsequent budget years. The interdisciplinary teams will typically require the commitment of several senior faculty supported by postdoctorals, graduate students and other technical experts over a several year period. The need for additional domestic doctoral-level engineering students is particularly critical in terms of future advanced energy R&D efforts. This program will be highly selective and only superior institutional proposals that fully meet these criteria will be funded.

The third program subactivity included in the university institutional agreements program is the minority institutions research and education program. Here, the intent is to develop new energy research capability at smaller, traditionally minority universities and colleges in order to broaden the base of participation and contributions to the National Energy Program by these institutions. An important related objective is to enhance the training received by minority science and engineering students working toward future careers in energy research and related fields.

Research projects supported in this program are based on the annual review of unsolicited research proposals submitted to the Office of Energy Research. In FY 1979, eleven research projects were supported with the following institutions; Howard University, Washington, D. C.; Atlanta University, Georgia; Tuskegee Institute, Alabama; North Carolina A&T State University, North Carolina; Alabama A&M University, Alabama; North Carolina Central University, North Carolina; Jackson State University, Mississippi; Prairie View A&M University, Texas; Bowie State College, Maryland; and Texas Southern University, Texas. Energy research supported in these projects ranged from basic energy science to environmental assessments, solar technology development, and coal conversion research. All projects included support for students. Total support in FY 1979 was \$654,450 (\$550,000 from ER and \$104,450 from ET), with a similar amount planned for FY 1980.

The budget request of \$7,700,000 in FY 1981 for the university institutional agreements program, an increase of \$5,400,000 over the total available in FY 1980 will provide continued support for three current university institutional awards (the University of Puerto Rico, Stanford University, and Purdue University), second year support for the two new projects initiated in FY 1980, and five new awards to be made in FY 1980. These new awards will principally emphasize joint research efforts between university research groups and industry on selected energy research problems with strong potential for industrial application. Cost sharing will be required from participating industries in this effort. The total of ten research awards in this program subactivity is considered the optimum number of awards in the program based on the number of meritorious proposals received and program staff oversight responsibilities. In the proposed new initiative for the support of goal-oriented, multidisciplinary research

programs, university awards would be made in response to a broad competitive solicitation provisions for follow-on support and the addition of new programs in subsequent budget years. This budget request will also provide support for fifteen research awards under the minority institutions research program, including replacement of eight awards that will end in FY 1979. The increase proposed for the support of minority energy research projects is consistent with the Department's goal of involving more minority scientists and engineers, including students, in the Nation's energy effort. In addition to the support for research projects, funds will also be provided to research groups at both universities and the Department's National Laboratories to conduct a special program of research apprenticeships for high school minority students interested in pursuing scientific or technical-related degrees in college. Over 500 apprenticeships are to be supported at the budget level requested. This activity is part of the government-wide effort led by the Office of Science and Technology Policy to stimulate broader interest in the minority communities in careers in science and engineering and to establish individual working relationships between students interested in such careers with active scientific and technical researchers. At the budget level requested for the overall university institutional agreements program, it is estimated that 200 university faculty members (average one-third time) and 350 advanced graduate students will be supported in energy research activities.

	<u>FY 1980</u> <u>Appropriation</u>	<u>FY 1981</u> <u>Base</u>	<u>FY 1981</u> <u>Request</u>
<u>University reactor fuel assistance</u>	\$1,700.	\$1,700	\$2,500

The objective of this program is to support specialized nuclear energy research and training facilities at selected universities; these are dual purpose reactor facilities, being utilized for both research and educational purposes. The facilities supported are not specifically duplicated elsewhere, either in the National Laboratories or in the private sector corporate laboratories.

There are currently 54 university research and training reactors in operation in the United States. These reactors were established under varying financial sponsorship, including private, state, and Federal funds. Some years ago, the former Atomic Energy Commission established a policy of providing funds to universities for the procurement of specialized reactor fuel and for support of a portion of reactor operating costs when the reactors are shared with neighboring, non-reactor-owning colleges and universities (reactor sharing).

Under this program, funds are provided for the fabrication of fuel elements for a small number of university research reactors and for university reactor operating costs associated with reactor sharing. The refueling requirements of the reactors vary from several times per year to once in several years. Several years ago the fuel supply for plate-type fuel became a serious problem. In 1977, the only domestic fabricator of plate type fuel for non-DOE reactors suspended its fabrication operation. Arrangements were then made to establish another company as a supplier. The reactors at the University of Michigan, University of Missouri, the Massachusetts Institute of Technology (MIT), the University of Virginia, Rhode Island Atomic Energy Commission and several other institutions are all dependent on plate-type fuel from this sole supplier. The major share of funding available under this program is now allocated for support of the company's fuel assembly line. The current schedule calls for delivery in FY 1980 of 16 fuel elements for Michigan, 26 elements for Missouri, 13 elements for MIT, and 15 elements for Rhode Island.

Seventeen of the university reactors are TRIGA reactors. They are fueled with TRIGA fuel elements for which a different company is the sole supplier. Seven TRIGA fuel elements are scheduled for procurement for Pennsylvania State University in FY 1980.

In conjunction with administration policies on non-proliferation and safeguards, the Nuclear Regulatory Commission has issued regulations limiting the quantity of highly enriched uranium (HEU) allowed on a reactor site. As a result, the Argonne National Laboratory is directing a program to initiate the use of low enriched uranium (LEU) fuel in research, training, and test reactors worldwide. Universities in the United States are active participants in this program, and are studying conversion of their reactors to LEU fuel. Establishment of the current supplier of plate-type fuel as a supplier of LEU fuel for the university reactors is anticipated.

In FY 1981, funds of \$2,500,000, an increase of \$800,000, are requested for this program. The major share of the funding is requested for support of university reactor fuel fabrication. Of this increase, \$625,000 is requested for tooling and other costs associated with production of LEU fuel elements and their use at university reactors. An amount of \$175,000 is requested for increased support for reactor sharing projects.

	<u>FY 1980</u> <u>Appropriation</u>	<u>FY 1981</u> <u>Base</u>	<u>FY 1981</u> <u>Request</u>
University/laboratory cooperative program	\$2,800	\$2,800	\$3,800

The university/laboratory cooperative program encompasses a wide variety of activities that bring college and university faculty and undergraduate and graduate students to the Department's Energy Technology Centers, National Laboratories, and other contractor operated facilities to participate in ongoing research programs and intensive instructional/learning programs on energy-related projects. The program is designed to increase the interactions and flow of information between university and Laboratory scientists and to increase the direct familiarity of university scientists with current developments and techniques in energy R&D. Among the specific activities supported through this program are summer or academic year research appointments for university faculty at a participating Departmental facility, support for student research participation including dissertation support, and faculty institutes and short courses. The use on a shared basis of unique Laboratory research equipment and facilities is also part of this program. This particularly benefits faculty and students from smaller colleges without such specialized and costly research equipment.

Funding is provided through this program to 12 National Laboratories and other contractor organizations. Special mention should be made of three such organizations. The Associated Western Universities, an organization of 32 member universities in the Rocky Mountain region, administers cooperative programs with 12 or more Department Laboratories and facilities in the western United States. The Northwest College and University Association for Science, a consortium of 52 colleges and universities plus seven industrial firms, operates special research and training programs which principally use the facilities at the Pacific Northwest Laboratory and the Hanford Engineering Development Laboratory at Richland, Washington. The Oak Ridge Associated Universities, a consortium of 45 universities located in the south and southeast, carries out faculty and student research and training programs at the Oak Ridge National Laboratory, the Savannah River Laboratory, and the Morgantown and Pittsburgh Energy Technology Centers. Other Laboratories which directly participate in the university/laboratory cooperative program include the Brookhaven National Laboratory, in Upton, Long Island, the Argonne National Laboratory in Chicago, Illinois, and the Ames National Laboratory at Ames, Iowa.

The budget request of \$3,800,000 represents an increase of \$1,000,000 over the FY 1980 appropriation. Of this amount, \$600,000 will be used to reinstate support for special training programs on energy-related subjects (principally at the Oak Ridge Associated Universities and at the Argonne National Laboratory) for faculty at smaller colleges and universities. At this level it is anticipated that over 750 faculty members and other researchers will be able to participate in short courses and summer institutes and through such participation to develop new and revise current academic courses on energy subjects. The remaining \$400,000 of the proposed increase will be used to expand the number of faculty and students conducting research efforts using the unique facilities and resources of the participating National Laboratories. In total, over 2,300 faculty and students will be involved in the university/laboratory cooperative program at the requested budget level. This request is the first significant budget increase in six years for this program effort.

Workload and staffing requirements for university/laboratory cooperative program are as follows:

Research proposals reviewed (per year).....	30
Awards administered (per year).....	12
Development and operation of Management Information System for participants in total program.....	2,300



	FY 1980	FY 1981	FY 1981
	<u>Appropriation</u>	<u>Base</u>	<u>Request</u>
<u>Program direction</u>	\$ 267	\$ 278	\$ 320

The FY 1981 request for personnel funding for university research support is \$320,000, an increase of \$53,000 over FY 1980. This amount provides for planned step increases, promotions, awards, and associated benefits for the existing personnel (five full-time permanent staff years and three other than full-time permanent staff-years).

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

	FY 1979 <u>Appropriation</u>	FY 1980 <u>Appropriation</u>	FY 1981 <u>Base</u>	FY 1981 <u>Request</u>
Technical program and policy analysis (ER)				
Program direction:		<sup>a/</sup>		
Operating expenses .....	<u>1,826</u>	<u>1,935</u>	<u>2,051</u>	<u>1,981</u>
Total .....	<u>1,826</u>	<u>1,935</u>	<u>2,051</u>	<u>1,981</u>

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

Summary of Changes

FY 1980 Appropriation enacted .....	\$1,935
Built-in increases and decreases:	
Pay cost supplemental .....	+ <u>116</u>
FY 1981 Base .....	\$2,051
Program increases and decreases:	
Net of transfer of positions to other ER programs, and increases in salaries, benefits, and other compensation required for remaining personnel .....	- <u>70</u>
FY 1981 Budget Request .....	\$1,981

The goal of the Technical Program and Policy Analysis (TPPA) activity is to provide the personnel resources required by the Director of Energy Research in order to carry out his responsibilities under the Department of Energy Organization Act (P.L. 95-91), or as mandated by the Secretary, in areas beyond the scope of the assigned Energy Research programs. The FY 1981 request of \$1,981,000, a decrease of \$70,000 from FY 1980, will provide salaries, benefits and related personnel expenses for 43 full time permanent positions, or 44 equivalent staff years of effort. This represents a decrease of eight positions which have been reassigned to other Energy Research (ER) program offices. The request will provide only for the in-house staff to carry out the analyses and studies required to fulfill the Director's responsibilities outlined below, and includes no funds for outside contracts.

Among the responsibilities assigned to the Director of Energy Research in the DOE Organization Act are: (1) monitoring the Department's research and development programs in order to advise the Secretary with regard to any undesirable gaps or duplications; (2) advising the Secretary with respect to the well-being and management of the Multipurpose Laboratories; (3) supervising or supporting research activities carried out by any of the Assistant Secretaries. Additional responsibilities assigned to the Director by the Secretary since formation of the Department include: (1) providing independent advice to the Secretary and Under Secretary on budgetary priorities for energy research and development programs; (2) providing support for the Energy Research Advisory Board, the Research and Development Coordination Council, and the Field and Laboratory Coordination Council; (3) preparation of R&D strategies for the development of specific energy technologies; (4) chairing the R&D Strategy Committee of the International Energy Agency; (5) providing policy and technical analyses relative to nuclear non-proliferation issues.

<sup>a/</sup> Reflects net comparability adjustment of \$-65,000 for shift of positions due to DOE reorganization. A payraise supplemental request of \$118,000 is pending.

During the past year, the personnel funded under TPPA carried out the second Technology Base Review, which assessed the basic and applied research, and exploratory development efforts throughout the Department. Strategies were prepared for the development of fission, fusion, solar, and geothermal energy, in connection with the FY 1981 Internal Review. Other accomplishments include coordination of the development of institutional plans for the Multipurpose Laboratories, lead mission assignments, and development of a system for authorizing the assignment of new work to them. Short-range evaluations of laboratory performance were also conducted. The Office of Energy Research also assisted in establishing a DOE Nuclear Non-Proliferation Policy Committee to provide high-level Departmental attention to nuclear non-proliferation issues, and carried out a number of analyses, both policy-oriented and technical in nature, of subjects related to non-proliferation.

The Department's requirements for expert advice, policy analyses, determination of priorities, plans, strategies, and coordination in the types of areas mentioned above are expected to continue to increase in FY 1981. The FY 1981 request will provide the minimum level of personnel resources needed to support the Department, and to allow the Director of Energy Research to meet his responsibilities in these areas.



Department of Energy  
 FY 1981 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,<br>Lawrence Berkeley Laboratory, Berkeley, California | 2. Project No. 80-ES-10   |
| 3. Date A-E work initiated: 2nd Qtr. FY 1980  | 5. Previous cost estimate: None<br>Date:  |
| 3a. Date physical construction starts: 1st Qtr. FY 1981   | 6. Current cost estimate: \$12,600<br>Less amount for PE&D: <u>0</u><br>Net cost estimate: \$12,600<br>Date: 1/80 |
| 4. Date construction ends: 4th Qtr. FY 1982   |   |

7. Financial schedule

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

8. Brief physical description of project

This project will provide a laboratory-office addition to Building 62 of approximately 46,000 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 500 kV Atomic Resolution Microscope (ARM), a computer control system, a bridge crane, and a glove-box, closed hood system. 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

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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 Å point-to-point resolution, will allow LBL to establish the capability for atomic resolution in this country.

The Atomic Resolution Microscope (ARM) must also include an energy-loss spectrometer attachment for high resolution chemical analysis in order to complement its detailed morphological information. Feeder microscopes are essential to screen specimens and determine optimum candidates for imaging in the ARM, and experimental microscopes will be utilized to test component modifications which assure state-of-the-art performance for the 500 kV machine. These facilities will also

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)

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.

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.

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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)

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 SHEET

Lawrence Berkeley Laboratory (LBL)

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

2. Project No. 80-ES-10

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10. Details of cost estimate\*

a. Engineering, design and inspection at about 15% of construction costs, item b .....		\$ 900
b. Construction costs .....		6,300
1. Improvements to land .....	\$ 233	
2. Building (46,000 sq. ft. gross at about \$118/sq. ft)....	5,428	
3. Special facilities .....	505	
4. Utilities .....	134	
c. Standard equipment .....		\$ 4,400
1. ARM & associated equipment .....	\$3,500	
2. Chemical sciences equipment .....	900	
d. Contingencies @ approximately 14% of items a & b. above .....		<u>1,000</u>
Total project costs .....		<u>\$12,600</u>

\*Based upon a completed conceptual design.

11. Method of performance

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

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

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

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

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

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

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.

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Department of Energy  
 FY 1981 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: Accelerator improvements and modifications,<br>Oak Ridge National Laboratory, Oak Ridge, Tennessee | 2. Project No. 81-E-304  |
| 3. Date A-E work initiated: 1st Qtr. FY 1981   | 5. Previous cost estimate: None<br>Date:   |
| 3a. Date physical construction starts: 2nd Qtr. FY 1981  | 6. Current cost estimate: \$200<br>Less amount for PE&D: <u>0</u><br>Net cost estimate: <u>\$200</u><br>Date: 1/80 |
| 4. Date construction ends: 2nd Qtr. FY 1982  |  |
| 7. <u>Financial schedule</u>   |  |

<u>Fiscal Year</u>	<u>Authorizations</u>	<u>Appropriations</u>	<u>Obligations</u>	<u>Costs</u>
1981	\$ 200	\$ 200	\$ 200	\$ 120
1982	0	0	0	80
1983	0	0	0	0

8. Brief physical description of project  
 A high resolution magnetic spectrograph capable of energy resolution of E/E  $10^{-4}$  will be installed. This instrument, an Elbek spectrometer, has been obtained from Los Alamos as excess property. A new power supply will be obtained. The camera box will be modified to accommodate position-sensitive detectors. Pumping systems will be installed, and the detectors interfaced to the data acquisition system.

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CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

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1. Title and location of project: Accelerator improvements and modifications,  
Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 81-E-304

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

To fully exploit the use of tandem accelerator facilities for future atomic collisions research, basic improvements which capitalize on the excellent ion sources and instruments available, are badly needed. The ORNL EN-tandem accelerator was originally installed in 1961 and 1962. The facility was planned for nuclear physics research with light ions. Since that time, the facility has evolved to the point that nearly 100 percent of the research is done with heavy ions and approximately 85 percent is atomic physics. Atomic collision experiments concerning highly ionized, heavy ions in various ionization-excitation states require the widest possible variety of heavy ion beams derived from high current sources possessing excellent ion optic beam quality and stability. The tandem laboratory presently possesses ion sources equal to or better than those of any other similar facility in the world. Much of this negative ion source development work was stimulated by the needs of the new tandem accelerator incorporated in the Holifield Heavy Ion Research Facility (HHIRF) but is equally useful for atomic collision research using the EN-tandem. Continued ORNL leadership in fast beam pulse techniques will make experiments possible where a pulsed beam interacts with a coincidentally pulsed high power laser.

The case for national atomic collisions facilities has been carefully considered in the Report of the Ad Hoc Panel on Accelerator-Related Atomic Physics Research, NAS/NRC. The findings and recommendations of this Panel are strongly supportive of this project. This is especially true of the Panel's recommendation for conversion of selected existing nuclear research accelerator laboratories and construction of installations dedicated to atomic physics.

The atomic physics program on the EN-tandem is now operated essentially as a national facility. A total of 62 scientists and students from 16 institutions have participated in these experiments in one year.

If this improvement were not funded, the Atomic Collision Program would be increasingly handicapped. The absence of a magnetic spectrograph would make it impossible to perform many important experiments now needed to advance the forefront of science.

CONSTRUCTION PROJECT DATA SHEETS

Oak Ridge National Laboratory (ORNL)

1. Title and location of project: Accelerator improvements and modifications,  
Oak Ridge National Laboratory, Oak Ridge, Tennessee

2. Project No. 81-E-304

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

The installation of this spectrograph will provide the ability to make very precise energy loss measurements in crystal channeling, in stopping power experiments, and for energy loss measurements in coincidence with inner-shell ionization or excitation, where energies relative to the primary beam energy for different charge states must be determined.

10. Details of cost estimate\*

	<u>Item Cost</u>	<u>Total Cost</u>
a. Engineering, design and inspection at 28% of construction costs .....		\$ 35
b. Construction costs .....		125
Magnetic spectrograph installation .....	\$ 125	
Subtotal .....		<u>160</u>
c. Contingency at 25% of above costs .....		<u>40</u>
Total project costs .....		\$ 200

\*Based on engineering study.

11. Method of performance:

Design and inspection will be performed by the operating contractor. Construction and procurement will be accomplished by the CPFF contractor and by the operating contractor as necessary, utilizing fixed-price sub-contracts to the extent feasible awarded on the basis of competitive bids. CPFF construction will be required because of the modification and reuse of existing equipment and the necessary coordination with ongoing experimental work.

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Department of Energy  
 FY 1981 CONGRESSIONAL BUDGET REQUEST

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

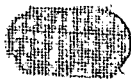
(Tabular dollars in thousands. Narrative material in whole dollars.)

Office of Basic Energy Sciences (OBES)

- |   |   |
|---|---|
| 1. Title and location of project: General plant projects, various locations | 2. Project No. 81-E-301   |
| 3. Date A-E work initiated: 1st Qtr. FY 1981                                | 5. Previous cost estimate: None<br>Date:  |
| 3a. Date physical construction starts: 2nd Qtr. FY 1981                     | 6. Current cost estimate: \$ 300<br>Less amount for PE&D: <u>0</u><br>Net cost estimate: \$ 300<br>Date: 1/80 |
| 4. Date construction ends: 4th Qtr. FY 1982                                 |   |
| 7. <u>Financial schedule</u>  |   |

<u>Fiscal Year</u>	<u>Obligations</u>	<u>Costs</u>			
		<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>After FY 1981</u>
Prior Year Projects	xxx	\$ 202	\$ 313	\$ 0	\$ 0
FY 1979 Projects	\$ 270	15	255	0	0
FY 1980 Projects	250	0	150	100	0
FY 1981 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



CONSTRUCTION PROJECT DATA SHEETS

Office of Basic Energy Sciences (OBES)

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

2. Project No. 81-E-301

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

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 significant R&D program is anticipated as a prerequisite for design and construction of the subprojects under consideration.

The currently estimated distribution of FY 1981 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 various locations:

Ames Laboratory .....\$ 275

Requirements include: upgrade of the campus warehouse roof (\$76,700); energy conservation modifications to the Development Building Laboratory Wing (\$15,800); addition of isolation valves on the utility risers of the Development Building (\$13,200); humidity generator upgrade for Spedding Hall and the Metallurgy and Development Buildings (\$39,700); upgrade of distilled water generating equipment (\$33,000); installation of lighting protection for the reactor building (\$26,500); upgrade of the electrical system to 480 volt operation at Spedding Hall (\$59,600); and miscellaneous small projects (\$10,500).

Notre Dame Radiation Laboratory .....\$ 25

This project would provide for building modifications (\$20,000) to the laboratory research space and equipment items including benches and fume hoods (\$5,000) in the new research addition to the laboratory.

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CONSTRUCTION PROJECT DATA SHEETS

Office of Basic Energy Sciences (OBES)

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

2. Project No. 81-E-301

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10. Details of cost estimates

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

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